Thu. Nov 1, 2018

Room1

Symposium | C. Crystal Plasticity: From Electrons to Dislocation Microstructure

[SY-C9] Symposium C-9

Chair: Vasily Bulatov(Physical and Life Sciences Directorate, Lawrence Livermore National Laboratory, United States of America)
9:45 AM - 11:00 AM Room1

[SY-C9] Interstitial Shuffling Mechanism for Solute-Induced Embrittlement of Titanium
○Daryl C. Chrzan （Department of Materials Science and Engineering, University of California, Berkeley, United States of America）

[SY-C9] Screw dislocation mediated solution strengthening of substitutional α-Ti alloys - First principles investigation
○Piotr Kwasniak （Warsaw University of Technology, Poland）

[SY-C9] Microstructural effects on strain rate sensitivity in dual-phase titanium alloys
○Sana Waheed[1], Zebang Zheng[2], Daniel S. Balint[1], Fionn P. E. Dunne[2] （1.Dept. of Mechanical Engineering, Imperial College London , UK, 2.Dept. of Materials, Imperial College London , UK）

[SY-C9] **Understanding thermal alleviation in cold dwell fatigue in titanium alloys using crystal plasticity model**
○Zebang Zheng[1], Adam Stapleton[2], Kate Fox[2], Fionn P.E. Dunne[1] （1.Dept. of Materials, Imperial College London, UK, 2.Rolls-Royce plc, UK）

Symposium | C. Crystal Plasticity: From Electrons to Dislocation Microstructure

[SY-C10] Symposium C-10

Chair: Tomohito Tsuru(Japan Atomic Energy Agency, Japan)
11:15 AM - 12:15 PM Room1

[SY-C10] First Principles Calculations of Dislocations in Model Engineering Alloys (Ni, Ni3Al, hcp-Ti, and a Refractory Metal BCC-HEA)
○Christopher Woodward （Air Force Research Laboratory, United States of America）

[SY-C10] **Hybrid QM/MM study of dislocation glide in tungsten in the presence of plasma components**
○Petr Grigorev[1], Tom Swinburne[2], James Kermode[1] （1.Warwick Centre for Predictive Modelling, UK, 2.Los Alamos National Laboratory, United States of America）

[SY-C10] First-principles Calculations of Deformation Twins in Hexagonal Titanium Alloys
○Daisuke Matsunaka, Ryosuke Amano （Dept. of Mechanical Engineering, Shinshu Univ., Japan）

Symposium | C. Crystal Plasticity: From Electrons to Dislocation Microstructure

[SY-C11] Symposium C-11

Chair: Nikhil Chandra Admal(University of California Los Angeles, United States of America)
2:00 PM - 3:30 PM Room1

[SY-C11] A Multi-Scale Dislocation Language - Data Mining, Statistical Analysis, and Steps Towards a Community-Driven Data Base
○Stefan Sandfeld （TU Bergakademie Freiberg, Germany）

[SY-C11] **The effect of dislocation character on dislocation line tension in bcc tungsten and its impact on kink-pair enthalpy**
○David Cereceda[1], Vasily Bulatov[3], Jaime Marian[2] （1.Dept. of Mechanical Engineering, Villanova University, United States of America, 2.Department of Materials Science and Engineering, University of California Los Angeles, United States of America, 3.Physical and Life Sciences Directorate, Lawrence Livermore National Laboratory, United States of America）

[SY-C11] Atomistic modeling of thermally activated plasticity in UO_2
Aurélien Soulié[1], ○Jean-Paul Crocombette[1], Antoine Kraych[1], Frédérico Garrido[2], Gaël Sattonnay[2], Emmanuel Clouet[1] （1.CEA Saclay, SRMP, France, 2.CSNSM, CNRS-IN2P3-Université Paris-Sud, France）

[SY-C11] **FTMP-based Simulations and Evaluation of Geometrically-Necessary Boundaries (GNBs) of Dislocation**
○Shiro Ihara, Tadashi Hasebe （Dept. of Mechanical Engineering, Kobe Univ., Japan）

[SY-C11] Improved phase field model of dislocation intersections
○Songlin Zheng[1], Yong Ni[2] （1.China Academy of Engineering Physics, China, 2.University of Science and Technology of China, China）

Symposium | C. Crystal Plasticity: From Electrons to Dislocation Microstructure

[SY-C12] Symposium C-12

Chair: Irene Beyerlein(University of California at Santa Barbara, United States of America)
4:00 PM - 5:15 PM Room1

[SY-C12] Modeling the interaction between martensitic phase transformations and dislocation dynamics
○Rachel Derby, Michael Budnitzki, Stefan Sandfeld （TU Bergakademie Freiberg, Germany）

[SY-C12] The effect of microscopic slip deformation on the yield stress in dispersion hardened alloys analyzed by using crystal plasticity FEM
○Yelm Okuyama[1], Masaki Tanaka[1], Tatsuya Morikawa[1], Tetsuya Ohashi[2] （1.Dept. of Materials Science and Engineering, Kyushu University, Japan, 2.Dept. of Engineering, Kitami Institute of Technology, Japan）

[SY-C12] Deformation Behaviour for Two-Phase Composites under Large Deformations using Micromechanical Analysis
○Srihari Dodla （Madanapalle Institute of Technology (MITS) Madanapalle, India）

[SY-C12] Dislocation dynamics simulation of FCC single crystals in high strain rate deformation
○Ronan MADEC （CEA, DAM, DIF, France）

[SY-C12] Comparison of two methods to cross-slip modeling by means of mathematical theory of moving curves
○Miroslav Kolar, Jan Kratochvíl, Petr Pauš, Michal Beneš （Czech Technical University in Prague, Czech Republic）

Room2

Symposium | E. Deformation and Fracture Mechanism of Materials

[SY-E9] Symposium E-9

Chairs: Andrej Ostapovec(Institute of Physics of Materials ASCR, Czech Republic), Yujie Wei(Chinese Academy of Sciences, China)
9:45 AM - 11:00 AM Room2

[SY-E9] **The motion of a single dislocation from molecular dynamics simulations and its physical interpretation**
○Yujie Wei[1,2], Shenyou Peng[1,2] （1.Chinese Academy of Sciences, China, 2.School of Engineering Sciences, University of Chinese Academy of Sciences, China）

[SY-E9] **Atomistic study on the super-elasticity of single crystal bulk NiTi shape memory alloy under adiabatic condition**
○Bing Wang[1], Guozheng Kang[1], Qianhua Kan[1], Wenping Wu[2], Kun Zhou[3], Chao Yu[1] （1.School of Mechanics and Engineering, Southwest Jiaotong University, China, 2.School of Civil Engineering, Wuhan University, China, 3.School of Mechanical and Aerospace Engineering, Nanyang Technological University, Singapore）

[SY-E9] Atomistic Modelling of Fracture with Non-Linear Elastic Boundary Conditions
○Punit Patel, James Kermode （University of Warwick, UK）

[SY-E9] **Atomistic simulation of the deformation and crack nucleation mechanisms in titanium alloys**
○Dongsheng Xu （Institute of Metal Research, Chinese Academy of Sciences, China）

Symposium | E. Deformation and Fracture Mechanism of Materials

[SY-E10] Symposium E-10

Chairs: Irene Beyerlein(University of California at Santa Barbara, USA), Dongsheng Xu(Institute of Metal Research, CAS, China)
11:15 AM - 12:30 PM Room2

[SY-E10] Study of atomic trajectories during twinning transformation in magnesium
○Andrej Ostapovec[1], Tomáš Káňa[1], Václav Paidar[2] （1.Institute of Physics of Materials ASCR, Czech Republic, 2.Institute of Physics ASCR, Czech Republic）

[SY-E10] **Understanding nanocontact plasticity through massive MD simulations**
○Jorge Alcala[1], Javier Varillas[2,1], Jordi Torner[2], Jan Očenášek[1] （1.Universidad Politecnica de Catalunya, Spain, 2.New Technologies Research Centre, Czech Republic）

[SY-E10] Atomistically informed mesoscale modeling of fracture
○Hamad ul Hassan[1], Johannes Möller[2,3], Erik Bitzek[2], Alexander Hartmaier1[1], Rebecca Janisch[1] （1.ICAMS, Ruhr-Universität Bochum, Germany, 2.Friedrich-Alexander Universität Erlangen-Nürnberg , Germany, 3.Fraunhofer Institut für Werkstoffmechanik, Freiburg, Germany）

[SY-E10] **Lattice Distortion Effect on Cross-Slip in High Entropy Alloys and Lennard-Jones Systems for Face-Centered Cubic**
○Chao-Chun Yen[1], Junping Du[2,3], Jia-An Lin[4], Yu-Chieh Lo[4] （1.National Tsing Hua University, Taiwan, 2.Kyoto University, Japan, 3.Osaka University, Japan, 4.National Chiao Tung University, Taiwan）

[SY-E10] **Atomic structure of gamma/alpha2 interface and**

its influence on plastic deformation of lamellar TiAl alloys

○Hao Wang[1], Aidong Tu[1], Yanxia Liu[2], Dongsheng Xu[1], Rui Yang[1] （1.Institute of Metal Research, CAS, China, 2.Dept. of Physics, Liaoning University, China）

Symposium | E. Deformation and Fracture Mechanism of Materials

[SY-E11] Symposium E-11

Chairs: Xiaoyu Yang(Computer network information center, CAS, China), Denise Reimann(ICAMS, Ruhr-Universität Bochum, Germany)
2:00 PM - 3:30 PM Room2

[SY-E11] Thermodynamically consistent directional distortional hardening of wrought Mg alloys: experimental investigation and constitutive modeling

○Baodong Shi[1], Yan Peng[1], Chong Yang[1], Jianliang Sun[1], Fusheng Pan[2] （1.NECSR, School of Mechanical Engineering, Yanshan Univ., China, 2.NERC-MA, Chongqing Univ., China）

[SY-E11] **A computational infrastructure for multiscale materials simulation**

○Xiaoyu Yang （Computer network information center of the Chinese Academy of Sciences, China）

[SY-E11] Using machine learning methods to homogenize damage from micro- to macroscale

Denise Reimann[1], Hamad ul Hassan[1], Tobias Glasmachers[2], ○Alexander Hartmaier[1] （1.ICAMS, Ruhr-Universität Bochum, Germany, 2.Institut für Neuroinformatik, Ruhr-Universität Bochum, Germany）

[SY-E11] Graph theory analysis of rich fiber-scale data yields very fast simulations of damage evolution in composites

jerry quek[2], ○brian n cox[1] （1.arachne consulting, United States of America, 2.IHPC, Singapore）

[SY-E11] A deep learning-based constitutive model for finite element analysis

Fariborz Ghavamian[1], ○Angelo Simone[2,1] （1.Delft University of Technology, Netherlands, 2.University of Padova, Italy）

Symposium | E. Deformation and Fracture Mechanism of Materials

[SY-E12] Symposium E-12

Chairs: Baodong Shi(NECSR, School of Mechanical Engineering, Yanshan Univ., China), Ligang Zhang(Central South University, China)
4:00 PM - 5:00 PM Room2

[SY-E12] **Diffusivities and atomic mobilities in bcc Ti-Mo-Nb-Ta-Zr alloys**

○Weimin Bai[1], Guanglong Xu[2], Libin Liu[1], Ligang Zhang[1] （1.School of Materials Science and Engineering, Central South Univ., China, 2.Tech Inst. for Advanced Materials &School of Materials Science and Engineering, Nanjing Tech Univ., China）

[SY-E12] Design of Ti-alloy by Integrating High Throughput Experiments and Calculations

○Ligang Zhang, Libin Liu, Di Wu （Central South University, China）

[SY-E12] Simulation of Plasticity in Amorphous Solids

○Shingo Urata[1], Takahiro Murashima[2], Shaofan Li[3] （1.Innovative Technology Research Center, Asahi Glass Co., Ltd (AGC)., Japan, 2.Dept. of Physics, Tohoku University, Japan, 3.Dept. of Civil and Environmetal Engineering, Univ. of California Berkeley, United States of America）

[SY-E12] Computational generation of the yield surfaces using stress based loading

○mayank chouksey, Sumit Basu （Indian Institute of Technology, Kanpur, India）

Room3

Symposium | F. From Microstructure to Properties: Mechanisms, Microstructure, Manufacturing

[SY-F9] Symposium F-9

Chair: Ernst Kozeschnik(Institute of Materials Science and Technology, TU Wien, Austria)
9:45 AM - 11:00 AM Room3

[SY-F9] Programmable Materials - tuning effective materials response

○Peter Gumbsch[1,2], Chris Eberl[1,3], Claudio Findeisen[1,2], Alexander Butz[1], Jan Pagenkopf[1,2] （1.Fraunhofer IWM, Germany, 2.Karlsruhe Institute of Technology (KIT), Germany, 3.Albert-Ludwigs-Universität Freiburg, Germany）

[SY-F9] **Equilibrium crystal shape of GaAs by ab-initio thermodynamics**

In Won Yeu[1,2], Gyuseung Han[1,2], Cheol Seong Hwang[2], ○Jung-hae Choi[1] （1.Center for Electronic Materials, Korea Institute of Science and Technology, Korea, 2.Department of Materials Science and Engineering, and Inter-university Semiconductor Research Center, Seoul National University, Korea）

[SY-F9] Elastic field of lattice defects in low-dimensional nano-carbon materials

○Xiao-Wen LEI[1], Akihiro NAKATANI[2], Tomoya TANIGUCHI[1] （1.Dept. of Mechanical Engineering, Univ. of Fukui, Japan, 2.Dept. of Adaptive Machine Systems, Osaka Univ. , Japan）

Symposium | F. From Microstructure to Properties: Mechanisms, Microstructure, Manufacturing

[SY-F10] Symposium F-10

Chair: Ricardo Lebensohn(Los Alamos National Laboratory, United States of America)
11:15 AM - 12:30 PM Room3

[SY-F10] **Data Analytics for Mining Process-Structure-Property Linkages for Hierarchical Materials**
○Surya Raju Kalidindi （Georgia Tech, United States of America）

[SY-F10] Maximization of strengthening effect of microscopic morphology in duplex elastoplastic solids
○Ikumu Watanabe[1], Gaku Nakamura[2], Kohei Yuge[2] （1.National Institute for Materials Science, Japan, 2.Seikei University, Japan）

[SY-F10] Assessment of formability limit diagram prediction by crystal plasticity finite element method
○Duancheng Ma （Leichtmetallkompetenzzentrum Ranshofen GmbH, Austria）

[SY-F10] Analysis of gradient microstructures using crystal plasticity
○Balaji Selvarajou, Jerry Quek Siu Sin （IHPC, Singapore, Singapore）

Symposium | F. From Microstructure to Properties: Mechanisms, Microstructure, Manufacturing

[SY-F11] Symposium F-11

Chair: Peter Gumbsch(Fraunhofer IWM, Germany)
2:00 PM - 3:30 PM Room3

[SY-F11] **Mesoscale plasticity models of polycrystalline materials for efficient computation of microstructure/property relationships**
○Ricardo Lebensohn （Los Alamos National Laboratory, United States of America）

[SY-F11] Development of a new consistent discrete Green operator for FFT-based methods to solve heterogeneous problems with eigenstrains
○Komlavi Senyo ELOH[1,2,3], Alain JACQUES[2,1], Stéphane BERBENNI[1,3] （1.University of Lorraine, France, 2.Institut Jean Lamour, France, 3.Laboratoire d'etudes de microstructures et de mécanique des matériaux, France）

[SY-F11] Efficient FFT-based Homogenisation without Linear Reference Medium
○Till Junge （EPFL, Mech. Engineering, Multiscale Mechanics Modeling, Switzerland）

[SY-F11] Multiscale modelling of the effective viscoplastic behavior of constituents of the mantle transition zone (Mg_2SiO_4 wadsleyite and ringwoodite): bridging atomic and polycrystal scales
Olivier Castelnau[1], Katell Derrien[1], Sebastian Ritterbex[2], Philippe Carrez[2], ○Patrick Cordier[2] （1.Process and Engineering in Mechanics and Materials, CNRS/ENSAM/CNAM, Paris, France, 2.Unité Matériaux et Transformations, CNRS / Univ. Lille, Lille, France）

[SY-F11] Scalable and Directionally-Sensitive Three-Dimensional Quantifying of Orientation and Dislocation Density Gradients in Crystal Plasticity Computer Simulations
○Markus Kuehbach, Franz Roters （Max-Planck-Institut fur Eisenforschung GmbH, Germany）

Symposium | F. From Microstructure to Properties: Mechanisms, Microstructure, Manufacturing

[SY-F12] Symposium F-12

Chair: Yasushi Shibuta(The University of Tokyo, Japan)
4:00 PM - 5:30 PM Room3

[SY-F12] Microstructure formation in large-scale molecular dynamics simulation
○Yasushi Shibuta[1], Shin Okita[1], Eisuke Miyoshi[2], Shinji Sakane[2], Tomohiro Takaki[2], Munekazu Ohno[3] （1.The University of Tokyo, Japan, 2.Kyoto Institute of Technology, Japan, 3.Hokkaido University, Japan）

[SY-F12] Directed assembly of structured nanoparticles through rapid micromixing
○Arash Nikoubashman[1], Nannan Li[2], Athanassios Z. Panagiotopoulos[2] （1.Johannes Gutenberg University of Mainz, Germany, 2.Princeton University, United States of America）

[SY-F12] Various interfaces related to twinning in hexagonal metals
○Vaclav Paidar[1], Andriy Ostapovets[2] （1.Institute of Physics AS CR Prague, Czech Republic, 2.Institute of Physics of Materials AS CR Brno, Czech Republic）

[SY-F12] Multiscale mean-field modelling of mechanochemical processes in heterogeneous

materials for energy storage

○Mikhail Poluektov[1], Łukasz Figiel[1,2] （1.International Institute for Nanocomposites Manufacturing, WMG, University of Warwick, UK, 2.Warwick Centre for Predictive Modelling, University of Warwick, UK）

[SY-F12] Impact of local symmetry breaking on the physical properties of tetrahedral liquids

○Rui Shi, Hajime Tanaka （University of Tokyo, Japan）

Room4

Symposium | G. Modeling Mechanical Behavior of Materials under Harsh Environments

[SY-G5] Symposium G-5

Chairs: Keonwook Kang(Yonsei University, Korea), Akiyuki Takahashi(Tokyo University of Science, Japan)
9:45 AM - 11:00 AM Room4

[SY-G5] Metallic materials under extreme pressure: Interplay of plasticity and phase transitions

○Nina Gunkelmann[1], Hoang-Thien Luu[1], Diego R. Tramontina[3], Carlos J. Ruestes[3], Yudi Rosandi[4], Herbert M. Urbassek[2] （1.Clausthal University of Technology, Germany, 2.University of Kaiserslautern, Germany, 3.National University of Cuyo, Argentine, 4.University of Padjadjaran, Indonesia）

[SY-G5] Dislocation dynamics modeling of fracture behavior with considering dislocation shielding effect

○Akiyuki Takahashi, Hayato Sugasawa, Masanori Nagura （Tokyo University of Science, Japan）

[SY-G5] Dynamic behaviors of dislocations and grain boundaries induced by phonon scattering in nanoscale

○Soon Kim, Sung Youb Kim （Dept. of Mechanical Engineering, UNIST, Korea）

[SY-G5] Investigation on 1/2<11-1>{112} and 1/2<11-1>{123} mixed dislocations in BCC iron by classical molecular dynamics

○Tomohisa Kumagai[1], Akiyoshi Nomoto[1], Akiyuki Takahashi[2] （1.Central Research Institute of Electric Power Industory, Japan, 2.Tokyo University of Science, Japan）

Symposium | G. Modeling Mechanical Behavior of Materials under Harsh Environments

[SY-G6] Symposium G-6

Chairs: Akiyuki Takahashi(Tokyo University of Science, Japan), Keonwook Kang(Yonsei University, Korea)
11:15 AM - 12:15 PM Room4

[SY-G6] Repulsive Correction in Tersoff Potential for Irradiated Si

○Youhwan Jo, Taeyeon Kim, Byeongchan Lee （Kyung Hee University, Korea）

[SY-G6] Phase-field modeling of microstructural evolution of Fe-Cr-Al system

○Kunok Chang （Kyung Hee Univ., Korea）

[SY-G6] Dissolution kinetics of ejecta in hydrogen at megabar pressure

○Arslan B. Mazitov[1,2], Artem R. Oganov[3,1,4], Alexey V. Yanilkin[1,2] （1.Dukhov Research Institute of Automatics (VNIIA), Moscow, Russian Federation, Russia, 2.Moscow Institute of Physics and Technology, Dolgoprudny, Russian Federation, Russia, 3.Skolkovo Institute of Science and Technology, Skolkovo Innovation Center, Moscow, Russian Federation, Russia, 4.International Center for Materials Discovery, Northwestern Polytechnical University, Xi’ an, China）

[SY-G6] MD simulation study of displacement damage in bulk wurtzite GaN by proton irradiation

○SangHyuk Yoo, Yongwoo Kim, Keonwook Kang （Dept. of Mechanical Engineering, Yonsei Univ., Korea）

Symposium | N. Towards Experimentally Relevant Time Scales: Methods for Extending Atomistic Simulation Times and Their Applications in Material Science

[SY-N5] Symposium N-5

Chair: Jutta Rogal(ICAMS Ruhr University Bochum, Germany)
2:00 PM - 3:30 PM Room4

[SY-N5] Understanding the impact of extended defects on the behaviour of C atoms: a multi technique approach

○Christophe Domain[1], charlotte S becquart[2] （1.EDF, France, 2. Univ.Lille, CNRS, INRA, ENSCL, UMR 8207, UMET, Unité Matériaux et Transformations, France）

[SY-N5] Localised on-the-fly Kinetic Monte Carlo

○Johannes Bulin （Fraunhofer-Institut SCAI, Germany）

[SY-N5] A Preconditioning scheme for Minimum Energy Path finding methods

○Stela Makri, James Kermode, Christoph Ortner （University of Warwick, UK）

[SY-N5] Temperature Programmed Molecular Dynamics - Accessing rare events using a combination of finite time sampling and bias potentials

○Abhijit Chatterjee （Dept. of Chemical Engineering, Indian Institute of Technology Bombay, India）

Symposium | N. Towards Experimentally Relevant Time Scales: Methods for Extending Atomistic Simulation Times and Their Applications in Material Science

[SY-N6] Symposium N-6

Chair: Chad W Sinclair(Dept. of Materials Engineering, University of British Columbia, Canada)
4:00 PM - 5:30 PM Room4

[SY-N6] **Modelling metals, alloys and cement paste across length and time scales**

○Laurent Karim Beland[1], Roger E Stoller[3], Yuri N Osetsky[3], Tingtao Zhou[2], Katerina Katerina Ioannidou[2], Franz-Josef Ulm[2], Roland Pellenq[2] (1.Queen's University, Canada, 2.Massachusetts Institute of Technology, United States of America, 3.Oak Ridge National Laboratory, United States of America)

[SY-N6] BCA-MD-KMC hybrid simulation for long time helium plasma irradiation inducing fuzzy nanostructure on tungsten

○Atsushi M Ito[1,2], Arimichi Takayama[1], Hiroaki Nakamura[1,3] (1.National Institute for Fusion Science, National Institutes of Natural Sciences, Japan, 2.The Graduate University for Advanced Studies, Japan, 3.Department of Electrical Engineering, Graduate School of Engineering, Nagoya University, Japan)

[SY-N6] Atomistic Modelling of Pipe Diffusion: a Direct Comparison of MD, KMC, aKMC and DMD

Frederic Houlle[1], Jutta Rogal[2], ○Erik Bitzek[1] (1.FAU Erlangen-Nuernberg, Germany, 2.ICAMS Ruhr University Bochum, Germany)

[SY-N6] Strategies for optimal construction of Markov chain representations of atomistic dynamics

○Danny Perez, Thomas Swinburne (Los Alamos National Laboratory, United States of America)

[SY-N6] Simulating the collective diffusion mechanism of amorphous solids at experimentally relevant time scales

○Yunjiang Wang[1,2], Shigenobu Ogata[3] (1.Institute of Mechanics, Chinese Academy of Sciences, China, 2.School of Engineering Science, University of Chinese Academy of Sciences, China, 3.Graduate School of Engineering Science, Osaka University, Japan)

Room5

Symposium | K. Multiscale Simulations of Catastrophic Phenomena: Toward Bridging between Materials Fracture and Earthquake

[SY-K1] Symposium K-1

Chairs: Momoji Kubo(Institute for Materials Research, Tohoku University, Japan), Tomoaki Niiyama(Kanazawa Univ., Japan)
11:15 AM - 12:30 PM Room5

[SY-K1] Supercomputer Post-K Project “Challenge of Basic Science - Exploring Extremes through Multi-Physics and Multi-Scale Simulations”

○Momoji Kubo (Tohoku Univ., Japan)

[SY-K1] Universal avalanche statistics across 16 decades in length: From nanocrystals (and neurons) to earthquakes and stars?

○Karin Dahmen (University of Illinois at Urbana Champaign, United States of America)

[SY-K1] Predicting avalanches and failure: wood and paper

○Mikko Alava, Juha Koivisto, Tero Mäkinen, Leevi Viitanen (Aalto University, Finland)

[SY-K1] System-spanning shear avalanches induced by thermal structural relaxation in metallic glasses

○Tomoaki Niiyama[1], Masato Wakeda[2], Tomotsugu Shimokawa[4], Shigenobu Ogata[3] (1.College of Science and Engineering, Kanazawa Univ., Japan, 2.Research Center for Structural Materials, National Institute for Materials Science, Japan, 3.Department of Mechanical Science and Bioengineering, Osaka University, Japan, 4.Faculty of Mechanical Engineering, Kanazawa University, Japan)

Symposium | K. Multiscale Simulations of Catastrophic Phenomena: Toward Bridging between Materials Fracture and Earthquake

[SY-K2] Symposium K-2

Chairs: Ferenc Kun(University of Debrecen, Hungary), Ian Main(University of Edinburgh, UK)
2:00 PM - 3:30 PM Room5

[SY-K2] Predictability of catastrophic failure in porous media

○Ian Main[1], Ferenc Kun[2], Jeremie Vasseur[3], Andrew Bell[1] (1.University of Edinburgh, UK, 2.University of Debrecen, Hungary, 3.Ludwig Maximilian University, Munich, Germany)

[SY-K2] Deciphering the dynamics of precursors to failure in quasi-brittle solids: an inspiration for understanding the statistics of earthquakes ?

○Laurent Ponson[1], Estelle Berthier[1], Vincent Démery[2] (1.Institut Jean le Rond d'Alembert, CNRS - Sorbonne University, Paris, France, 2.Gulliver, CNRS - ESPCI, Paris, France)

[SY-K2] Avalanche precursors and fracture strength in the

limit of high disorder

○Ferenc Kun[1,2], Viktória Kádár[1] （1.Department of Theoretical Physics, University of Debrecen, Hungary, 2.Institute for Nuclear Research (Atomki), Debrecen, Hungary）

[SY-K2] Jump statistics of epicenters in thermally induced cracking of fiber bundles

○Naoki Yoshioka[1], Ferenc Kun[2], Nobuyasu Ito[1,3] （1.RIKEN Center for Computational Science, Japan, 2.Department of Theoretical Physics, University of Debrecen, Hungary, 3.Department of Applied Physics, Graduate Schoold of Engineering, The University of Tokyo, Japan）

[SY-K2] Time dependent fracture under unloading in a fiber bundle model

○Reka Korei, Ferenc Kun （Department of Theoretical Physics, University of Debrecen, Hungary）

Symposium | K. Multiscale Simulations of Catastrophic Phenomena: Toward Bridging between Materials Fracture and Earthquake

[SY-K3] Symposium K-3

Chairs: Takahiro Hatano(University of Tokyo, Japan), Akio Nakahara(Nihon Univ., Japan)
4:00 PM - 5:30 PM Room5

[SY-K3] Creep of strongly disordered materials: Plasticity, damage and approach to failure

○Michael Zaiser, David Fernandez Castellanos （Inst,. of Materials Simulation, Dept of Materials Science, FAU University of Erlangen-Nuremberg, Germany）

[SY-K3] **Creep rupture and Omori-Utsu law: Fiber bundle model approach**

○Takahiro Hatano[1], Subhadeep Roy[2] （1.University of Tokyo, Japan, 2.Norwegian University of Science and Technology, Norway）

[SY-K3] **Temperature dependent shear friction in metallic glass**

○Akio Ishii[1], Tomoaki Niiyama[2], Takahiro Hatano[3], Tomotsugu Shimokawa[2], Shigenobu Ogata[1] （1.Osaka Univ., Japan, 2.Kanazawa Univ., Japan, 3.Tokyo Univ., Japan）

[SY-K3] Mechanism of controlled crack formation induced by memory effect of clay paste

○Akio Nakahara[1], Rokuya Hayashi[1], Tomoki Hiraoka[1], Yousuke Matsuo[1], So Kitsunezaki[2] （1.Nihon Univ., Japan, 2.Nara Women's University, Japan）

[SY-K3] Effects of Shockwave-Induced Nanobubble Collapse on Precision Polishing : Molecular Dynamics Study

○yoshimasa aoyama[1], Jingxiang Xu[2], Yuske Ootani[1], Nobuki Ozawa[1], Momoji Kubo[1] （1.Dept. of Materials Science, Tohoku Univ., Japan, 2.Dept. of Mechanical Engineering, Shanghai Ocean Univ., China）

Symposium | O. Tribology and Interface: Multi-Scale, Multi-Physics, and Multi-Chemistry Phenomena in Friction, Lubrication, Wear, and Adhesion

[SY-O9] Symposium O-9

Chairs: Yusuke Ootani(Tohoku University, Japan), Shuichi Uehara(Tohoku University, Japan)
9:45 AM - 11:00 AM Room5

[SY-O9] **Combined experimental and computational study on the superlubricity mechanism of 2D Materials at the microscale**

○Tianbao Ma （Tsinghua University, China）

[SY-O9] Quantum chemistry vs. rheology of some EMIM-based ionic liquids

Szerena Kisztina Ujvari[1,2], Konstantinos Gkagkas[1], ○Andras Vernes[2,3] （1.Advanced Material Research Division, Toyota Motor Europe NV/SA, Technical Center, Hoge Wei 33B, 1930 Zaventem, Belgium, 2.AC2T research GmbH, Viktor-Kaplan-Str. 2/C, 2700 Wiener Neustadt, Austria, 3.Institute of Applied Physics, TU Wien, Wiedner Hauptstr. 8-10/134, 1040 Vienna, Austria）

[SY-O9] Lubrication with a refrigerant : a challenge made possible thanks to fluid/surface chemistry

Stéphane TROMP[1], Laurent JOLY[2], Manuel COBIAN[3], ○Nicolas FILLOT[1] （1.Univ Lyon, INSA-Lyon, , CNRS UMR5259, LaMCoS, F-69621 Villeurbanne, France, 2.Univ Lyon, Universite Claude Bernard Lyon 1, CNRS, Institut Lumiere Matiere, F-69622 Villeurbanne, France, 3.Univ Lyon, Ecole Centrale de Lyon, ENISE, ENTPE, CNRS UMR5513, Laboratory of Tribology and System Dynamics, F-69134 Ecully, France）

[SY-O9] Meso-scale SPH simulation for friction and wear between elastic-plastic solids with various asperities

○Natsuko Nakagawa Sugimura[1,2], Le Van Sang[2], Yuji Mihara[1], Hitoshi Washizu[2] （1.Dept. of Mechanical Engineering, Tokyo City Univ., Japan, 2.Grad. Sch. of Simulation Studies, Univ. of Hyogo,, Japan）

Room6

Symposium | A. Advances in Materials Theory for Multiscale Modeling

[SY-A9] Symposium A-9

Chair: Eliot Fried(Okinawa Institute of Science and Technology, Japan)
9:45 AM - 11:00 AM Room6

[SY-A9] Group-theoretical construction for constitutive equation of the first strain gradient elasticity

○Ryuichi Tarumi[1], Shunsuke Kobayashi[2], Yoji Shibutani[2] （1.Graduate School of Engineering Science, Osaka Univ., Japan, 2.Dept. of Mechanical Engineering, Osaka Univ., Japan）

[SY-A9] Physically based strain gradient plasticity model for length scale dependent yield strength

○Peter Gudmundson （Department of Solid Mechanics, KTH Royal Institute of Technology, Sweden）

[SY-A9] **FTMP-based Seamless Description of Deformation-Fracture Transitions**

○Tadashi Hasebe （Kobe Univ., Japan）

[SY-A9] On the crucial role played by instantaneous and hidden multifield features of lattice dynamics in their nonlocal pseudocontinuum modeling

○Miguel Charlotte （University of Toulouse, Institute Clement Ader, CNRS -- UMR 5312 INSA/UPS/ISAE-SupAero/Mines Albi, France）

Symposium | A. Advances in Materials Theory for Multiscale Modeling

[SY-A10] Symposium A-10

Chair: Steve Fitzgerald(University of Leeds, UK)
11:15 AM - 12:30 PM Room6

[SY-A10] Interdiffusion and atomic mobilities in fcc Ag-Mg, Ag-Mn and Ag-Mg-Mn alloy

○Qianhui Min[1], Yuling Liu[1], Yong Du[1], Huixin Liu[1], Li Chen[1], Biao Hu[3], Changfa Du[2], Zhoushun Zheng[2] （1.Powder Metallurgy Research Institute,Central South University, China, 2.School of mathematics and statistics,Central South University, China, 3.School of Material Science and Engineering, Anhui University Of Science And Technology, China）

[SY-A10] **Stacking and Multilayered Nature of Martensite in Copper Based Shape Memory Alloys**

○Osman ADIGUZEL （Firat University , Turkey）

[SY-A10] Mesoscale understanding of ionic conduction in yttria stabilized zirconia

○Abhijit Chatterjee （Dept. of Chemical Engineering, Indian Institute of Technology Bombay, India）

[SY-A10] cancellation

[SY-A10] Accelerating stochastic simulations with path integrals

○Steve Fitzgerald （University of Leeds, UK）

Room7

Symposium | I. Multiscale Modeling of Grain Boundary Dynamics, Grain Growth and Polycrystal Plasticity

[SY-I9] Symposium I-9

Chairs: Yuri Mishin(George Mason University, United States of America), Yang Xiang(Hong Kong University of Science and Technology, Hong Kong)
9:45 AM - 11:00 AM Room7

[SY-I9] Grain Boundary Microstates Under Irradiation: A Moment in Time?

○Mitra L Taheri （Drexel University, Department of Materials Science &Engineering, United States of America）

[SY-I9] The Role of Grain Boundaries under Long-Time Radiation

○Jing Luo[1], Yichao Zhu[1], Xu Guo[1], Yang Xiang[3], Stephen Jonathan Chapman[2] （1.Dalian University of Technology, China, 2.Mathematical Institute, University of Oxford, UK, 3.Department of Mathematics, The Hong Kong University of Science and Technology, Hong Kong）

[SY-I9] Quantifying point defect fluxes to interfaces and the role of interface structure

○Shen J Dillon （University of Illinois , United States of America）

Symposium | I. Multiscale Modeling of Grain Boundary Dynamics, Grain Growth and Polycrystal Plasticity

[SY-I10] Symposium I-10

Chair: Saryu Fensin(Los Alamos National Lab, United States of America)
11:15 AM - 12:15 PM Room7

[SY-I10] Structure and Mobility of Dissociated Cacancies at Twist Grain Boundaries and Screw Dislocations in Ionic Compounds

○Blas Pedro Uberuaga, Enrique Martinez, Kedarnath Kolluri, Xiang-Yang Liu （Los Alamos National Laboratory, United States of America）

[SY-I10] Reverse engineering the kinetics of grain growth

Mingyan Wang[1], Jules Dake[1], Søren Schmidt[2], ○Carl Krill[1] （1.Institute of Micro and Nanomaterials, Ulm University, Germany, 2.Dept. of Physics, Technical University of Denmark, Denmark）

Symposium | I. Multiscale Modeling of Grain Boundary Dynamics, Grain Growth and Polycrystal Plasticity

[SY-I11] Symposium I-11

Chairs: Bob Svendsen(RWTH Aachen University, Germany), Jeremy K Mason(University of California, Davis, United States of America)
2:00 PM - 3:30 PM Room7

[SY-I11] Recent advances in the Full-Field modeling of microstructural evolutions using a finite-element level set integrated framework.

○Daniel Pino Munoz, Thomas Toulorge, Charbel Moussa, Nathalie Bozzolo, Marc Bernacki （Mines ParisTech / PSL Research University, France）

[SY-I11] The effect of strong anisotropic grain boundary energy and mobility on microstructure formation and evolution: mesoscale modeling and simulation

○Brandon Runnels[1], Josep Maria Gras Ribot[1], Ian Chesser[2] （1.University of Colorado Colorado Springs, United States of America, 2.Carnegie Mellon University, United States of America）

[SY-I11] A Machine Learning Exploration of Grain Boundary Mobility Mechanisms

Leila Khalili[1], Eric R Homer[2], ○Srikanth Patala[1] （1.North Carolina State University, United States of America, 2.Brigham Young University, United States of America）

Symposium | I. Multiscale Modeling of Grain Boundary Dynamics, Grain Growth and Polycrystal Plasticity

[SY-I12] Symposium I-12

Chairs: Blas Pedro Uberuaga(Los Alamos National Laboratory, United States of America), Chris P Race(University of Manchester, UK)
4:00 PM - 5:15 PM Room7

[SY-I12] Formation and shrinkage of grain boundary loops in two-dimensional colloidal crystals

Francois Lavergne, Arran Curran, Dirk Aarts, ○Roel Dullens （University of Oxford, UK）

[SY-I12] Growth and characterization of two-dimensional poly(quasi)crystals

○Petri Hirvonen[1], Gabriel Martine La Boissonière[2], Zheyong Fan[1], Cristian Achim[3], Nikolas Provatas[4], Ken R. Elder[5], Tapio Ala-Nissila[1,6] （1.Dept. of Applied Physics, Aalto Univ., Finland, 2.Dept. of Mathematics and Statistics, McGill Univ., Canada, 3.Dept. of Chemical Engineering, Univ. of Concepción, Chile, 4.Dept. of Physics, McGill Univ., Canada, 5.Dept. of Physics, Oakland Univ., United States of America）

[SY-I12] A Parallel Algorithm for High Resolution 3D Phase Field Simulations of Polycrystalline Solidification

○Pavel Strachota, Aleš Wodecki （Czech Technical University in Prague, Czech Republic）

[SY-I12] Properties of β / ω phase interfaces in Ti and their implications on mechanical properties and ω morphology

○Shuo Cao[1], Qing-Miao Hu[1], Rui Yang[1], Yong Jiang[2] （1.Institute of Metal Research, Chinese Academy of Science , China, 2.Central South University, China）

Room8

Symposium | D. Data-Driven and Physics-Informed Materials Discovery and Design

[SY-D1] Symposium D-1

Chair: Daniel Urban(Fraunhofer IWM, Germany)
9:45 AM - 11:00 AM Room8

[SY-D1] **Data-Driven Discovery of new materials**

○Isao Tanaka （Dept. Materials Science and Engineering, Kyoto Univ. , Japan）

[SY-D1] Machine Learning and Materials Discovery*

○Gus Hart （Brigham Young University, United States of America）

[SY-D1] Data-Driven Materials Design in an Industrial Environment

○Thomas Eckl, Lothar Kunz, Benedikt Ziebarth （Robert Bosch GmbH, Germany）

Symposium | D. Data-Driven and Physics-Informed Materials Discovery and Design

[SY-D2] Symposium D-2

Chair: Tilmann Hickel(MPIE, Germany)
11:15 AM - 12:30 PM Room8

[SY-D2] Using Machine-Learning to Create Predictive Material Property Models

○Chris Wolverton （Northwestern University, United States of America）

[SY-D2] Designing mesoscale structures of Li-ion battery electrode using FIB-SEM image via machine learning

○Yoichi Takagishi, Tatsuya Yamaue （Kobelco Research Institute Inc., Japan）

[SY-D2] **Stability Engineering of Halide Perovskite via Machine Learning**

○Wan-Jian YIN, Wanjian YIN （Soochow University,

China）

[SY-D2] Systematic evaluation of ionization potentials of divalent cation binary oxides

○Yoyo Hinuma[1,2,3], Hiroyuki Hayashi[2,3], Yu Kumagai[4], Isao Tanaka[2,3], Fumiyasu Oba[2,5] （1.Center for Frontier Science, Chiba Univ., Japan, 2.Center for Materials Research by Information Integration, National Institute for Materials Science, Japan, 3.Department of Materials Science and Engineering, Kyoto Univ., Japan, 4.Materials Research Center for Element Strategy, Tokyo Institute of Technology, Japan, 5.Laboratory for Materials and Structures, Institute of Innovative Research, Tokyo Institute of Technology, Japan）

Symposium | D. Data-Driven and Physics-Informed Materials Discovery and Design

[SY-D3] Symposium D-3

Chair: Daryl Chrzan(UC Berkeley, USA)
2:00 PM - 3:30 PM Room8

[SY-D3] Finding the needle in the haystack: Materials discovery through high-throughput ab initio computing and data mining

○Geoffroy Hautier （Universite catholique de Louvain, Belgium）

[SY-D3] High-entropy alloys investigation using machine-learned potentials

○Tatiana Kostiuchenko, Alexander Shapeev （Dept. of Material Science and Engeneering , Skolkovo Institute of Science and Technology, Moscow, Russia）

[SY-D3] Stability evaluation of high-entropy alloys via accurate on-lattice model

○Evgenii Meshkov[1], Ivan Novoselov[1], Alexander Shapeev[2], Alexey Yanilkin[1] （1.All-Russian Research Institute of Automatics (VNIIA), Russia, 2.Skolkovo Institute of Science and Technology, Russia）

[SY-D3] Atomistically informed atomic mobility databases for continuum diffusion simulations

○Katrin Abrahams[1], Daniel Gaertner[2], Maximilian Grabowski[3], Irina Roslyakova[1], Oleg Shchyglo[1], Sergiy V. Divinski[2], Ingo Steinbach[1] （1.Scalebridging Thermodynamic and Kinetic Simulation (ICAMS), Ruhr-University Bochum, Germany, 2.Institute of Materials Physics, University of Münster, Germany, 3.Atomistic Modelling and Simulation (ICAMS), Ruhr-University Bochum, Germany）

[SY-D3] The European Materials Modelling Council: standardization, interoperability and data management tools for materials modelling

○Luca Bergamasco[1], Emanuele Ghedini[2], Gerhard Goldbeck[3], Eliodoro Chiavazzo[1], Pietro Asinari[1] （1.Politecnico di Torino, Italy, 2.Università di Bologna, Italy, 3.Goldbeck Consulting Ltd, UK）

Symposium | D. Data-Driven and Physics-Informed Materials Discovery and Design

[SY-D4] Symposium D-4

Chair: Minoru Otani(AIST, Japan)
4:00 PM - 5:30 PM Room8

[SY-D4] Exploration of large ab initio data spaces to design structural materials with superior mechanical properties

○Joerg Neugebauer, Jan Janssen, Tilmann Hickel, Blazej Gabowski （Max-Planck-Institut fuer Eisenforschung, Germany）

[SY-D4] Toward a machine learning aided interatomic potential for multi-element alloys: Application to binary compounds

○Doyl Dickel, David Francis, Christopher Barrett （Mississippi State University, United States of America）

[SY-D4] **Machine Learning potentials for modeling iradiation defects in iron and tungsten**

○Alexandra Goryaeva[1], Jean-Bernard Maillet[2], Mihai-Cosmin Marinica[1] （1.DEN-Service de Recherches de Métallurgie Physique, CEA, Université Paris-Saclay, 91191 Gif-sur-Yvette, France, 2.CEA-DAM DIF, 91297 Arpajon Cedex, France）

[SY-D4] Effect of friction and ductility on relaxation dynamics and mechanical memory of crumpled materials

○Mehdi Habibi, Eric van Bruggen （Wageningen University, Netherlands）

[SY-D4] Big-data insights into solute-GB segregation

○Liam Huber, Blazej Grabowski, Joerg Neugebauer （MPIE, Germany）

Room9

Symposium | H. Multiscale Mechanics of Polymers, Soft Matter and Network Materials

[SY-H7] Symposium H-7

Chair: Patrick R. Onck(Univ. of Groningen, Netherlands)
9:45 AM - 11:00 AM Room9

[SY-H7] Computational modeling approach for the

rational design of DNA nanostructures

○Do-Nyun Kim, Jae Young Lee, Jae Gyung Lee, Young-Joo Kim, Kyung Soo Kim, Chanseok Lee （Department of Mechanical and Aerospace Engineering, Seoul National University, Korea）

[SY-H7] Quantitative Multiscale Modelling of Bionano Interface

○Vladimir Lobaskin[1], Stefano Poggio[1], David Power[1], Hender Lopez[2] （1.School of Physics, University College Dublin, Ireland, 2.Institute Laue-Langevin, Grenoble, France）

[SY-H7] Multiscale modelling of intrinsically-disordered proteins

Ankur Mishra, Henry De Vries, Hamid Jafarinia, Erik Van der Giessen, ○Patrick R. Onck （University of Groningen, Netherlands）

[SY-H7] Tracing the interplay of polymer topology and hydrodynamics

○Lisa B. Weiss[1], Arash Nikoubashman[2], Christos N. Likos[1] （1.University of Vienna, Austria, 2.Johannes Gutenberg University Mainz, Germany）

Symposium | H. Multiscale Mechanics of Polymers, Soft Matter and Network Materials

[SY-H8] Symposium H-8

Chair: Patrick R. Onck(Univ. of Groningen, Netherlands)
11:15 AM - 12:30 PM Room9

[SY-H8] Modeling and Simulation of DNA Foldback Intercoil Structure

○Moon Ki Kim, Byung Ho Lee, Soojin Jo （School of Mechanical Engineering, Sungkyunkwan University, Korea）

[SY-H8] DNA-particle vitrimer systems

○francesco sciortino （Sapienza Universita' di Roma, Italy）

[SY-H8] Relation between Macroscopic Flows in a Contraction-Expansion Channel and Dynamics of Well-Entangled Polymer Chains

○Takeshi Sato, Takashi Taniguchi （Dept. of Chemical Engineering, Kyoto Univ., Japan）

[SY-H8] Origin of large scale spatial organization of DNA-polymer in bacterial chromosomes.

○Apratim Chatterji[1], Tejal Agarwal[2], Manjunath G.P.[3], Farhat Habib[4] （1.IISER-Pune, India 411008, India, 2.IISER-Pune, India, 411008, India, 3.NYU, USA, United States of America, 4.Inmobi, Bangalore, India 560103., India）

Symposium | H. Multiscale Mechanics of Polymers, Soft Matter and Network Materials

[SY-H9] Symposium H-9

Chair: Kees Storm(Eindhoven University of Technology, Netherlands)
2:00 PM - 3:30 PM Room9

[SY-H9] **Micromechanics and instabilities in soft composite materials**

○Stephan Rudykh （University of Wisconsin - Madison, United States of America）

[SY-H9] Deformation analysis of UV curing 3d printed materials by combined molecular dynamics-finite element method

Jiwon Jung, Chanwook Park, ○Gunjin Yun （Seoul National University, Korea）

[SY-H9] Modelling and 3D Printing Kelvin Cell Acoustic Metamaterial

○Huina MAO[1], Peter Göransson[1], John Kennedy[2], Henry Rice[2], Umberto Iemma[3] （1.Dept. of Aeronautical and Vehicle Engineering, KTH Royal Institute of Technology, Sweden, 2.Dept. of Mechanical and Manufacturing Engineering, Trinity College Dublin, Ireland, 3.Engineering Department, Roma Tre University, Italy）

[SY-H9] Theoretical approach for EUV resist fabrication: DFT-MD-FDM study

○Muyoung Kim[1], Junghwan Moon[1], Joonmyung Choi[3], Sungwoo Park[1], Byunghoon Lee[3], Changyoung Jeong[3], Maenghyo Cho[2,1] （1.Divison of Multiscale Mechanical Design, School of Mechanical and Aerospace Engineering, Seoul National University, Korea, 2.Institute of Advanced Machines and Design, Seoul National University, Korea, 3.SAMSUNG ELECTRONICS CO., LTD, Korea）

Symposium | H. Multiscale Mechanics of Polymers, Soft Matter and Network Materials

[SY-H10] Symposium H-10

Chair: Kees Storm(Eindhoven University of Technology, Netherlands)
4:00 PM - 5:30 PM Room9

[SY-H10] In silico design of self-assembly nanostructured polymer systems by multiscale molecular modelling

○Maurizio Fermeglia （University of Trieste , Italy）

[SY-H10] Dynamical properties of suspensions of star block-copolymers in shear flow.

○Diego Felipe Jaramillo - Cano[1], Manuel Camargo[2],

Christos N. Likos[1] （1.Faculty of Physics, University of Vienna, Austria, 2.CICBA, Universidad Antonio Nariño - Campus Farallones, Colombia）

[SY-H10] Heterogeneous flow and internal friction in amorphous carbon

○Richard Jana[1], Lars Pastewka[1], Daniele Savio[2], Volker L Dehringer[3], Gábor Csányi[3], Julian von Lautz[2], Michael Moseler[2], Peter Gumbsch[2,4] （1.Albert Ludwigs Universitaet Freiburg, Germany, 2.Fraunhofer-Institut für Werkstoffmechanik IWM, Germany, 3.University of Cambridge, UK, 4.Institue for Applied Materials, Karlsruhe Institute of Technology, Germany）

[SY-H10] **Increasing the thermal conductivity of polymer nanocomposites filled with carbon nanotubes via molecular dynamics simulation**

○Yangyang Gao[1], Liqun Zhang[1], Florian Müller-Plathe[2] （1.Beijing University of Chemical Technology, China, 2.Technische Universität Darmstadt, Germany）

[SY-H10] **Thermal transport in polymer-based nanocomposite materials across multiple scales**

Rajat Srivastava, ○Matteo Fasano, Shahin Mohammadnejad, Hernan Chavez Thielemann, Eliodoro Chiavazzo, Pietro Asinari （Energy Department, Politecnico di Torino, Italy）

Room10

Symposium | B. Challenges in the Multiscale Modelling of Radiation Effects in Nuclear Materials

[SY-B5] Symposium B-5

Chair: Jean-Paul Crocombette(CEA, Univ. Paris-Saclay, France)
9:45 AM - 11:00 AM Room10

[SY-B5] He impurities in boron carbide : structure, kinetics, and Raman signatures

○Guido Roma, Kevin Gillet, Anton Schneider, Jean-Paul Crocombette （CEA, Univ. Paris-Saclay, France）

[SY-B5] Irradiation damage in nuclear graphite at the atomic scale

○Alain Chartier[1], Laurent Van Brutzel[1], Justin Pageot[2] （1.DEN, Service de la Corrosion et du Comportement des Materiaux dans leur Environment, CEA Saclay, France, 2.DEN, Service d’ Etudes des Materiaux Irradies, CEA Saclay, France）

[SY-B5] Using computational modeling to understand radiation damage tolerance in complex oxides both from the bottom-up and the top-down

○Blas Pedro Uberuaga （Los Alamos National Laboratory, United States of America）

[SY-B5] **Development of defect mechanics-based multi-scale simulation techniques for reliability study of high performance electronic devices in radiation environments**

○Yukeun Eugene Pak[1], Youjung Seo[2], Dhaneshwar Mishra[1], Keonwook Kang[3], Jihyun Kim[4] （1.Advanced Institutes Convergence Technology, Korea, 2.Seoul National University, Korea, 3.Yonsei University, Korea, 4.Korea University , Korea）

Symposium | B. Challenges in the Multiscale Modelling of Radiation Effects in Nuclear Materials

[SY-B6] Symposium B-6

Chair: Jaime Marian(University of California Los Angeles, United States of America)
11:15 AM - 12:30 PM Room10

[SY-B6] Ion Irradiation as a Surrogate for Reactor Irradiation: The Expected and the Surprises

○Gary S Was[1], Zhijie Jiao[1], David Woodley[1], Stephen Taller[1], Gerrit Vancoevering[1], Anthony Monterrosa[1], Elizabeth Getto[4], Brian Wirth[2], Arthur Motta[3] （1.University of Michigan, United States of America, 2.University of Tennessee, United States of America, 3.Pennsylvania State University, United States of America, 4.United Stated Naval Academy, United States of America）

[SY-B6] **Dose Effect on the Irradiation Induced Loop Density and Burgers Vector in Ion-Irradiated Ferritic/Martensitic Steel HT9 Through In-Situ TEM**

Ce Zheng[1], Stuart Maloy[2], ○Djamel Kaoumi[1] （1.North Carolina State University, United States of America, 2.Los Alamos National Laboratory, United States of America）

[SY-B6] **Novel Deformation Mechanism of Helium Irradiated Copper**

○WEIZHONG HAN （Xi'an Jiaotong University, China）

[SY-B6] Isotope effect on quantum diffusion of interstitial hydrogen in face-centered cubic metals

○Hajime Kimizuka[1], Shigenobu Ogata[1,2], Motoyuki Shiga[3] （1.Osaka University, Japan, 2.Kyoto University, Japan, 3.Japan Atomic Energy Agency, Japan）

Symposium | B. Challenges in the Multiscale Modelling of Radiation Effects in Nuclear Materials

[SY-B7] Symposium B-7

Chair: Marjorie Bertolus(CEA/DEN/DEC, Centre CEA de Cadarache, France)
2:00 PM - 3:30 PM Room10

[SY-B7] Thermal properties of fluorite-type metal dioxides: CeO_2, ThO_2, UO_2, NpO_2, PuO_2 and AmO_2
○Masato Kato （Japan Atomic Energy Agency, Japan）

[SY-B7] **SCIANTIX: A new inert gas behaviour module ready for use**
○Davide Pizzocri, Tommaso Barani, Lelio Luzzi （Politecnico di Milano, Italy）

[SY-B7] Modeling swelling in U_3Si_2 nuclear fuel using a multi-scale computational approach
○Larry Aagesen[1], Karim Ahmed[2], Benjamin Beeler[1], Daniel Schwen[1], Yongfeng Zhang[1] （1.Idaho National Laboratory, United States of America, 2.Texas A&M University, United States of America）

[SY-B7] Why Multiscale Modeling of Nuclear Fuel is Absolutely Essential and Why it is so Challenging
○Michael R Tonks[1], Yongfeng Zhang[2], David Andersson[3], Simon Phillpot[1], Christopher Stanek[3] （1.University of Florida, United States of America, 2.Idaho National Laboratory, United States of America, 3.Los Alamos National Laboratory, United States of America）

Symposium | B. Challenges in the Multiscale Modelling of Radiation Effects in Nuclear Materials

[SY-B8] Symposium B-8

Chair: Guang-Hong Lu(Beihang University, China)
4:00 PM - 5:30 PM Room10

[SY-B8] Kinetic Monte Carlo study of tungsten fuzz formation under low energy helium irradiation
○Zhangcan Yang, Yingzhao He, Quansong Peng （School of Energy and Power Engineering, Huazhong University of Science and Technology, China）

[SY-B8] Constrained thermodynamic model for multi-component alloys under irradiation: A matrix formulation from first-principles Hamiltonian
○Duc Nguyen-Manh[1], J.S Wrobel[2], A. Fernandez_Caballero[3], S.L. Dudarev[1] （1.Materials Science and Scientific Computing Department, Culham Centre for Fusion Energy, UKAEA, UK, 2.Faculty of Materials Science and Engineering, Warsaw University of Technology, Poland, 3.School of Mechanical Aerospace and Civil Engineering, University of Manchester , UK）

[SY-B8] Kinetic Monte-Carlo Simulations of Radiation Damage in W(Re,Os) Alloys
○Matthew James Lloyd[1,2], David Armstrong[1], Enrique Martinez Saez[3], Duc Nguyen-Manh[2] （1.Department of Materials, University of Oxford, UK, 2.Culham Centre for Fusion Energy, UK, 3.Los Alamos National Laboratory, United States of America）

[SY-B8] Modeling Re-precipitate hardening in neutron irradiated W and W-Re alloys: from point defects to macroscopic hardening
Chen-Hsi Huang[1], Leili Gharaee[2], Paul Erhart[2], ○Jaime Marian[1] （1.University of California Los Angeles, United States of America, 2.Chalmers University, Sweden）

[SY-B8] In-situ TEM of Formation Processes of Defects in Tungsten under Irradiation: Comparison between Electron and Self-ion Irradiations
○Kazuto Arakawa （Shimane University, Japan）

Symposium | C. Crystal Plasticity: From Electrons to Dislocation Microstructure

[SY-C9] Symposium C-9

Chair: Vasily Bulatov(Physical and Life Sciences Directorate, Lawrence Livermore National Laboratory, United States of America)

Thu. Nov 1, 2018 9:45 AM - 11:00 AM Room1

[SY-C9] Interstitial Shuffling Mechanism for Solute-Induced Embrittlement of Titanium

○Daryl C. Chrzan （Department of Materials Science and Engineering, University of California, Berkeley, United States of America）

[SY-C9] Screw dislocation mediated solution strengthening of substitutional α-Ti alloys - First principles investigation

○Piotr Kwasniak （Warsaw University of Technology, Poland）

[SY-C9] Microstructural effects on strain rate sensitivity in dual-phase titanium alloys

○Sana Waheed[1], Zebang Zheng[2], Daniel S. Balint[1], Fionn P. E. Dunne[2] （1.Dept. of Mechanical Engineering, Imperial College London , UK, 2.Dept. of Materials, Imperial College London , UK）

[SY-C9] Understanding thermal alleviation in cold dwell fatigue in titanium alloys using crystal plasticity model

○Zebang Zheng[1], Adam Stapleton[2], Kate Fox[2], Fionn P.E. Dunne[1] （1.Dept. of Materials, Imperial College London, UK, 2.Rolls-Royce plc, UK）

(Thu. Nov 1, 2018 9:45 AM - 11:00 AM Room1)

[SY-C9] Interstitial Shuffling Mechanism for Solute-Induced Embrittlement of Titanium

Invited

○Daryl C. Chrzan （Department of Materials Science and Engineering, University of California, Berkeley, United States of America）

The exceptional sensitivity of the strength of Ti alloys to low concentrations of interstitial O arises from a mechanism akin to steric hindrance [1]. The equilibrium interstitial sites of the O atoms are highly distorted and compressed during the passage of a dislocation. The presence of an O atom at this site resists this distortion and compression inhibiting the passage of the dislocation and strengthening the metal. However, this strength increase is also correlated with embrittlement of the metal. We identify a dislocation-induced interstitial shuffling mechanism that can explain the observed O-induced embrittlement of Ti [2]. Molecular dynamics simulations show that the passage of a dislocation can move a fraction of the O interstitials from their equilibrium octahedral sites into adjacent hexahedral sites. The excess number of O interstitials in hexahedral sites is metastable and will eventually return to equilibrium. However, simulations of the dislocation/O interstitial interaction predict that an O atom in the hexahedral site presents a weaker obstacle to dislocation slip than an O atom in the octahedral site. Under typical strain rates, the time between dislocation passage on the slip plane is less than the estimated typical residence time for an O atom in the hexahedral site. The implication is that the passage of the first dislocation on the slip plane leads to softening for the subsequent dislocations. Subsequent dislocations may the further soften the slip plane through the same mechanism. This slip plane softening is expected to lead to planar slip, and the stress concentrations associated with planar slip then lead to the embrittlement of the metal. This work is supported by the U. S. Office of Naval Research under grant N00014-16-1-2304 and employed computational resources of the National Science Foundation under grant ACI-1053575.

[1] Q. Yu *et al.*, Science 347, 635-639 (2015).

[2] M. Poschmann *et al.*, to be published.

(Thu. Nov 1, 2018 9:45 AM - 11:00 AM Room1)

[SY-C9] Screw dislocation mediated solution strengthening of substitutional α-Ti alloys - First principles investigation

○Piotr Kwasniak （Warsaw University of Technology, Poland）

The mechanical properties of hexagonal Ti alloys depend substantially on the glide of <*a*> type screw dislocations. The configurations and stabilities of these line defects are, however, known only in pure Ti and Ti + O solutions, where the locking-unlocking mechanism and a strong pinning effect control their activity. In this study, we investigated the unclear, screw dislocation mediated solution strengthening of substitutional α-Ti alloys. To this end, a first principle computational scheme was used to determine the structures and energies of the considered line defects during planar and cross-slip processes in the vicinity of the solute element. Two phenomena were determined that are crucial in terms of plastic deformation: (i) enhanced

polymorphism of the dislocation cores leading to multiple new core configurations, and (ii) relatively large positive and negative interaction energies between the solutes and the line defects. Both these effects are strongly affected by the valence configuration of the alloying elements. Due to their pronounced structure and energy variations, dislocation planar and cross slip processes can occur under different scenarios, through diverse non-planar core geometries. The calculations performed also indicate In as a potential alloy element for improving both the strength and ductility of Ti by stabilizing a special, compact core geometry able to spread on an arbitrary glide plane with a low energy barrier. All of the above effects are discussed in terms of the physical factors (solute size misfit, stacking fault energy and electronic structure) that affect the energy and geometry of dislocation cores.

(Thu. Nov 1, 2018 9:45 AM - 11:00 AM Room1)

[SY-C9] Microstructural effects on strain rate sensitivity in dual-phase titanium alloys

○Sana Waheed[1], Zebang Zheng[2], Daniel S. Balint[1], Fionn P. E. Dunne[2] (1.Dept. of Mechanical Engineering, Imperial College London , UK, 2.Dept. of Materials, Imperial College London , UK)

Cold dwell fatigue failure in titanium alloys is a major concern in aero-engine applications and is inherently linked to the strain rate sensitivity (SRS) of the material. Recent crystal plasticity finite element (CPFE) work has shown the material SRS to be influenced by a number of microstructural factors [1]. However, these higher-level modelling studies do not include discrete aspects of slip and considerably overestimate the material rate sensitivity as compared to experimental studies. Thus, the significance and mechanism of microstructural effects on experimentally observed strain rate sensitivity in titanium alloys remain unclear.

In this study, a planar discrete dislocation plasticity (DDP) model is set up explicitly incorporating dislocation penetration across phase boundaries and material heterogeneity arising from alpha and beta titanium phases to simulate realistic microstructures. Stress relaxation tests are performed to investigate microstructural effects, such as the presence of colony or basketweave microstructures, textured or non-textured crystallography and grain size effects, on the material strain rate sensitivity. The SRS coefficients obtained from the simulations match closely with experimental values. It is found that changing the microstructure from pure alpha, colony to basketweave, and reducing alpha grain sizes leads to a significant reduction in material rate sensitivity, whereas dislocation penetration is found to not be as significant as previously considered for small hold strains. The mechanistic basis for these effects is argued to be changes in dislocation mean free-path and the total amount of plasticity in the specimen. Finally, DDP results are compared with corresponding CPFE simulations, to show that discrete aspects of slip and hardening mechanisms have to be accounted for to capture experimentally observed rate sensitivity. These results provide increased understanding of the mechanism of cold dwell fatigue failure in titanium alloys and are relevant for the design of dwell-insensitive microstructures.

(Thu. Nov 1, 2018 9:45 AM - 11:00 AM Room1)

[SY-C9] Understanding thermal alleviation in cold dwell fatigue in titanium alloys using crystal plasticity model

○Zebang Zheng[1], Adam Stapleton[2], Kate Fox[2], Fionn P.E. Dunne[1] （1.Dept. of Materials, Imperial College London, UK, 2.Rolls-Royce plc, UK）

Dwell fatigue facet nucleation has been investigated in isothermal rig disc spin tests and under anisothermal in-service engine conditions in titanium alloy IMI834 using α-HCP homogenised and faithful α-β lamellar microstructure crystal plasticity representations. The empirically observed facet nucleation and disc failure at low stress in the isothermal spin tests has been explained and originates from the material rate sensitivity giving rise to soft grain creep accumulation and hard grain basal stresses which increase with fatigue cycling until facet nucleation. The α-HCP homogenised model is not able to capture this observed behaviour at sensible applied stresses. In contrast to the isothermal spin tests, anisothermal in-service disc loading conditions generate soft grain slip accumulation predominantly in the first loading cycle after which no further load shedding nor soft grain creep accumulation is observed, such that the behaviour is stable, with no further increase in hard grain basal stress so that facet nucleation does not occur, as observed empirically. The *thermal alleviation*, which derives from in-service loading conditions and gives the insensitivity to dwell fatigue dependent on the temperature excursions, has been explained. A stress-temperature map for IMI834 alloy has been established to demarcate the ranges for which the propensity for dwell fatigue facet nucleation is high, threatening or low.

Symposium | C. Crystal Plasticity: From Electrons to Dislocation Microstructure

[SY-C10] Symposium C-10

Chair: Tomohito Tsuru(Japan Atomic Energy Agency, Japan)

Thu. Nov 1, 2018 11:15 AM - 12:15 PM Room1

[SY-C10] First Principles Calculations of Dislocations in Model Engineering Alloys (Ni, Ni3Al, hcp-Ti, and a Refractory Metal BCC-HEA)

○Christopher Woodward （Air Force Research Laboratory, United States of America）

[SY-C10] Hybrid QM/MM study of dislocation glide in tungsten in the presence of plasma components

○Petr Grigorev[1], Tom Swinburne[2], James Kermode[1] （1.Warwick Centre for Predictive Modelling, UK, 2.Los Alamos National Laboratory, United States of America）

[SY-C10] First-principles Calculations of Deformation Twins in Hexagonal Titanium Alloys

○Daisuke Matsunaka, Ryosuke Amano （Dept. of Mechanical Engineering, Shinshu Univ., Japan）

(Thu. Nov 1, 2018 11:15 AM - 12:15 PM Room1)

[SY-C10] First Principles Calculations of Dislocations in Model Engineering Alloys (Ni, Ni3Al, hcp-Ti, and a Refractory Metal BCC-HEA)

Invited

○Christopher Woodward （Air Force Research Laboratory, United States of America）

In order to understand the “chemistry of deformation” an adequate description of the strain field near the center (core) of dislocations is required. While continuum elasticity methods have been very successful in describing long-range stress fields of dislocations these methods diverge in the core region. Atomistic methods have shown that the forces produced at the dislocation core and their coupling to the applied stress can have a dramatic effect on plasticity. However, atomistic methods are limited by the fidelity of the assumed interaction model and for this reason are at best semi-empirical. Here the Lattice Greens Function is used with Density Functional Theory to calculate the equilibrium core structure of isolated screw dislocation in four model-engineering alloys. These include Ni, $L1_2$ Ni_3Al, and a c+a pyramidal dislocation in hcp Ti. Pipe diffusion along the dissociated partial dislocations in Ni has been evaluated for self-diffusion and Co solutes. Recent progress extending a 3-d lattice Greens function to model screw dislocations in a refractory bcc high entropy (high concentration solid solutions) will be reviewed.

(Thu. Nov 1, 2018 11:15 AM - 12:15 PM Room1)

[SY-C10] Hybrid QM/MM study of dislocation glide in tungsten in the presence of plasma components

○Petr Grigorev[1], Tom Swinburne[2], James Kermode[1] （1.Warwick Centre for Predictive Modelling, UK, 2.Los Alamos National Laboratory, United States of America）

Tungsten has been chosen as the diverter armour material in ITER and is the main candidate material for plasma-facing components for future fusion reactors.Interaction of plasma components with the material is unavoidable and will lead to degradation of the performance and the lifetime of the in-vessel components.From this point of view it is important to gain an understanding of dislocation mobility as well as the influence of fusion plasma components (H and He) on the mechanism.

Dislocation glide is governed by the localised rearrangement of atoms inside the dislocation core but is tightly coupled to the stress and strain fields on larger length scale.Thus, a correct description of the process requires chemically accurate treatment of the dislocation core atoms together with the use of the systems large enough to accommodate the corresponding stress fields.On the one hand, Density Functional Theory (DFT) provides an accurate description of the interatomic bonding, however the computational cost of the method does not allow one to study large enough systems and requires usage of periodic cells (i. e. with dislocation dipoles and quadrupoles with complex symmetry). On the other hand, classical interatomic potentials are much more computationally affordable allowing to study systems of required size, but the accuracy and transferability of the description of dislocation core is poor, especially for multi-element systems.

In this study we use a hybrid multiscale approach, namely quantum mechanics/molecular mechanics

(QM/MM) combining an accurate local QM description of the dislocation core atoms with a classical model for the rest of the system. We apply a recently developed QM/MM implementation of the virtual work principle to compute energy barriers. The effect of H and He atoms in the material on the dislocation core structure together with the energetics of dislocations and impurities are investigated. The obtained results are analysed by comparison with pure DFT studies from literature together with machine learning based Gaussian Approximation Potential (GAP) model.

(Thu. Nov 1, 2018 11:15 AM - 12:15 PM Room1)

[SY-C10] First-principles Calculations of Deformation Twins in Hexagonal Titanium Alloys

○Daisuke Matsunaka, Ryosuke Amano （Dept. of Mechanical Engineering, Shinshu Univ., Japan）

Because of the excellent strength-to-density ratio and the high corrosion resistance, titanium (Ti) and Ti alloys have attracted much attention as aerospace and biomedical materials. One of the methods to improve mechanical properties of Ti is addition of solid solution atoms. For example, the tensile and fatigue strengths of Ti increase with oxygen content, although compromising ductility and toughness. For further development of titanium alloys, detailed understanding of effects of alloying elements on individual deformation modes, various slip and deformation twinning, in hexagonal alpha-titanium alloys is important.
In this study, we investigate twin boundaries and interaction of solute atoms such as Al in alpha-titanium alloys by first-principles calculations. For {11-22} twin, the mirror glide structure is stable, compared with the mirror reflection one and the {10-12} twin boundary. While the {10-12} twin boundary can migrate easily, the energy barrier for migration of the {11-22} twin boundary is relatively high. The interaction of solute atoms with the {10-12} twin boundary depends on the distance and the corresponding boundary sites, i.e., expansion and compression sites. On the other hand, the interaction of solute atoms with the {11-22} twin boundary is complex due to the mirror glide boundary structure.

Symposium | C. Crystal Plasticity: From Electrons to Dislocation Microstructure

[SY-C11] Symposium C-11

Chair: Nikhil Chandra Admal(University of California Los Angeles, United States of America)

Thu. Nov 1, 2018 2:00 PM - 3:30 PM Room1

[SY-C11] A Multi-Scale Dislocation Language - Data Mining, Statistical Analysis, and Steps Towards a Community-Driven Data Base

○Stefan Sandfeld （TU Bergakademie Freiberg, Germany）

[SY-C11] The effect of dislocation character on dislocation line tension in bcc tungsten and its impact on kink-pair enthalpy

○David Cereceda[1], Vasily Bulatov[3], Jaime Marian[2] （1.Dept. of Mechanical Engineering, Villanova University, United States of America, 2.Department of Materials Science and Engineering, University of California Los Angeles, United States of America, 3.Physical and Life Sciences Directorate, Lawrence Livermore National Laboratory, United States of America）

[SY-C11] Atomistic modeling of thermally activated plasticity in UO_2

Aurélien Soulié[1], ○Jean-Paul Crocombette[1], Antoine Kraych[1], Frédérico Garrido[2], Gaël Sattonnay[2], Emmanuel Clouet[1] （1.CEA Saclay, SRMP, France, 2.CSNSM, CNRS-IN2P3-Université Paris-Sud, France）

[SY-C11] FTMP-based Simulations and Evaluation of Geometrically-Necessary Boundaries (GNBs) of Dislocation

○Shiro Ihara, Tadashi Hasebe （Dept. of Mechanical Engineering, Kobe Univ., Japan）

[SY-C11] Improved phase field model of dislocation intersections

○Songlin Zheng[1], Yong Ni[2] （1.China Academy of Engineering Physics, China, 2.University of Science and Technology of China, China）

(Thu. Nov 1, 2018 2:00 PM - 3:30 PM Room1)

[SY-C11] A Multi-Scale Dislocation Language - Data Mining, Statistical Analysis, and Steps Towards a Community-Driven Data Base

Invited

○Stefan Sandfeld （TU Bergakademie Freiberg, Germany）

Dislocations are simplistic objects: they are one-dimensional, their motion is constrained by the crystallography and they are surrounded by a stress field that decays with 1/r. However, once dislocations start to interact with themselves or with other microstructures, their collective behavior becomes extremely complex. This - despite the apparent simplicity of the individual object - is still far from completely being understood.

Simulation methods, such as the Molecular Dynamics (MD) or the Discrete Dislocation Dynamics (DDD) have been very successfull in predicting the evolution of dislocation microstructures along with the resulting structure-property relations. However, up to now, there is no common "language" that allows to directly compare different dislocation structures - not even if they are obtained from the same simulation method. This makes statistical analysis and data mining on the level of the dislocations difficult.

An overview over state of the art methods for analyzing systems of dislocations will be given. Subsequently, the "Multi-scale Dislocation Language" (MuDiLingo) will be introduced, which allows to extract important geometrical properties of dislocations along with the corresponding energies. Based on examples from MD and DDD it will be shown (i) how this approach can be used to quantitatively compare dislocation microstructures, (ii) how valuable input for simulation methods on higher length scales can be provided by data-mining, and (iii) how MuDiLingo will enable us to create a data base of dislocation data, which might be of great benefit to the community.

(Thu. Nov 1, 2018 2:00 PM - 3:30 PM Room1)

[SY-C11] The effect of dislocation character on dislocation line tension in bcc tungsten and its impact on kink-pair enthalpy

○David Cereceda[1], Vasily Bulatov[3], Jaime Marian[2] （1.Dept. of Mechanical Engineering, Villanova University, United States of America, 2.Department of Materials Science and Engineering, University of California Los Angeles, United States of America, 3.Physical and Life Sciences Directorate, Lawrence Livermore National Laboratory, United States of America）

In addition to the well-characterized elastic contribution, the energy of a dislocation contains an inelastic, or ‘core’, term that reflects the loss of validity of elasticity theory at dislocation segments. While the elastic part is known to be symmetric about its maximum value for the edge orientation (minimum for screw), in bcc metals, the core energy displays an asymmetry that can be characterized using atomistic calculations. In kink-pair configurations on screw dislocations, this asymmetry leads to a difference in energy between ‘right’ and ‘left’ kinks that is not captured in elastic models. In this work, we calculate dislocation segment self-energies as a function of dislocation character in bcc tungsten and kink-pair enthalpies as a function of stress. To avoid finite-size artifacts in atomistic simulations, we develop continuum models of kink-pair configurations based on full elasticity and line tension approaches, parameterized with a substrate Peierls potential and dislocation self-energies obtained from atomistic calculations.

The elastic and line tension models represent specific situations of the environment of these kink-pair configurations, and we discuss our results in terms of the range of validity of each as well as the effect of self-energy asymmetry on kink-pair enthalpy. To match the continuum results to direct atomistic simulations, we vary the core radius of elasticity theory and discuss the implications of the values obtained.

(Thu. Nov 1, 2018 2:00 PM - 3:30 PM Room1)

[SY-C11] Atomistic modeling of thermally activated plasticity in UO_2

Aurélien Soulié[1], ○Jean-Paul Crocombette[1], Antoine Kraych[1], Frédérico Garrido[2], Gaël Sattonnay[2], Emmanuel Clouet[1] （1.CEA Saclay, SRMP, France, 2.CSNSM, CNRS-IN2P3-Université Paris-Sud, France）

We investigate the thermally activated glide mobility of dislocations in uranium dioxide (UO_2) from an atomistic point of view using a variable charge many-body empirical potential, the Second Moment Tight-Binding potential with charge equilibration (SMTB-Q). In order to determine the main glide system, we model the dislocation core structures for edge and screw orientations lying in different glide planes. Uncommon core structures with a double periodicity and a charge alternation are obtained. Straight dislocations motion is first considered to obtain the Peierls stress of each dislocation. We then address the thermally activated motion of the dislocations by the nucleation of kink pairs. Atomistic simulations give us the structure as well as the formation and migration energies of kink pairs. This information is finally combined with an elastic interaction model for kink pairs to obtain the dislocation velocities and the evolution of the critical resolved shear stress as a function of temperature. These quantities are compared to experimental critical resolved shear stress and dislocation velocity measured on urania single crystals.

Reference : Acta Materialia 150, 248-261 (2018)

(Thu. Nov 1, 2018 2:00 PM - 3:30 PM Room1)

[SY-C11] FTMP-based Simulations and Evaluation of Geometrically-Necessary Boundaries (GNBs) of Dislocation

○Shiro Ihara, Tadashi Hasebe （Dept. of Mechanical Engineering, Kobe Univ., Japan）

Rational as well as practically-feasible treatments of spatio-temporally distributed discrete dislocation ensembles have been a long-standing issue and still a challenging problem inevitable in completion of multiscale modeling of metallic materials. Unlike 2D cases, which cannot be simply reduced down to continuously-distributed density function-like pictures, 3D counterparts need to deal, more or less, with its configurational complexities explicitly. We have recently been tackling these based on FTMP (Field Theory of Multiscale Plasticity), focusing on continuum descriptions of dislocation aggregates. Among others, quantitative stability/instability assessments of wall structures are critically important, in the sense that they substantially dominates both the micro/macro mechanical properties of the material systems concerned. The present study targets GNBs (Geometrically Necessary Boundaries) in terms of their stability/instability criteria and some dynamic interactions with in-coming dislocations, whose details about the consisting dislocations recently have been experimentally identified and theoretically evaluated by Hong, Winther, et al. Dislocation dynamics simulations on five typical GNBs, i.e., GNBs 2, 3, 4, 7 and 8, are conducted by utilizing Zbib code

and ParaDis code, and FTMP-based evaluations are performed against them. Duality diagram representations revealed a possible overall picture that governs the GNBs, i.e., all the GNBs exhibit a common tendency to converge ultimately to a single point, i.e., the ideal value for a hexagonal network-based GNB that yields the lowest energy as well as the smallest incompatibility, located in the most lower-left on the diagram.

(Thu. Nov 1, 2018 2:00 PM - 3:30 PM Room1)

[SY-C11] Improved phase field model of dislocation intersections

○Songlin Zheng[1], Yong Ni[2] (1.China Academy of Engineering Physics, China, 2.University of Science and Technology of China, China)

Revealing the long-range elastic interaction and short-range core reaction between intersecting dislocations is crucial for understanding dislocation-based strain hardening mechanisms in crystalline solids. Phase field model (PFM) has shown great potential in modeling dislocation dynamics with employing the continuum microelasticity theory to describe the elastic interactions and incorporating the -surface into the crystalline energy to enable the core reactions. Since the crystalline energy is approximately formulated by linear superposition of interplanar potential of each slip plane in the previous PFM, it does not fully account for the reactions between dislocations gliding in intersecting slip planes. In this study, an improved PFM of dislocation intersections is proposed through updating the crystalline energy by coupling the potential of two intersecting planes, and then applied to study the collinear interaction compared with the previous PFM model. Collinear annihilation captured only in the improved PFM is found to strongly affect the junction formation and plastic flow in multislip systems. The results indicate that the improvement is essential for PFM of dislocation intersections.

Symposium | C. Crystal Plasticity: From Electrons to Dislocation Microstructure

[SY-C12] Symposium C-12

Chair: Irene Beyerlein(University of California at Santa Barbara, United States of America)

Thu. Nov 1, 2018 4:00 PM - 5:15 PM Room1

[SY-C12] Modeling the interaction between martensitic phase transformations and dislocation dynamics

○Rachel Derby, Michael Budnitzki, Stefan Sandfeld （TU Bergakademie Freiberg, Germany）

[SY-C12] The effect of microscopic slip deformation on the yield stress in dispersion hardened alloys analyzed by using crystal plasticity FEM

○Yelm Okuyama[1], Masaki Tanaka[1], Tatsuya Morikawa[1], Tetsuya Ohashi[2] （1.Dept. of Materials Science and Engineering, Kyushu University, Japan, 2.Dept. of Engineering, Kitami Institute of Technology, Japan）

[SY-C12] Deformation Behaviour for Two-Phase Composites under Large Deformations using Micromechanical Analysis

○Srihari Dodla （Madanapalle Institute of Technology (MITS) Madanapalle, India）

[SY-C12] Dislocation dynamics simulation of FCC single crystals in high strain rate deformation

○Ronan MADEC （CEA, DAM, DIF, France）

[SY-C12] Comparison of two methods to cross-slip modeling by means of mathematical theory of moving curves

○Miroslav Kolar, Jan Kratochvíl, Petr Pauš, Michal Beneš （Czech Technical University in Prague, Czech Republic）

(Thu. Nov 1, 2018 4:00 PM - 5:15 PM Room1)

[SY-C12] Modeling the interaction between martensitic phase transformations and dislocation dynamics

○Rachel Derby, Michael Budnitzki, Stefan Sandfeld （TU Bergakademie Freiberg, Germany）

Two of the most important deformation mechanisms in TRIP-Steel are the martensitic phase transformations (MT) and elastic/plastic deformation due to the motion of dislocations. Martensitic phase transformations are desirable because they enhance the strength of TRIP-steels, however, dislocations can lower the strength of the material. These two phenomena are strongly coupled due to their contributions of strain to the system, resulting in an effect on the final macroscopic properties of the material. Thus, both dislocations and phase transformations must be considered simultaneously when modeling TRIP-Steels.

While MD simulations are inherently able to treat both dislocations and MT, such simulations suffer from a high computational cost and, hence, are not able to reach relevant time scales. Phenomenological continuum models for plasticity can be coupled with phase field approaches for the MT and can reach larger time scales; they do not capture the dynamics of the dislocations.

In our model, the dynamics of dislocations is described by a continuum dislocation dynamics (CDD) model, where instead of individual dislocations, a dislocation density is considered. This approach reduces the computational cost and enables the modeling of larger length scales. We use a coupled CDD/phase field approach to study the interaction of dislocation plasticity and the martensitic phase transformations. Our main focus is on the influence of different initial values and on the history dependence of the material. This will allow us to discuss, among others, what happens to dislocations in regions that undergo a MT - an information of big importance for continuum models operating on larger length scales.

(Thu. Nov 1, 2018 4:00 PM - 5:15 PM Room1)

[SY-C12] The effect of microscopic slip deformation on the yield stress in dispersion hardened alloys analyzed by using crystal plasticity FEM

○Yelm Okuyama[1], Masaki Tanaka[1], Tatsuya Morikawa[1], Tetsuya Ohashi[2] （1.Dept. of Materials Science and Engineering, Kyushu University, Japan, 2.Dept. of Engineering, Kitami Institute of Technology, Japan）

The relationship between yield stress and the distribution of microscopic plastic deformation was investigated in dispersion hardened alloys using crystal plasticity FEM. Dispersed particles were randomly distributed in a 3D box in the calculation model. A plate region was extracted from the 3D box, and was used as a finite element model. The length factor in the Orowan equation was determined form the particle distribution in the 3D box. The critical resolved shear stress in local was set to a function of the length factor in the model. The length factor was defined as the average spacing of the particles, which surround the element, on the slip plane. The crystal plasticity analysis elucidates that the initiation and propagation of local slip deformation depends on the length factor. In this study, the relationship between the length factor and macroscopic mechanical response, *i.e.* yield stress and work hardening rate, is discussed.

(Thu. Nov 1, 2018 4:00 PM - 5:15 PM Room1)

[SY-C12] Deformation Behaviour for Two-Phase Composites under Large Deformations using Micromechanical Analysis

○Srihari Dodla （Madanapalle Institute of Technology (MITS) Madanapalle, India）

This study presents a micromechanics approach for the elasto-viscoplastic behaviour of eutectic materials and structures. In this approach, the high-fidelity generalised method of cells (HFGMC) is applied for the prediction of the effective behaviour of two cold-drawn Cu-Ag composites with different drawing strains and to obtain the field (deformation gradient and stress) distributions in the composite. Both phases (Cu or Ag) are rate-dependent crystal plasticity material constituents. HFGMC is applied for analysing the deformation behaviour of two-phase Cu-Ag composites under uniaxial compression. The micromechanical analysis has been verified by comparison with experimental and finite element simulation results. Results in terms of deformation behaviour and field distributions are given for two different cold-drawn composites.

(Thu. Nov 1, 2018 4:00 PM - 5:15 PM Room1)

[SY-C12] Dislocation dynamics simulation of FCC single crystals in high strain rate deformation

○Ronan MADEC （CEA, DAM, DIF, France）

In the range of high strain rate deformations from 10^4 to 10^6 s^{-1} or more, the mobile dislocation density significantly increases and some dislocations may reach a large fraction of sound velocity. The extent of this mobile dislocation multiplication stage depends upon material, experimental or simulation conditions. It also strongly depends on the initial dislocation density. When the total dislocation density reaches a certain value, it may saturate [1].

Molecular dynamics simulations are well suited for very high strain rates (10^7 s^{-1} or more). Hoverver, owing to the extremely small volumes and simulation times, it cannot deal with smaller strain rates. As a consequence, another type of simulation is needed for strain rates below 10^6 s^{-1} and dislocation dynamics simulations appears to be the most suitable method for this purpose.

The first dislocation dynamics studies at high strain rates were performed in small volumes (2-5 microns) of copper single crystals [2-5]. The dislocation fluxes and artefacts such as self annihilations were not carefully handled [6]. In addition, plastic strains were quite small (less than 0.2%) for such volume sizes and the saturation of the mobile dislocation density was difficult to reach even for the lowest strain rate. Nevertheless, the effect of inertia above 10^3 s^{-1} [2] and, above all, the importance of cross-slip [3-5] were established.

With growing computing power, larger volumes and deformations can be reached and the end of the multiplication stage of high strain rate deformation can be reached. So this topic deserves being revisited. Results about dislocation velocities, mobile and total dislocation densities, as well as the anisotropic response of copper single crystal as a function of stain rate and the effect of cross-slip will be discussed.

[1] L. Zepeda-Ruiz, A. Stukowski, T. Oppelsturp, V.V. Bulatov, Nature 550, 492-495 (2017)
[2] Z.Q. Wang, I.J. Beyerlein, R. Lesar, Phil. Mag. 87, 2263-2279 (2007)

[3] Z.Q. Wang, I.J. Beyerlein, R. Lesar, Model. Simul. Mater. Sci. Eng. 15, 675-690 (2007)
[4] Z.Q. Wang, I.J. Beyerlein, R. Lesar, Phil. Mag. 88, 1321-1343 (2008)
[5] Z.Q. Wang, I.J. Beyerlein, R. Lesar, Int. J. Plast. 25 26-48 (2009)
[6] R. Madec, B. Devincre, L. Kubin, Solid mechanics and its applications 115, 35-44 (2004)

(Thu. Nov 1, 2018 4:00 PM - 5:15 PM Room1)

[SY-C12] Comparison of two methods to cross-slip modeling by means of mathematical theory of moving curves

○Miroslav Kolar, Jan Kratochvíl, Petr Pauš, Michal Beneš （Czech Technical University in Prague, Czech Republic）

The contribution focuses on the comparison of two different methods of dislocation cross-slip modeling, both based on the theory of evolving curves. The cross-slip is understood as deterministic, stress-driven dislocation process. In certain geometrical configuration, the criterion based on evaluation of driving stresses in the primary plane and in the cross-slip plane is employed. As an illustrative example, we consider a scenario where the cross-slip is forced by the repulsive stress exerted by a spherical obstacle with realistic repulsive stress. The result of this scenario is the double cross-slip.

The employed model for the dislocation motion can be schematically written as the curvature driven flow in the form

normal velocity = curvature + force.

In the first method, the dislocation motion law is based on the isometric projection. The cross-slip plane is tilted to the primary plane so that dislocation motion remains planar. When the dislocation enters the cross-slip plane, the appropriate physical quantities are recalculated accordingly.

The second method is based on the exploitation of the model of curves evolving on smooth surfaces and driven by the geodesic curvature. The smoothness of the the glide surface is ensured by regularizing the sharp interfaces between the primary plane and the cross-slip plane.

For both methods, the dislocations are described as parametrized curves. In numerical simulations, the flowing finite volume method is used. The results of the numerical simulations for both methods are compared to demonstrate their agreement.

Symposium | E. Deformation and Fracture Mechanism of Materials

[SY-E9] Symposium E-9

Chairs: Andrej Ostapovec(Institute of Physics of Materials ASCR, Czech Republic), Yujie Wei(Chinese Academy of Sciences, China)

Thu. Nov 1, 2018 9:45 AM - 11:00 AM Room2

[SY-E9] The motion of a single dislocation from molecular dynamics simulations and its physical interpretation

○Yujie Wei[1,2], Shenyou Peng[1,2] （1.Chinese Academy of Sciences, China, 2.School of Engineering Sciences, University of Chinese Academy of Sciences, China）

[SY-E9] Atomistic study on the super-elasticity of single crystal bulk NiTi shape memory alloy under adiabatic condition

○Bing Wang[1], Guozheng Kang[1], Qianhua Kan[1], Wenping Wu[2], Kun Zhou[3], Chao Yu[1] （1.School of Mechanics and Engineering, Southwest Jiaotong University, China, 2.School of Civil Engineering, Wuhan University, China, 3.School of Mechanical and Aerospace Engineering, Nanyang Technological University, Singapore）

[SY-E9] Atomistic Modelling of Fracture with Non-Linear Elastic Boundary Conditions

○Punit Patel, James Kermode （University of Warwick, UK）

[SY-E9] Atomistic simulation of the deformation and crack nucleation mechanisms in titanium alloys

○Dongsheng Xu （Institute of Metal Research, Chinese Academy of Sciences, China）

(Thu. Nov 1, 2018 9:45 AM - 11:00 AM Room2)

[SY-E9] The motion of a single dislocation from molecular dynamics simulations and its physical interpretation

Invited

○Yujie Wei[1,2], Shenyou Peng[1,2] (1.Chinese Academy of Sciences, China, 2.School of Engineering Sciences, University of Chinese Academy of Sciences, China)

The dependence of dislocation mobility on stress is the fundamental ingredient for the deformation in crystalline materials. Strength and ductility, the two most important properties characterizing mechanical behavior of crystalline metals, are in general governed by dislocation motion. Experimentally, recording the position of a moving dislocation in a short time window is still challenging, and direct observation to deduce the speed-stress relationship of dislocations is still missing. Here we report the motion of an obstacle-free twinning partial dislocation in face centred cubic crystals with spatial resolution at the angstrom scale and temporal picosecond temporal information. The dislocation exhibits two limiting speeds: The first is subsonic and occurs when the resolved shear stress is on the order of hundreds of megapascal. While the stress is raised to gigapascal level, an abrupt jump of dislocation velocity occurs, from subsonic to supersonic regime. The two speed limits are governed respectively by the local transverse and longitudinal phonons associated with the stressed dislocation, as the two types of phonons influence dislocation gliding at different stress levels. In contrast, the kinetics of a screw dislocation is distinct from that of edges. We demonstrate that a screw dislocation can move steadily at the speed of shear wave velocity, or even move supersonically.

(Thu. Nov 1, 2018 9:45 AM - 11:00 AM Room2)

[SY-E9] Atomistic study on the super-elasticity of single crystal bulk NiTi shape memory alloy under adiabatic condition

○Bing Wang[1], Guozheng Kang[1], Qianhua Kan[1], Wenping Wu[2], Kun Zhou[3], Chao Yu[1] (1.School of Mechanics and Engineering, Southwest Jiaotong University, China, 2.School of Civil Engineering, Wuhan University, China, 3.School of Mechanical and Aerospace Engineering, Nanyang Technological University, Singapore)

The temperature-induced phase transition and the super-elasticity (from the stress-induced phase transition) of equiatomic single crystal bulk NiTi shape memory alloys are investigated by the molecular dynamics method. By the simulation to the thermo-mechanical response of the single crystal NiTi alloy along the $<001>_{B2}$ under the compression/unloading and an adiabatic condition, the temperature change and the nucleation and growth of martensite transformation during the compression/unloading are discussed. The simulated results of molecular dynamics show that the single crystal bulk NiTi shape memory alloy exhibits a significant temperature change during the martensite transformation and its reverse under an adiabatic condition; moreover, a localized instability occurs apparently in the process of martensite transformation, which is closely related to the nucleation and growth rates of martensite phase; finally the effect of model size and strain rate on the thermo-mechanical response of the single crystal bulk NiTi alloy is also discussed, and no instability is observed in the simulated stress-strain curves if the model size is relatively larger, e.g., $8V_0$ and $13.824V_0$.

(Thu. Nov 1, 2018 9:45 AM - 11:00 AM Room2)

[SY-E9] Atomistic Modelling of Fracture with Non-Linear Elastic Boundary Conditions

○Punit Patel, James Kermode （University of Warwick, UK）

Atomistic simulations of crack propagation are key to understanding the fracture behaviour of materials. Cracks involve strong coupling across the scales, with bond breaking on the quantum scale driven by long range stress fields. Current QM methods are limited to simulation sizes too small to accurately describe fracture dynamics and improved QM/MM methods are able to adequately capture elastic effects [1]. However these methods are still heavily limited temporally and to coarse grain into the continuum scale while maintaining the overall fracture dynamics an expanded multiscale approach is required.
Applications in covalently bonded single crystals to complex alloys are underway. Screened classical potentials [2] predict a brittle response in both silicon carbide (SiC) and diamond, giving confidence in their applicability. DFT SiC surface energy calculations produced predictions in good agreement with experiment [3]. Extension of a multiscale approach for fracture includes a novel approach in correcting for finite domain boundary conditions, in which a non-linear continuum boundary correction is applied to help reduce the required system size, in order to compute energy barriers for crack extension bridging DFT and long time scale MD [4].

[1] N. Bernstein *et al.*, Rep. Prog. Phys. 72, 026501 (2009).
[2] L. Pastewka *et al.*, Phys. Rev. B. 87, 205410 (2013).
[3] G. Sernicola *et al.*, Nat. Commun. 8, 108 (2017)
[4] P. Patel, L. Pastewka, C. Ortner and J. R. Kermode, In Prep, (2018)

(Thu. Nov 1, 2018 9:45 AM - 11:00 AM Room2)

[SY-E9] Atomistic simulation of the deformation and crack nucleation mechanisms in titanium alloys

○Dongsheng Xu （Institute of Metal Research, Chinese Academy of Sciences, China）

Titanium alloys are widely used in aero-space and chemical industries, but due to the complicated hierarchical microstructure formed in these systems, the deformation and fatigue life control is not easy. Multi-scale simulations were carried out on the deformation and microstructure evolution of titanium alloys in order to understand deformation and fatigue behavior under different conditions. The dislocation nucleation, interaction, debris accumulation and their effects on the deformation and fatigue crack nucleation were investigated. It was shown that, upon cyclic deformation, point defects and small dislocation loops can be formed in slip band by dipolar reaction. This will consume mobile dislocations, and make the operating slip system hardened; at the same time, they can provide deformation mechanism upon further increase of the stress. Comparing with perfect lattice, the lattice with point defects under tension perpendicular to the slip plane can be weakened by these point defects, therefore they may serve as fatigue crack nucleation sites and propagating paths. These understanding gained by simulations may provide important clue to the fatigue resistance design for titanium alloys.

Symposium | E. Deformation and Fracture Mechanism of Materials

[SY-E10] Symposium E-10

Chairs: Irene Beyerlein(University of California at Santa Barbara, USA), Dongsheng Xu(Institute of Metal Research, CAS, China)

Thu. Nov 1, 2018 11:15 AM - 12:30 PM Room2

[SY-E10] Study of atomic trajectories during twinning transformation in magnesium

○Andrej Ostapovec[1], Tomáš Káňa[1], Václav Paidar[2] （1.Institute of Physics of Materials ASCR, Czech Republic, 2.Institute of Physics ASCR, Czech Republic）

[SY-E10] Understanding nanocontact plasticity through massive MD simulations

○Jorge Alcala[1], Javier Varillas[2,1], Jordi Torner[2], Jan Očenášek[1] （1.Universidad Politecnica de Catalunya, Spain, 2.New Technologies Research Centre, Czech Republic）

[SY-E10] Atomistically informed mesoscale modeling of fracture

○Hamad ul Hassan[1], Johannes Möller[2,3], Erik Bitzek[2], Alexander Hartmaier1[1], Rebecca Janisch[1] （1.ICAMS, Ruhr-Universität Bochum, Germany, 2.Friedrich-Alexander Universität Erlangen-Nürnberg , Germany, 3.Fraunhofer Institut für Werkstoffmechanik, Freiburg, Germany）

[SY-E10] Lattice Distortion Effect on Cross-Slip in High Entropy Alloys and Lennard-Jones Systems for Face-Centered Cubic

○Chao-Chun Yen[1], Junping Du[2,3], Jia-An Lin[4], Yu-Chieh Lo[4] （1.National Tsing Hua University, Taiwan, 2.Kyoto University, Japan, 3.Osaka University, Japan, 4.National Chiao Tung University, Taiwan）

[SY-E10] Atomic structure of gamma/alpha2 interface and its influence on plastic deformation of lamellar TiAl alloys

○Hao Wang[1], Aidong Tu[1], Yanxia Liu[2], Dongsheng Xu[1], Rui Yang[1] （1.Institute of Metal Research, CAS, China, 2.Dept. of Physics, Liaoning University, China）

(Thu. Nov 1, 2018 11:15 AM - 12:30 PM Room2)

[SY-E10] Study of atomic trajectories during twinning transformation in magnesium

○Andrej Ostapovec[1], Tomáš Káňa[1], Václav Paidar[2] (1.Institute of Physics of Materials ASCR, Czech Republic, 2.Institute of Physics ASCR, Czech Republic)

Deformation twinning is important mode of plastic deformation in magnesium and its alloys. Study of twinning mechanisms has long tradition. However, there is still opened questions in this field. There is some speculations in the literature, which connects possibility of non-Schmid behavior of mechanical twinning to type of atomic trajectories during twinning transformation. However, such theoretical considerations often use simplified descriptions of atomic motions. For instance, some authors made conclusions about macroscopic behaviour of twinning on the basis of linear or circular atomic trajectories. In a broader picture, real atomic paths should be quite complicated. They are consequence of disconnection glide along twin boundary. In this study we would like to discuss atomic trajectories obtained from modeling using EAM potentials as well as from ab-initio calculations.

(Thu. Nov 1, 2018 11:15 AM - 12:30 PM Room2)

[SY-E10] Understanding nanocontact plasticity through massive MD simulations

○Jorge Alcala[1], Javier Varillas[2,1], Jordi Torner[2], Jan Očenášek[1] (1.Universidad Politecnica de Catalunya, Spain, 2.New Technologies Research Centre, Czech Republic)

This presentation concerns comprehensive molecular dynamics (MD) simulations of nanocontact plasticity in body-centered cubic (BCC) and face-centered cubic (FCC) crystals. The main focus is on the understanding of the evolution of the nanoscale material hardness with increasing tip penetration through detailed analyses of the distinct defect nucleation processes which result in the formation of a permanent imprint. It is shown that the gradual development of an entangled defect structure essentially governs the evolution of material pileup at the contact boundary, a feature that explains the different FCC and BCC imprint morphologies and topographies that develop depending on loading orientation. The present analyses provide a fundamental background to understand why BCC surfaces are harder than FCC surfaces at the nanoscale, including the role of the elastic response of the indented crystals. Novel MD simulations for crystals containing a preexisting (dense) dislocation network further confirm the pivotal role of the incepted defects upon indenter tip penetration. Our analyses contribute to the understanding of indentation size effects in submicrometer-sized material volumes, where a physical rationale to the validity of strain gradient plasticity and geometrically necessary dislocations is essentially lacking. Finally, our investigation leads to the finding of a general correlation between the nanohardness and the yield strength measured at the nanoscale under uniaxial loading conditions.

(Thu. Nov 1, 2018 11:15 AM - 12:30 PM Room2)

[SY-E10] Atomistically informed mesoscale modeling of fracture

○Hamad ul Hassan[1], Johannes Möller[2,3], Erik Bitzek[2], Alexander Hartmaier1[1], Rebecca Janisch[1] （1.ICAMS, Ruhr-Universität Bochum, Germany, 2.Friedrich-Alexander Universität Erlangen-Nürnberg , Germany, 3.Fraunhofer Institut für Werkstoffmechanik, Freiburg, Germany）

At the engineering scale, continuum mechanics provides an efficient way to model fracture based on stresses, stress intensity factors, and energy release rates. At the atomic scale, in contrast, the breaking of atomic bonds is caused by critical forces acting on individual atoms. Therefore, a scaling methodology is required to apply information from atomistic scale to the continuum level problems, which are governed by engineering length and time scales.

Fracture at the continuum level can be described using state of the art methods such as cohesive zone-based modeling, which requires a material-specific traction-separation law (T-S law). Here, we present a mesh independent approach for atomistic-to-continuum level scaling of the stress and displacement measures, which are used in the T-S law. Our approach is based on a detailed analysis of the forces acting between the atoms in front of a crack tip, as well as between two semi-infinite half-crystals. Such a constellation is used to calculate the properties of cohesive zones based on atomistic simulations. The analysis shows, that the interatomic forces at a crack tip can be directly related to the restoring tractions between the two planar surfaces. This allows for an unambiguous scaling of the critical stresses and displacements, from GPa / Åon the atomic level, to the order of hundreds of MPa and nm on the mesoscale. A series of finite element simulations are performed for K_I loading based on the scaled input data for the T-S law and the critical stress intensity factors are calculated and compared with results from the atomistic simulations. We demonstrate and examine the ability of the atomistically informed finite element simulation to directly reproduce results from atomistic simulations.

(Thu. Nov 1, 2018 11:15 AM - 12:30 PM Room2)

[SY-E10] Lattice Distortion Effect on Cross-Slip in High Entropy Alloys and Lennard-Jones Systems for Face-Centered Cubic

○Chao-Chun Yen[1], Junping Du[2,3], Jia-An Lin[4], Yu-Chieh Lo[4] （1.National Tsing Hua University, Taiwan, 2.Kyoto University, Japan, 3.Osaka University, Japan, 4.National Chiao Tung University, Taiwan）

The superior mechanical properties of high-entropy alloys (HEAs) make an outstanding success in material science and engineering. In recent years, more efforts have been devoted to the effect of severe lattice distortion, which is one of the core effects of HEAs. Previous studies have shown the impacts of severe lattice distortion on plastic deformation, including the influences on nucleation and propagation of dislocation. One of the most common mechanism is cross-slip in metals, which is a fundamental process of screw dislocation motion and plays an important role in dislocation annihilation and work hardening. However, there is no sufficient reference so far that can provide a clear correlation between the cross-slip and lattice distortion in HEAs. This may result from the difficulties of finding the cause of local lattice strain through experimental approach. Nevertheless, atomistic simulations can overcome the dilemma. Here, we create a binary system containing two different sizes of atoms. In order to focus on the lattice distortion caused only by size difference, a large-scale molecular dynamics simulation is performed using Lennard-Jones potentials to provide a size-controllable system where different sizes of atoms are assumed to be the same chemical potential. Therefore, we can systematically discuss the influence of the lattice distortion on cross-slip of HEAs. Furthermore, we apply nudged elastic band method on modified embedded-atom method potentials of CoCrFeMnNi and Lennard-Jones potentials to calculate the activation energy of cross slip for screw

dislocation respectively, and compare both results for further investigation.

(Thu. Nov 1, 2018 11:15 AM - 12:30 PM Room2)

[SY-E10] Atomic structure of gamma/alpha2 interface and its influence on plastic deformation of lamellar TiAl alloys

○Hao Wang[1], Aidong Tu[1], Yanxia Liu[2], Dongsheng Xu[1], Rui Yang[1] （1.Institute of Metal Research, CAS, China, 2.Dept. of Physics, Liaoning University, China）

TiAl alloys with the γ-TiAl/α_2-Ti_3Al lamellar structure exhibit excellent high temperature performance. However, the strong anisotropy of the lamellae leads to the strong dependence of mechanical properties, in particular the fatigue behavior, on lamella orientation, thickness, volume fraction, etc. In the present work, molecular dynamics with the embedded-atom potential is employed to investigate the energy of both the coherent and incoherent γ / α_2 interfaces. The interface coherency is found to depend on the volume ratio of the γ lamellae over the $\alpha_2$lamellae, resulting in a critical volume ratio, below/above which the interface is coherent/incoherent. Loading perpendicular and parallel to the lamella interface indicates that the yield strength of coherent interface is higher than that of the incoherent interface. Plastic deformation mostly occurs first in the γ region and transmits to the α_2 region via dislocations or twinning across the γ / α_2 interface. Subsequent fracture behavior also depends on the γ / α_2 volume ratio. With the coherency and incoherency interfaces, crack nucleates within the γ region and at the γ / α_2 interface, respectively. The present result thus contribute to the evaluation of the structural stability and the improvement of mechanical performance of TiAl alloys.

Symposium | E. Deformation and Fracture Mechanism of Materials

[SY-E11] Symposium E-11

Chairs: Xiaoyu Yang(Computer network information center, CAS, China), Denise Reimann(ICAMS, Ruhr-Universität Bochum, Germany)

Thu. Nov 1, 2018 2:00 PM - 3:30 PM Room2

[SY-E11] Thermodynamically consistent directional distortional hardening of wrought Mg alloys: experimental investigation and constitutive modeling

○Baodong Shi[1], Yan Peng[1], Chong Yang[1], Jianliang Sun[1], Fusheng Pan[2] （1.NECSR, School of Mechanical Engineering, Yanshan Univ., China, 2.NERC-MA, Chongqing Univ., China）

[SY-E11] A computational infrastructure for multiscale materials simulation

○Xiaoyu Yang （Computer network information center of the Chinese Academy of Sciences, China）

[SY-E11] Using machine learning methods to homogenize damage from micro- to macroscale

Denise Reimann[1], Hamad ul Hassan[1], Tobias Glasmachers[2], ○Alexander Hartmaier[1] （1.ICAMS, Ruhr-Universität Bochum, Germany, 2.Institut für Neuroinformatik, Ruhr-Universität Bochum, Germany）

[SY-E11] Graph theory analysis of rich fiber-scale data yields very fast simulations of damage evolution in composites

jerry quek[2], ○brian n cox[1] （1.arachne consulting, United States of America, 2.IHPC, Singapore）

[SY-E11] A deep learning-based constitutive model for finite element analysis

Fariborz Ghavamian[1], ○Angelo Simone[2,1] （1.Delft University of Technology, Netherlands, 2.University of Padova, Italy）

(Thu. Nov 1, 2018 2:00 PM - 3:30 PM Room2)

[SY-E11] Thermodynamically consistent directional distortional hardening of wrought Mg alloys: experimental investigation and constitutive modeling

Invited

○Baodong Shi[1], Yan Peng[1], Chong Yang[1], Jianliang Sun[1], Fusheng Pan[2] （1.NECSR, School of Mechanical Engineering, Yanshan Univ., China, 2.NERC-MA, Chongqing Univ., China）

As a lightweight structural material, magnesium alloy exhibits strong anisotropy due to texture, which limits its use in energy-saving lightweight structures. This pronounced anisotropy cannot be captured by only classical isotropic or kinematic hardening due to the constant shape evolution of yield surfaces during plastic deformation. Therefore, the shape evolution of yield surface, named as distortional hardening is the main approach to capture the anisotropic behavior of Mg alloy. Moreover, stress state is changing during forming process such as deep drawing, i.e., the loading history effect during plastic deformation cannot be ignored. Thus, focusing on loading path dependent distortional hardening of AZ31 Mg alloy, experimental investigation on the evolution of anisotropy is performed, moreover, a constitutive model with distortional evolution of yield surfaces is developed based on elasto-plasticity theory at finite strain. Thermodynamical consistency is proved. The anisotropic mechanical behavior of AZ31 Mg alloy is demonstrated after model parameters calibrated with experiments.

(Thu. Nov 1, 2018 2:00 PM - 3:30 PM Room2)

[SY-E11] A computational infrastructure for multiscale materials simulation

○Xiaoyu Yang （Computer network information center of the Chinese Academy of Sciences, China）

Bridging materials models and passing materials-related data and information across length scales is critical for the quantitative and predictive modelling of materials development. However, lacking of acceptable linkage software and tools is an obstacle. It is recommended in the report by the Minerals, Metals &Materials Society that “establishing an infrastructure for multiscale materials data is the first programmatic recommendations”. Currently we are developing such an infrastructure to address this need based on a high-throughput computational infrastructure MatCloud[1]. The core of this multiscale simulation infrastructure is a linking software tool and technologies that contains a workflow designer and a workflow engine. The workflow designer aims to support the design of simulations involving running quantum mechanics scale ABINIT simulation and molecular scale LAMMPS simulation by drag &drop approach. The workflow engine is responsible for parsing and processing the workflow of multiscale materials simulation created by the workflow designer. As a test case, the multiscale materials simulation linking tool will be used to develop a particular interatomic potential through data-driven approach. In this talk, we will report our progress and challenges encountered.

Reference:

[1]. Yang X. et al , MatCloud: A High-throughput Computational Infrastructure for Integrated Management of Materials Simulation, Data and Resources, Computational Materials Science, Volume 146, 15 April 2018,

Pages 319-333, https://doi.org/10.1016/j.commatsci.2018.01.039

(Thu. Nov 1, 2018 2:00 PM - 3:30 PM Room2)

[SY-E11] Using machine learning methods to homogenize damage from micro- to macroscale

Denise Reimann[1], Hamad ul Hassan[1], Tobias Glasmachers[2], ○Alexander Hartmaier[1] (1.ICAMS, Ruhr-Universität Bochum, Germany, 2.Institut für Neuroinformatik, Ruhr-Universität Bochum, Germany)

Micromechanical models are in general able to describe microstructural influences, such as texture and grain size distribution, on damage evolution. A homogenization from the micro to the macro scale is, however, conceptually demanding. Hence, a new approach involving machine learning algorithms is suggested. In this work, numerical data based on micromechanical simulations is used to train the machine learning algorithm, which in turn describes macroscopic damage evolution as function of loading conditions and microstructure. The micromechanical simulations are based on representative volume elements (RVE) of realistic microstructure models, using crystal plasticity and damage mechanics to describe plastic deformation and damage evolution on the grain level.
Local quantities from these RVE simulations, such as stress, strain and damage, are homogenized into global averages. The trained machine learning algorithm is then able to predict global damage evolution as a function of the macroscopic loading state (e.g. equivalent strains, equivalent and hydrostatic stresses), elastic-plastic material properties and microstructure information (e.g. grains size distribution, crystallographic texture, etc.). The results are compared with well-accepted closed-form damage models such as Chaboche or Lemaître for validation. Furthermore, different machine learning algorithms such as artificial neural networks, support vector machines and random forest are used and their results are compared with each other as well.

(Thu. Nov 1, 2018 2:00 PM - 3:30 PM Room2)

[SY-E11] Graph theory analysis of rich fiber-scale data yields very fast simulations of damage evolution in composites

jerry quek[2], ○brian n cox[1] (1.arachne consulting, United States of America, 2.IHPC, Singapore)

Simple mechanistic arguments suggest that the loci of cracks that initiate and propagate among fine-scale, stochastic, heterogeneous material domains might be predictable by fast graph theoretic methods, without executing explicit fracture mechanics simulations. Here we explore the usefulness of graph theoretic methods for analyzing the microcracking that develops in continuous fiber composites loaded transversely to the fiber direction. We use graph theoretic methods to analyze rich data published elsewhere for two types of fiber composite. The data describe the irregularity of the spatial distribution of the fiber population, and meandering of fibers within the population, which is seen when the fibers are tracked along the nominal fiber direction. Graph analysis yields very fast predictions of the likely sites of crack initiation in the fiber composite, as well as plausible indications of the likely direction in which an initiated crack will grow, the developing shape of the crack, and the frequency of instances of fibers that will bridge the crack obliquely, thereby raising the composite fracture resistance. From the results of the graph analysis, we infer a stochastic population of effective defects in the composite, whose location and effective strength are related to the

Euclidean and topological characteristics of the fiber population in the vicinity of the defect. We propose that, if the predicted distribution of defects is entered as an initial material condition in an homogenized finite element simulation of the composite, then the important effects of the stochastic fiber distribution, in regard to crack initiation, preferred directions of growth, and toughening due to fiber-bridging, can be captured in a simulation of tractable size. This strategy carries the pertinent spatial information content of any measured random distribution of fibers into a simulation in which the fibers are not represented explicitly.

(Thu. Nov 1, 2018 2:00 PM - 3:30 PM Room2)

[SY-E11] A deep learning-based constitutive model for finite element analysis

Fariborz Ghavamian[1], ○Angelo Simone[2,1] (1.Delft University of Technology, Netherlands, 2.University of Padova, Italy)

A deep learning model is simply a function that maps a given input to a desired output. In spite of the simple nature of a deep learning model, over the past decade it has revolutionized natural language processing (NLP) and image understanding (IU). One can name three fundamental reasons to explain this astonishing accomplishment: 1) availability of large amount of data for NLP and IU over the past decade; 2) the fact that the performance of a deep learning model keeps increasing by increasing the training data (unlike other machine learning models); and 3) the recently available hardware and software infrastructures which are tailored for deep learning.

In this contribution we leverage the power of deep learning to construct a deep learning-based constitutive model. More specifically, we develop a novel neural network architecture which is tailored for simulations of history-dependent material behavior, and we discuss its implementation in a finite element model.

A possible application of this deep learning-based constitutive model is to serve as an efficient surrogate to a representative volume element (RVE) in a multi-scale finite element analysis. In this application large amount of training data can readily be generated from the RVE. As a proof of concept, we train our deep learning model on a set of data collected from a viscoplastic constitutive model and employ it a finite element model. Through numerical experiments we show that the structural level response of the finite element model is adequately approximated when using the deep learning-based constitutive model in place of the viscoplastic one.

Symposium | E. Deformation and Fracture Mechanism of Materials

[SY-E12] Symposium E-12

Chairs: Baodong Shi(NECSR, School of Mechanical Engineering, Yanshan Univ., China), Ligang Zhang(Central South University, China)

Thu. Nov 1, 2018 4:00 PM - 5:00 PM Room2

[SY-E12] Diffusivities and atomic mobilities in bcc Ti-Mo-Nb-Ta-Zr alloys

○Weimin Bai[1], Guanglong Xu[2], Libin Liu[1], Ligang Zhang[1] （1.School of Materials Science and Engineering, Central South Univ., China, 2.Tech Inst. for Advanced Materials &School of Materials Science and Engineering, Nanjing Tech Univ., China）

[SY-E12] Design of Ti-alloy by Integrating High Throughput Experiments and Calculations

○Ligang Zhang, Libin Liu, Di Wu （Central South University, China）

[SY-E12] Simulation of Plasticity in Amorphous Solids

○Shingo Urata[1], Takahiro Murashima[2], Shaofan Li[3] （1.Innovative Technology Research Center, Asahi Glass Co., Ltd (AGC)., Japan, 2.Dept. of Physics, Tohoku University, Japan, 3.Dept. of Civil and Environmetal Engineering, Univ. of California Berkeley, United States of America）

[SY-E12] Computational generation of the yield surfaces using stress based loading

○mayank chouksey, Sumit Basu （Indian Institute of Technology, Kanpur, India）

(Thu. Nov 1, 2018 4:00 PM - 5:00 PM Room2)

[SY-E12] Diffusivities and atomic mobilities in bcc Ti-Mo-Nb-Ta-Zr alloys

○Weimin Bai[1], Guanglong Xu[2], Libin Liu[1], Ligang Zhang[1] (1.School of Materials Science and Engineering, Central South Univ., China, 2.Tech Inst. for Advanced Materials &School of Materials Science and Engineering, Nanjing Tech Univ., China)

Titanium and its alloys are widely used in biomedical field due to the low elastic modulus comparable to bone as well as high specific strength and high corrosion resistance. β-type (with bcc structure) and near β titanium alloys comprising non-toxic and non-allergic elements have been extensively investigated in the past decades to achieve low Young's modulus and good mechanical properties. Researchers suggested that Zr, Nb, Ta and Mo are the most desirable alloying elements in β-type bio-Ti alloys which have ability to effectively increase strength and reduce elastic modulus according to electronic structural calculations. Recently, a number of low-modulus biomedical β-titanium alloys have been developed, for example, Ti-29Nb-13Ta-4.6Zr (TNTZ), Ti-24Nb-4Zr-7.9Sn and Ti-8Mo-4Nb-2Zr.

Diffusivities play important roles when we manipulate above phase transformations and control microstructure development. The diffusion paths and phase fractions during homogenization and precipitation are precisely predicted with the help of thermodynamic and kinetic data by means of the Thermo-Calc and DICTRA software [2,3]. The microstructure evolution during heat treatment can be not only statistically explained via the classical nucleation and growth model equipped with accurate diffusivities, but also represented by the phase field modeling allying with diffusion kinetic database of multi- component and multi-phase systems.

In this work, the diffusivities of sub-ternary systems in Ti-Mo-Nb-Ta-Zr were extracted from composition profiles of diffusion couples using Whittle-Green [4] and Hall [5] methods. Based on the experimental results and thermodynamic descriptions, a self-consistent atomic mobility database of bcc Ti-Mo-Nb-Ta-Zr alloys were assessed using DICTRA software. All the kinetic descriptions were further verified by comprehensive comparisons between various model-predicted diffusion properties and the experimental data. The general agreement validates the potential application of the present atomic mobility database to simulate the diffusion in higher orders.

[1] J.-O. Andersson and J. Ågren, J. Appl. Phys. 72 (1992) 1350-1355.

[2] J.-O. Andersson et al., Calphad. 26 (2002) 273-312.

[3] D.P. Whittle and A. Green, Scr. Metall. 8 (1974) 883-884

[4] L.D. Hall, J. Chem. Phys. 21 (1953) 87-89.

(Thu. Nov 1, 2018 4:00 PM - 5:00 PM Room2)

[SY-E12] Design of Ti-alloy by Integrating High Throughput Experiments and Calculations

○Ligang Zhang, Libin Liu, Di Wu （Central South University, China）

The Speed for development of next materials is too slow and it has been emerging as the bottleneck for the innovation of the manufacturing technology. However, application of the computer and information technology to the materials science and engineering has made it possible for us to estimate the properties for single phases, model the microstructure evolutions, and predict the material properties. On the other hand, in order to verify the calculation results, we should develop and use the high throughput methods. In this talk, we introduce some new progress in materials calculation and high throughput experiments, especially the high throughput determination of the phase diagram, diffusion coefficients, and thermal-physical properties, and the high throughput verification of the response of the materials microstructure and properties to the compositions and heat treatment temperatures. Some preliminary results on the attempt of development of high strength and high toughness Ti alloys has been introduced.

(Thu. Nov 1, 2018 4:00 PM - 5:00 PM Room2)

[SY-E12] Simulation of Plasticity in Amorphous Solids

○Shingo Urata[1], Takahiro Murashima[2], Shaofan Li[3] （1.Innovative Technology Research Center, Asahi Glass Co., Ltd (AGC)., Japan, 2.Dept. of Physics, Tohoku University, Japan, 3.Dept. of Civil and Environmetal Engineering, Univ. of California Berkeley, United States of America）

A Multiscale model to simulate mechanical response of amorphous solids has been developed by coupling molecular mechanics and finite element method. In this method, an atomistic-based representative sampling cell (RS-cell) is embedded into each element to represent inelastic deformations in amorphous materials. Because the method employs a Parrinello-Rahman molecular dynamics based Cauchy-Born rule to construct an atomistically-informed constitutive model at continuum level, it is possible to quantitatively measure amorphous plastic deformations. In other words, the method intrinsically embeds a potential shear-transformation-zone (STZ), and thus the evolution of RS-cells can naturally allow molecular clusters having irreversible microstructure rearrangements at microscale in response to applied loads without using any phenomenological modeling. By using the proposed method, we obtained inelastic hysteresis loops for the amorphous materials under cyclic loading and also shear band formation at macroscale by using the Lennard-Jones binary glass (LJBG) model. In addition, we extended the method to apply to silicate glasses by considering electrostatic interaction. We would also demonstrate fracture simulation of the oxide glasses by coupling the method with Multiscale Cohesive Zone Model.

(Thu. Nov 1, 2018 4:00 PM - 5:00 PM Room2)

[SY-E12] Computational generation of the yield surfaces using stress based loading

○mayank chouksey, Sumit Basu （Indian Institute of Technology, Kanpur, India）

Ductile fracture in metals proceeds through nucleation, growth and coalescence of microvoids. Determination of the yield surface of a ductile porous material is necessary to simulate onset and evolution of ductile damage in a metal. Since the early work by Gurson where yield function for concentric spherical void inside a spherical RVE was considered, several extensions have emerged. It has been shown that the void

shape and anisotropy of the bulk matrix modify the yield function significantly. All these predictions of yield rely on limit analysis of the RVE based on the upper bound theorem and Hill-Mandal homogenization. These models have not accounted for onset of yield through localization of plastic strain.

Recently the competition between localization and uniform yield via the Gurson model has been compared. We have extended this work by performing stress controlled computational homogenization over sub-spaces of the principal stress space, to probe the yield surface of perfectly plastic materials with different void shapes. A special four-noded user element is developed in ABAQUS, that, is tied to a RVE with periodic boundary condition, restrained rigid body rotation and subjected to either macroscopic deformation gradient or Cauchy stress. The macroscopic plastic dissipation rate is monitored to detect yield. As a result, yield due to both uniform plastic deformation and localization are captured. We have compared the results of our computationally determined yield surfaces with the theoretical upper bound estimates. We show that over a significant section of the principal stress sub-space, localization modifies the yield surface. For prolate voids, localization hastens yield while for oblate it is delayed over estimates provided by models based on the upper bound theorem. The comparison gives us a rich insight into the competition between macroscopic yield through uniform proliferation of plasticity and localization.

Symposium | F. From Microstructure to Properties: Mechanisms, Microstructure, Manufacturing

[SY-F9] Symposium F-9

Chair: Ernst Kozeschnik(Institute of Materials Science and Technology, TU Wien, Austria)

Thu. Nov 1, 2018 9:45 AM - 11:00 AM Room3

[SY-F9] Programmable Materials - tuning effective materials response

○Peter Gumbsch[1,2], Chris Eberl[1,3], Claudio Findeisen[1,2], Alexander Butz[1], Jan Pagenkopf[1,2]
（1.Fraunhofer IWM, Germany, 2.Karlsruhe Institute of Technology (KIT), Germany, 3.Albert-Ludwigs-Universität Freiburg, Germany）

[SY-F9] Equilibrium crystal shape of GaAs by ab-initio thermodynamics

In Won Yeu[1,2], Gyuseung Han[1,2], Cheol Seong Hwang[2], ○Jung-hae Choi[1] （1.Center for Electronic Materials, Korea Institute of Science and Technology, Korea, 2.Department of Materials Science and Engineering, and Inter-university Semiconductor Research Center, Seoul National University, Korea）

[SY-F9] Elastic field of lattice defects in low-dimensional nano-carbon materials

○Xiao-Wen LEI[1], Akihiro NAKATANI[2], Tomoya TANIGUCHI[1] （1.Dept. of Mechanical Engineering, Univ. of Fukui, Japan, 2.Dept. of Adaptive Machine Systems, Osaka Univ. , Japan）

(Thu. Nov 1, 2018 9:45 AM - 11:00 AM Room3)

[SY-F9] Programmable Materials - tuning effective materials response

Invited

○Peter Gumbsch[1,2], Chris Eberl[1,3], Claudio Findeisen[1,2], Alexander Butz[1], Jan Pagenkopf[1,2] (1.Fraunhofer IWM, Germany, 2.Karlsruhe Institute of Technology (KIT), Germany, 3.Albert-Ludwigs-Universität Freiburg, Germany)

The design of materials and materials microstructures to specific materials properties requires mechanistic materials modelling over multiple length scales to avoid tedious trial-and-error procedures and excessive experimentation. The feasibility of such multiscale modelling has now been demonstrated in several cases including the explicit modelling of the microstructural evolution during processing. As an example, I will explain the manufacturing process of a steel component, for which the local microstructure and the resulting material properties after deep drawing can be predicted.

On the component level, locally different processing conditions result in locally different materials properties which are often dealt with as a nuisance. I would like to take this further and ask whether we are able to design materials such that their locally varying properties are used for component functionality. Conceptually this can be regarded as locally *programming a material* to achieve component functionality. It will require large-scale structural optimization, predictive materials models for materials with significantly varying properties. I will give examples how this can be achieved. The approach can most easily be demonstrated using additively built metamaterials. With such metamaterials one can even go further and design them such that their effective materials properties can still be changed after manufacturing to achieve intrinsically *programmable materials*.

(Thu. Nov 1, 2018 9:45 AM - 11:00 AM Room3)

[SY-F9] Equilibrium crystal shape of GaAs by ab-initio thermodynamics

In Won Yeu[1,2], Gyuseung Han[1,2], Cheol Seong Hwang[2], ○Jung-hae Choi[1] (1.Center for Electronic Materials, Korea Institute of Science and Technology, Korea, 2.Department of Materials Science and Engineering, and Inter-university Semiconductor Research Center, Seoul National University, Korea)

The growth of the III-V compound semiconductors on Si is crucial to adapt their superior electronic properties to the silicon-based CMOS technology. In order to achieve the high-quality hetero-epitaxy preventing defects such as dislocation, crack, and anti-phase boundary, the selective area growth (SAG) method has been developed. To optimize this process, the atomic scale understanding is essential in terms of both the thermodynamics and kinetics. In this study, we establish a thorough methodology to calculate the surface energy as a function of temperature (T) and pressure (P) for the III-V compound materials in the combined framework of density functional theory (DFT) calculations and thermodynamics [1], which is competitive compared the previous DFT studies providing the surface energy as a function of chemical potential. Then, we construct the equilibrium crystal shape of GaAs as a function of T and P, including the effects of surface vibration. The calculated equilibrium shapes in various T and P conditions are compared with the experimentally grown shapes and explained in the viewpoint of the surface vibration, twin formation and kinetic factors.

[1] In Won Yeu *et al.,* Sci. Rep. 7, 10691 (2017).

(Thu. Nov 1, 2018 9:45 AM - 11:00 AM Room3)

[SY-F9] Elastic field of lattice defects in low-dimensional nano-carbon materials

○Xiao-Wen LEI[1], Akihiro NAKATANI[2], Tomoya TANIGUCHI[1] (1.Dept. of Mechanical Engineering, Univ. of Fukui, Japan, 2.Dept. of Adaptive Machine Systems, Osaka Univ. , Japan)

Carbon atoms build themselves into different materials such as fullerenes, diamond nano-thread, carbon nanotube (CNT), and graphene sheet (GS) in nanometer-scale. The materials are formally classified into point, line, and surface materials, which correspond to zero-, one- and two-dimensional materials, respectively. Many literatures report that the lattice defects affected mechanical properties and electronic properties. Lattice defects in such low-dimensional nano-carbon are limited into special atomic structures rather than bulk (three-dimensional) materials, but the properties of these low-dimensional materials depend on the lattice defects as well as bulk materials. Continuum theory, such as dislocation theory, has been developed sophisticatedly for very long years. In low-dimensional materials, however, theoretical approaches for lattice defects are just developing. In this study we discuss the elastic field of lattice defects in low-dimensional nano-carbon, e.g. Stone-Wales (SW) defects on single-walled carbon nanotubes (SWCNTs) and GS. The various equilibrium configurations of atomistic models with defects are obtained using LAMMPS. The site potential energy and stress distribution of each atom are evaluated in the vicinity of defects. We also measure a curvature and bond length to identify the out-of-plane deformation and in-plane deformation. We also study the dependence of elastic field on the chirality of CNT and the interaction of two SW defects in details. Formation energy significantly depends on chirality, i.e. diameter, of nanotube as well as the orientation and position of SW defect in SWCNT and GS. The results obtained for atomistic models are compared with an classical analytical solutions of plane stress which is established ideally with assumption of only in-of-plane deformation, and the effect of out-of-plane deformation of low-dimensional nano-carbon is discussed.

Symposium | F. From Microstructure to Properties: Mechanisms, Microstructure, Manufacturing

[SY-F10] Symposium F-10

Chair: Ricardo Lebensohn(Los Alamos National Laboratory, United States of America)

Thu. Nov 1, 2018 11:15 AM - 12:30 PM Room3

[SY-F10] **Data Analytics for Mining Process-Structure-Property Linkages for Hierarchical Materials**

○Surya Raju Kalidindi （Georgia Tech, United States of America）

[SY-F10] Maximization of strengthening effect of microscopic morphology in duplex elastoplastic solids

○Ikumu Watanabe[1], Gaku Nakamura[2], Kohei Yuge[2] （1.National Institute for Materials Science, Japan, 2.Seikei University, Japan）

[SY-F10] Assessment of formability limit diagram prediction by crystal plasticity finite element method

○Duancheng Ma （Leichtmetallkompetenzzentrum Ranshofen GmbH, Austria）

[SY-F10] Analysis of gradient microstructures using crystal plasticity

○Balaji Selvarajou, Jerry Quek Siu Sin （IHPC, Singapore, Singapore）

(Thu. Nov 1, 2018 11:15 AM - 12:30 PM Room3)

[SY-F10] Data Analytics for Mining Process-Structure-Property Linkages for Hierarchical Materials

Invited

○Surya Raju Kalidindi （Georgia Tech, United States of America）

A majority of the materials employed in advanced technologies exhibit hierarchical internal structures with rich details at multiple length and/or structure scales (spanning from atomic to macroscale). Collectively, these features of the material internal structure are here referred to as the material structure, and constitute the central consideration in the development of new/improved hierarchical materials. Although the core connections between the material’s structure, its evolution through various manufacturing processes, and its macroscale properties (or performance characteristics) in service are widely acknowledged to exist, establishing this fundamental knowledge base has proven effort-intensive, slow, and very expensive for most material systems being explored for advanced technology applications. The main impediment arises from lack of a broadly accepted framework for a rigorous quantification of the material’s structure, and objective (automated) identification of the salient features that control the properties of interest. This presentation focuses on the development of data science algorithms and computationally efficient protocols capable of mining the essential linkages from large ensembles of materials datasets (both experimental and modeling), and building robust knowledge systems that can be readily accessed, searched, and shared by the broader community. The methods employed in this novel framework are based on digital representation of material’s hierarchical internal structure, rigorous quantification of the material structure using n-point spatial correlations, objective (data-driven) dimensionality reduction of the material structure representation using data science approaches (e.g., principal component analyses), and formulation of reliable and robust process-structure-property linkages using various regression techniques. This new framework is illustrated through a number of case studies.

(Thu. Nov 1, 2018 11:15 AM - 12:30 PM Room3)

[SY-F10] Maximization of strengthening effect of microscopic morphology in duplex elastoplastic solids

○Ikumu Watanabe[1], Gaku Nakamura[2], Kohei Yuge[2] （1.National Institute for Materials Science, Japan, 2.Seikei University, Japan）

An inverse analysis method based on nonlinear finite element analysis is developed to find an optimized morphology of periodic microstructure for improving the macroscopic mechanical properties in duplex elastoplastic solids. Here a gradient-based computational optimization method and two types of homogenization methods are employed. In this study, the optimization problem is defined as the maximization of the sum of macroscopic external works for several macroscopic deformation modes, enabling us to obtain a high strength material. The morphologic strengthening effect is discussed through a comparison with experiments and classical theories.
In a homogenization method based on finite element analysis, a representative volume element of an objective microstructure is modeled with finite elements and the deformation analysis is conducted under periodic boundary condition in control of macroscopic stress or strain. As the numerical results, the deformation state of microstructure is obtained along with the corresponding macroscopic material response. By coupling with this computational homogenization method and a mathematical optimization

method, the microstructure corresponding to a required performance can be found efficiently.
In this study, a computational optimization method for microstructure is applied to maximize the strength of a dual-component elastoplastic solid. A standard metal plasticity is employed to describe the material responses of each components and the material constants are determined from the macroscopic experiments of the corresponding single-component materials. For optimization calculations, the distributions of two densities are considered with node-based discretization under a constraint condition to finally segregate two components. And here simple strain-constant analytical homogenization method, so-called mixture rule, is applied to handle the mixture state during the optimization process.

(Thu. Nov 1, 2018 11:15 AM - 12:30 PM Room3)

[SY-F10] Assessment of formability limit diagram prediction by crystal plasticity finite element method

○Duancheng Ma （Leichtmetallkompetenzzentrum Ranshofen GmbH, Austria）

This study is inspired by the recent development of “virtual material testing laboratory” in which the main equipment are full field crystal plasticity models. Ample examples have demonstrated its applications to sheet forming operations. In those applications, the mechanical anisotropy originated from the crystallographic texture can be adequately described, such as r-values and earing. Formability is also another very important property in sheet metal forming, which yet have not been equipped in these virtual laboratories. Though theoretical models for formability can be dated back to 1800s, all popular models at the moment suffer respective limitations. In this study, we make an attempt to the prediction of formability limit diagram by crystal plasticity finite element method, with the objective of overcoming the limitations posed by the current theoretical models. The focus is placed on the texture dependence of the formability limit diagram

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(Thu. Nov 1, 2018 11:15 AM - 12:30 PM Room3)

[SY-F10] Analysis of gradient microstructures using crystal plasticity

○Balaji Selvarajou, Jerry Quek Siu Sin （IHPC, Singapore, Singapore）

Gradients in microstructural features such as grain size, initial dislocation density and crystallographic texture occur in many engineering applications such as shot peened regions and heat affected zone of welds. While such microstructures may be desirable to improve mechanical properties, modelling of such microstructures require integration of appropriate length scales into the constitutive model. Crystal plasticity finite element method (CPFEM) offers an appropriate route to integrate the crystallographic and grain shape/size effects into the same descriptor for deformation; thus it allows for the probing of the deformation behaviour of complex gradient microstructures. In this work, we implement a CPFEM model that accounts for the effect of the grain boundaries and thus bringing in a length scale effect. The model is used to perform mesoscale simulations of realistic microstructures. Emphasis is on the role of the distribution of grain size, shape and crystallographic texture on the deformation behaviour. Corroboration with the fracture behaviour of such microstructures are also made.

Symposium | F. From Microstructure to Properties: Mechanisms, Microstructure, Manufacturing

[SY-F11] Symposium F-11

Chair: Peter Gumbsch(Fraunhofer IWM, Germany)

Thu. Nov 1, 2018 2:00 PM - 3:30 PM Room3

[SY-F11] **Mesoscale plasticity models of polycrystalline materials for efficient computation of microstructure/property relationships**

○Ricardo Lebensohn （Los Alamos National Laboratory, United States of America）

[SY-F11] Development of a new consistent discrete Green operator for FFT-based methods to solve heterogeneous problems with eigenstrains

○Komlavi Senyo ELOH[1,2,3], Alain JACQUES[2,1], Stéphane BERBENNI[1,3] （1.University of Lorraine, France, 2.Institut Jean Lamour, France, 3.Laboratoire d'etudes de microstructures et de mé canique des matériaux, France）

[SY-F11] Efficient FFT-based Homogenisation without Linear Reference Medium

○Till Junge （EPFL, Mech. Engineering, Multiscale Mechanics Modeling, Switzerland）

[SY-F11] Multiscale modelling of the effective viscoplastic behavior of constituents of the mantle transition zone (Mg_2SiO_4 wadsleyite and ringwoodite): bridging atomic and polycrystal scales

Olivier Castelnau[1], Katell Derrien[1], Sebastian Ritterbex[2], Philippe Carrez[2], ○Patrick Cordier[2] （1.Process and Engineering in Mechanics and Materials, CNRS/ENSAM/CNAM, Paris, France, 2.Unité Matériaux et Transformations, CNRS / Univ. Lille, Lille, France）

[SY-F11] Scalable and Directionally-Sensitive Three-Dimensional Quantifying of Orientation and Dislocation Density Gradients in Crystal Plasticity Computer Simulations

○Markus Kuehbach, Franz Roters （Max-Planck-Institut fur Eisenforschung GmbH, Germany）

(Thu. Nov 1, 2018 2:00 PM - 3:30 PM Room3)

[SY-F11] Mesoscale plasticity models of polycrystalline materials for efficient computation of microstructure/property relationships

Invited

○Ricardo Lebensohn （Los Alamos National Laboratory, United States of America）

Models based on crystal plasticity are increasingly used in engineering applications to obtain microstructure-sensitive mechanical response of polycrystalline materials. Three key elements of these models are: a proper consideration of the single crystal plastic deformation mechanisms, a representative description of the microstructure, and an appropriate scheme to connect the microstates with the macroscopic response. The latter can be based on homogenization (e.g. self-consistent methods [1]), which relies on a statistical description of the microstructure, or be full-field solutions, which requires a spatial description of the microstructure (e.g. spectral methods [2]). Full-field models are numerically intensive, making their direct embedding in multiscale calculations computationally demanding. On the other hand, they can be used to generate reference solutions for assessment of homogenization-based approaches. In this talk we will review our recent efforts to develop material models based on polycrystal plasticity to capture anisotropic strength, along with their integration with emerging characterization methods in Experimental Mechanics (e.g. [3]), and their embedding in Finite Elements formulations (e.g. [4]) to solve problems involving complex geometries and boundary conditions with microstructure-sensitive material response.

[1] R.A. Lebensohn, C.N. Tomé and P. Ponte Castañeda: "Self-consistent modeling of the mechanical behavior of viscoplastic polycrystals incorporating intragranular field fluctuations". *Phil. Mag.* 87, 4287-4322 (2007).
[2] R.A. Lebensohn, A.K. Kanjarla and P. Eisenlohr: "An elasto-viscoplastic formulation based on fast Fourier transforms for the prediction of micromechanical fields in polycrystalline materials". *Int. J. Plast.* 32-33, 59-69 (2012).
[3] R. Pokharel, J. Lind, A.K Kanjarla, R.A. Lebensohn, S.F. Li, P. Kenesei, R.M. Suter and A.D. Rollett: “Polycrystal plasticity: comparison between grain scale observations of deformation and simulations”. *Ann. Rev. Cond. Matter Phys.* 5, pp. 317-346 (2014).
[4] J. Segurado, R.A. Lebensohn, J. Llorca and C.N. Tomé: "Multiscale modeling of plasticity based on embedding the viscoplastic self-consistent formulation in implicit finite elements". *Int. J. Plast.* 28, 124-140 (2012).

(Thu. Nov 1, 2018 2:00 PM - 3:30 PM Room3)

[SY-F11] Development of a new consistent discrete Green operator for FFT-based methods to solve heterogeneous problems with eigenstrains

○Komlavi Senyo ELOH[1,2,3], Alain JACQUES[2,1], Stéphane BERBENNI[1,3] （1.University of Lorraine, France, 2.Institut Jean Lamour, France, 3.Laboratoire d'etudes de microstructures et de mécanique des matériaux, France）

A new expression of the periodized discrete Green operator using the Discrete Fourier Transform method and consistent with the Fourier grid is derived from the classic "Continuous Green Operator" in order to

avoid the problem refered to as "aliasing" inherent to Discrete Fourier Transform methods. It is shown that the easy use of the conventional continous Fourier transform of the modified Green operator for heterogeneous materials with eigenstrains leads to spurious oscillations when computing the local responses of composite materials close to materials discontinuities like interfaces, dislocations, edges...We also focus on the calculation of the displacement field and its associated discrete Green operator which may be useful for materials characterisation methods like diffraction techniques.
The development of these new consistent discrete Green operators in the Fourier space allows to eliminate oscillations while retaining similar convergence capability. For illustration, the new discrete Green operators are implemented in a fixed-point algorithm for heterogeneous periodic composites knows as the Moulinec and Suquet (1994,1998) "basic scheme" that we extended to consider eigenstrain fields, as in Anglin, Lebensohn and Rollett(2014). Numerical examples are reported, such as the computation of the local stresses and displacement of composite materials with homogeneous or heterogeneous elasticiy combined with dilatational eigenstrain or representing prismatic dislocation loops. The mechanical fields obtained for cubic-shaped inclusion, spherical Eshelby and inhomogeneity, are compared with analytical solutions and the discretization method using the classic Green operator.

(Thu. Nov 1, 2018 2:00 PM - 3:30 PM Room3)

[SY-F11] Efficient FFT-based Homogenisation without Linear Reference Medium

○Till Junge （EPFL, Mech. Engineering, Multiscale Mechanics Modeling, Switzerland）

In the field of computational homogenisation of periodic representative volume elements (RVE), over the last two decades, fast Fourier transform (FFT)-based spectral solvers have emerged as a promising alternative to the finite element method (FE).
Most spectral methods are based on work of Moulinec and Suquet [1] and split an RVE's response into that of a linear reference medium and a periodic fluctuation due to heterogeneities. The main advantage of this formulation over FE is that it can be both significantly faster and memory-saving. The two main problems are 1) the choice of the reference medium, which is typically based on heuristics, non-trivial and has a strong impact on the method's convergence (A bad choice can render the method non-convergent), and 2) convergence is not uniform. Numerous studies have suggested mitigations to both of these problems (e.g. [2]), but they have remained substantial disadvantages compared to the more expensive, but also more robust FE.
Recent work by Zeman et al. [3] proposes a new formulation for spectral solvers which dispenses with the linear reference problem and converges unconditionally. We present Spectre, an open implementation of this novel method and use it to show that the new approach is more computationally efficient than its linear reference medium-based predecessors, converges in the presence of arbitrary phase contrast - including porosity - and eliminates or drastically reduces Gibbs ringing.

[1] H. Moulinec and P. Suquet. A numerical method for computing the overall response of nonlinear composites with complex microstructure. Computer Methods in Applied Mechanics and Engineering, 157(1):69-94, 1998
[2] M. Kabel, et al. Efficient fixed point and Newton-Krylov solvers for FFT-based homogenization of elasticity at large deformations. Computational Mechanics, 54:1497-1514, 2014
[3] J. Zeman, et al. A finite element perspective on non-linear FFT-based micromechanical simulations. Int. J. Num. Meth. Eng., 2016

(Thu. Nov 1, 2018 2:00 PM - 3:30 PM Room3)

[SY-F11] Multiscale modelling of the effective viscoplastic behavior of constituents of the mantle transition zone (Mg_2SiO_4 wadsleyite and ringwoodite): bridging atomic and polycrystal scales

Olivier Castelnau[1], Katell Derrien[1], Sebastian Ritterbex[2], Philippe Carrez[2], ○Patrick Cordier[2] (1.Process and Engineering in Mechanics and Materials, CNRS/ENSAM/CNAM, Paris, France, 2.Unité Matériaux et Transformations, CNRS / Univ. Lille, Lille, France)

The Earth mantle transition zone (an envelope of the Earth's interior between 410 and 660 km depth) is constituted by more than half from wadsleyite and ringwoodite. Waldseyite is present up to 525km depth, whereas ringwoodite appears below. In the transition zone, pressure ranges from 14 GPa to 24GPa, and temperature lies between 1880° K and 1900° K. Estimation of the viscoplastic behavior of these constituents, and the link with their microstructure (crystallographic texture), is crucial to better understand the structure of large scale convection cells in the mantle responsible for plate tectonic.

In this work, the viscoplastic behavior of wadsleyite and ringwoodite polycrystalline aggregates (cm scale) is obtained by bridging several scale transition models, starting from very fine scale (nm) of the dislocation core structure. This presentation will emphasize the grain-polycrystal scale transition.

Deformation resulting from thermally activated dislocation glide has been modeled in wadsleyite and ringwoodite at high pressures, for a wide range of temperatures, and under laboratory and *in situ* (*i.e.* mantle) strain-rates conditions. The model relies on the structure and kink pairs nucleation enthalpies of the rate controlling screw dislocations which have been modeled using the Peierls-Nabarro-Galerkin method and an elastic interaction model. Corresponding single slip critical resolved shear stresses (CRSS), and associated constitutive equations have been deduced from Orowan's equation in order to describe the average viscoplastic behavior at the grain scale, for all available slip systems.

These data are then implemented in two grain-polycrystal scale transition models, a statistical one (Second-Order Viscoplatic Self-Consistent scheme) allowing rapid evaluation of the effective viscosity of the polycrystalline aggregates, and a full-field method (FFT based method) allowing investigating many inter- and intra-granular features such as stress and strain localization in a typical microstructure, heterogeneous activation of slip systems, etc. Calculations have been performed for pressure, temperature, and strain-rates conditions corresponding to laboratory and *in situ* conditions. The obtained effective behavior is in very good match with available experimental data.

(Thu. Nov 1, 2018 2:00 PM - 3:30 PM Room3)

[SY-F11] Scalable and Directionally-Sensitive Three-Dimensional Quantifying of Orientation and Dislocation Density Gradients in Crystal Plasticity Computer Simulations

○Markus Kuehbach, Franz Roters （Max-Planck-Institut fur Eisenforschung GmbH, Germany）

In-grain orientation and dislocation density gradients, especially those building up at grain and phase boundaries, tune to significant extent a variety of microstructure evolution mechanisms: the nucleation and incipient stage of discontinuous dynamic recrystallization, deformation texture evolution, or phase transformations to name but a few. Despite being additionally also of relevance for stress and strain partitioning, their comprehensive quantification in three dimensions, though, has received little attention so far and remains elusive.

In this work we report on higher-order neighbor- and signed-distance-based techniques for quantifying such gradients; resulting in a tool applicable to point-cloud-based data. These are tracked for instance via integration point cloud sets in finite-strain-formalism full-field crystal plasticity computer simulations. Exemplarily, as such an evaluation of dislocation gradients resulting from Crystal Plasticity deformation simulations using the DAMASK spectral solver [1, 2] will be presented and their relevance for discontinuous dynamic recrystallization discussed.

[1] P. Eisenlohr, M. Diehl, R.A. Lebensohn, F. Roters: A spectral method solution to crystal elasto-viscoplasticity at finite strains, International Journal of Plasticity 46 (2013), 37 - 53

[2] P. Shanthraj, P. Eisenlohr, M. Diehl, F. Roters: Numerically robust spectral methods for crystal plasticity simulations of heterogeneous materials, International Journal of Plasticity 66 (2015) 31 - 45

Symposium | F. From Microstructure to Properties: Mechanisms, Microstructure, Manufacturing

[SY-F12] Symposium F-12

Chair: Yasushi Shibuta(The University of Tokyo, Japan)

Thu. Nov 1, 2018 4:00 PM - 5:30 PM Room3

[SY-F12] Microstructure formation in large-scale molecular dynamics simulation

○Yasushi Shibuta[1], Shin Okita[1], Eisuke Miyoshi[2], Shinji Sakane[2], Tomohiro Takaki[2], Munekazu Ohno[3] （1.The University of Tokyo, Japan, 2.Kyoto Institute of Technology, Japan, 3.Hokkaido University, Japan）

[SY-F12] Directed assembly of structured nanoparticles through rapid micromixing

○Arash Nikoubashman[1], Nannan Li[2], Athanassios Z. Panagiotopoulos[2] （1.Johannes Gutenberg University of Mainz, Germany, 2.Princeton University, United States of America）

[SY-F12] Various interfaces related to twinning in hexagonal metals

○Vaclav Paidar[1], Andriy Ostapovets[2] （1.Institute of Physics AS CR Prague, Czech Republic, 2.Institute of Physics of Materials AS CR Brno, Czech Republic）

[SY-F12] Multiscale mean-field modelling of mechanochemical processes in heterogeneous materials for energy storage

○Mikhail Poluektov[1], Łukasz Figiel[1,2] （1.International Institute for Nanocomposites Manufacturing, WMG, University of Warwick, UK, 2.Warwick Centre for Predictive Modelling, University of Warwick, UK）

[SY-F12] Impact of local symmetry breaking on the physical properties of tetrahedral liquids

○Rui Shi, Hajime Tanaka （University of Tokyo, Japan）

(Thu. Nov 1, 2018 4:00 PM - 5:30 PM Room3)

[SY-F12] Microstructure formation in large-scale molecular dynamics simulation

Invited

○Yasushi Shibuta[1], Shin Okita[1], Eisuke Miyoshi[2], Shinji Sakane[2], Tomohiro Takaki[2], Munekazu Ohno[3] (1.The University of Tokyo, Japan, 2.Kyoto Institute of Technology, Japan, 3.Hokkaido University, Japan)

Microstructure formation is discussed on the basis of large-scale molecular dynamics (MD) simulations of nucleation, solidification and subsequent grain grow for pure iron [1-3]. After the nucleation and solidification, the time change of volume of grains is directly estimated for 2D and 3D grain growths [1]. For the 2D grain growth, grains with seven and more neighboring grains generally grow larger, whereas those with five and less neighboring grains shrink and disappear [2], which basically agrees with von Neumann-Mullins law. For the 3D grain growth, threshold number of neighboring grains is estimated to be approximately 14 [2]. Moreover, the physical origin of the deviation from the ideal grain growth is investigated by the direct estimation of the reduced mobility (i.e., the product of the intrinsic grain boundary mobility and the grain boundary energy) and the geometric factor [3]. The new insights based on large-scale MD simulations up to billion atoms are achieved for the first time owing to a multi-graphics processing unit (GPU) parallel computation on the GPU-rich supercomputer.

[1] Y. Shibuta, et al., Nature Comm. 8 (2017) 10. [2] S. Okita, Y. Shibuta, ISIJ Int. 56 (2016) 2199. [3] S. Okita et al., submitted.

(Thu. Nov 1, 2018 4:00 PM - 5:30 PM Room3)

[SY-F12] Directed assembly of structured nanoparticles through rapid micromixing

○Arash Nikoubashman[1], Nannan Li[2], Athanassios Z. Panagiotopoulos[2] (1.Johannes Gutenberg University of Mainz, Germany, 2.Princeton University, United States of America)

Tailored nanoparticles are increasingly sought after for many scientific and technological applications, such as optoelectronic devices and highly selective catalysts. However, both research and commercialization of these materials has been impeded by the lack of suitable fabrication techniques. One promising approach for overcoming this hurdle is flash nanoprecipitation, where (soft) nanoparticles are assembled through rapid micromixing of polymers in solution with a miscible poor solvent. This continuous process allows for high yields as well as precise control over particle size and morphology. We employed multiscale computer simulations of this process to understand its underlying mechanisms and to efficiently explore parameter space. We first performed explicit solvent molecular dynamics (MD) simulations of a bead-spring polymer model to study the microscopic properties of the fabrication process. Then, we fed the MD data into a kinetic Monte Carlo algorithm to reach macroscopic length- and timescales. We discovered that the nanoparticle size can be reliably tuned through the initial polymer concentration and the mixing rate. Further, we were able to fabricate a wide variety of structured colloids, such as Janus and core-shell particles, when polymer blends were used in the feed stream.

(Thu. Nov 1, 2018 4:00 PM - 5:30 PM Room3)

[SY-F12] Various interfaces related to twinning in hexagonal metals

○Vaclav Paidar[1], Andriy Ostapovets[2] (1.Institute of Physics AS CR Prague, Czech Republic, 2.Institute of Physics of Materials AS CR Brno, Czech Republic)

The {10-12} twin mode is the one most commonly activated in hexagonal metals. A primary part of the lattice transition from the matrix to the twin orientation is shear deformation that converts the [0001] direction of the hexagonal axis in the matrix to a direction almost parallel to the [10-10] direction perpendicular to the $<a>$ axis in the basal plane in the twin. In addition to primary mechanical twinning also several types of double-twins were observed as, for example, {10-11}-{10-12} or {10-12}-{10-12}. Surprisingly, the last one can occur in magnesium with the c/a ratio smaller than $\sqrt{3}$ but also in zinc with the c/a ratio larger than $\sqrt{3}$. Various types of symmetrical and asymmetrical interfaces including also basal/basal or prismatic/prismatic boundaries will be discussed and their impact on materials properties will be envisaged.

(Thu. Nov 1, 2018 4:00 PM - 5:30 PM Room3)

[SY-F12] Multiscale mean-field modelling of mechanochemical processes in heterogeneous materials for energy storage

○Mikhail Poluektov[1], Łukasz Figiel[1,2] (1.International Institute for Nanocomposites Manufacturing, WMG, University of Warwick, UK, 2.Warwick Centre for Predictive Modelling, University of Warwick, UK)

Performance enhancement of energy storage devices, e.g. batteries, requires careful selection of materials. The microstructure of such materials can undergo a complex electro-chemo-mechanical cycling during battery exploitation, which involves extreme volumetric expansion of the active material during the chemical reaction. The expansion is causing mechanical stress, which, in turn, influences the kinetics of chemical reactions even up to their arrest [3]. Thus, to predict the mechanochemical behaviour of a multi-material battery electrode, both the multi-physics phenomena and microstructure must be taken into account.

Up to now, the major focus has been on development of coupling models between mechanics, diffusion and chemical reactions, e.g. [4], particularly, chemical reactions, such as lithiation and oxidation, that take place at a surface, e.g. [1-2]. When localised reactions are modelled, the thermodynamic consistency has to be maintained and the velocity of the chemical reaction front should not violate the entropy production inequality and the balance laws. One such model is based on the chemical affinity tensor [2]. This model was used to predict the kinetics and the arrest of the reaction front in free-standing Si particles of a battery anode [5].

The model presented in this talk builds on [5] and accounts for the lithiation kinetics of a collection of particles inside an effective matrix material. The battery microstructure is modelled using the multiscale mean-field framework based on the incremental Mori-Tanaka method. This is the first application of a multiscale mean-field technique to modelling lithiation reaction front kinetics in a complex anode microstructure within the finite-strain framework, and to linking the intraparticle kinetics with the macroscopic response of the battery.

Acknowledgements
Financial support from the EU H2020 project Sintbat (685716) is gratefully acknowledged.

References
[1] ZW Cui, F Gao, JM Qu (2013) J Mech Phys Solids 61:293-310
[2] AB Freidin, EN Vilchevskaya, IK Korolev (2014) Int J Eng Sci 83:57-75
[3] K van Havenbergh, S Turner, N Marx, G van Tendeloo (2016) Energy Technol 4:1005-1012
[4] VI Levitas, H Attariani (2014) J Mech Phys Solids 69:84-111
[5] M Poluektov, AB Freidin, L Figiel (2018) Int J Eng Sci accepted

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(Thu. Nov 1, 2018 4:00 PM - 5:30 PM Room3)

[SY-F12] Impact of local symmetry breaking on the physical properties of tetrahedral liquids

○Rui Shi, Hajime Tanaka （University of Tokyo, Japan）

Water and silica are the most important materials with local tetrahedral symmetry. They have similar crystalline polymorphs and exhibit anomalous density maximum in the liquid state. However, water and silica also show very different characteristics. For instance, the density of water varies much more sharply than that of liquid silica near the maximum as temperature changes. More notably, silica is a very good glass-former, but water is an extremely poor one. The physical origins of these similarities and differences still remain elusive, due to the lack of a microscopic understanding of the structural ordering in these two important liquids. Here, by accessing microscopic structural information by computer simulations, we reveal that local translational symmetry breaking is responsible for the density anomalies. On the other hand, the difference in the degree of local orientational symmetry breaking between water and silica, which originates from the difference in their bonding nature, causes not only the difference in the sharpness of density anomalies, but also their distinct glass-forming abilities. Our work not only shows the crucial roles of local translational and orientational symmetry breaking in the physical properties of the two extremely important materials, water and silica, but also provides a unified scenario applicable for other tetrahedral liquids such as Si, Ge, C, BeF_2, and GeO_2.

Symposium | G. Modeling Mechanical Behavior of Materials under Harsh Environments

[SY-G5] Symposium G-5

Chairs: Keonwook Kang(Yonsei University, Korea), Akiyuki Takahashi(Tokyo University of Science, Japan)

Thu. Nov 1, 2018 9:45 AM - 11:00 AM Room4

[SY-G5] Metallic materials under extreme pressure: Interplay of plasticity and phase transitions

○Nina Gunkelmann[1], Hoang-Thien Luu[1], Diego R. Tramontina[3], Carlos J. Ruestes[3], Yudi Rosandi[4], Herbert M. Urbassek[2] （1.Clausthal University of Technology, Germany, 2.University of Kaiserslautern, Germany, 3.National University of Cuyo, Argentine, 4.University of Padjadjaran, Indonesia）

[SY-G5] Dislocation dynamics modeling of fracture behavior with considering dislocation shielding effect

○Akiyuki Takahashi, Hayato Sugasawa, Masanori Nagura （Tokyo University of Science, Japan）

[SY-G5] Dynamic behaviors of dislocations and grain boundaries induced by phonon scattering in nanoscale

○Soon Kim, Sung Youb Kim （Dept. of Mechanical Engineering, UNIST, Korea）

[SY-G5] Investigation on 1/2<11-1>{112} and 1/2<11-1>{123} mixed dislocations in BCC iron by classical molecular dynamics

○Tomohisa Kumagai[1], Akiyoshi Nomoto[1], Akiyuki Takahashi[2] （1.Central Research Institute of Electric Power Industory, Japan, 2.Tokyo University of Science, Japan）

(Thu. Nov 1, 2018 9:45 AM - 11:00 AM Room4)

[SY-G5] Metallic materials under extreme pressure: Interplay of plasticity and phase transitions

Invited

○Nina Gunkelmann[1], Hoang-Thien Luu[1], Diego R. Tramontina[3], Carlos J. Ruestes[3], Yudi Rosandi[4], Herbert M. Urbassek[2] （1.Clausthal University of Technology, Germany, 2.University of Kaiserslautern, Germany, 3.National University of Cuyo, Argentine, 4.University of Padjadjaran, Indonesia）

Shock waves are ubiquitous in various fields of activity including space science and engineering. They are of key interest for materials engineering, where shock-induced phase transitions may be used to produce new materials with increased strength which might be stable at ambient conditions.

As prototypical materials, we consider iron and iron-carbon alloys showing a pressure induced phase transformation from the bcc to the hexagonal close-packed phase at around 13 GPa depending on the carbon content. We study waves in polycrystalline Fe using an interatomic potential that faithfully incorporates this phase transition at the desired equilibrium pressure.

Our simulations show that the phase transformation is preceded by plastic activity, leading to the so-called 3-wave structure: An elastic compression wave is followed by a plastic wave which then leads to a phase-transformation front. We show that the phase transformation from bcc to hcp and vice-versa helps to drive twinning and decreases the probability of multiple spallation and crack formation. In agreement with experiments, the fracture surface is influenced by the phase transition showing smooth spall surfaces.

Despite large differences in material properties, shock waves in aluminium nanofoams exhibit, similar to polycrystalline iron, a 3-wave structure indicating three wave regimes: an elastic precursor is pursued by plastic activity in the filaments before eventually the foam structure is crushed and a compact material results. The collapse of the foam is well described by an analytical compaction model.

(Thu. Nov 1, 2018 9:45 AM - 11:00 AM Room4)

[SY-G5] Dislocation dynamics modeling of fracture behavior with considering dislocation shielding effect

○Akiyuki Takahashi, Hayato Sugasawa, Masanori Nagura （Tokyo University of Science, Japan）

Ductile-brittle transition (DBT) in ferric steels is a critical issue to ensure the structural integrity of nuclear power plants. The DBT is believed to be caused by the shielding effect of dislocations at the crack tip. Therefore, in order to make a deep understanding of the fracture behavior and the DBT mechanisms, it is necessary to develop a computational method that can take into account the dislocation nucleation, the dislocation behavior and the stress of dislocation around the crack tip, and can derive the fracture toughness as a result of dislocation-crack interactions. This paper presents a dislocation dynamics (DD) simulation technique for the fracture toughness calculation with the consideration of dislocation shielding effect. In this study, the crack is represented with discrete dislocations, and the crack problem is solved using the DD method. The dislocation nucleation from the crack tip is simply modeled with a critical shear stress in the immediate vicinity of the crack tip. The nucleated dislocations move in the material, and produce the stress at the crack tip. The complex system of crack-dislocation interactions can be solved only with the DD

method. In the DD method, the stress intensity factor at the crack tip can be easily computed by calculating the Peach-Koehler force, which is normally calculated in the DD simulations, acting at the crack tip dislocation. When the stress intensity factor reaches a critical value, the fracture toughness is determined by the applied stress. To demonstrate the potential of the developed DD method, we performed a simulation of dislocation shielding with various dislocation mobility, which imitates the temperature dependence of dislocation behavior and fracture toughness. The numerical result clearly shows that the higher dislocation mobility gives higher fracture toughness, which is qualitatively in agreement with experimental results.

(Thu. Nov 1, 2018 9:45 AM - 11:00 AM Room4)

[SY-G5] Dynamic behaviors of dislocations and grain boundaries induced by phonon scattering in nanoscale

○Soon Kim, Sung Youb Kim （Dept. of Mechanical Engineering, UNIST, Korea）

Conventional dislocation dynamics based on continuum theory is limited in its ability to describe motion of dislocations in nanoscale. This is because discrete characteristics are no longer ignored in nanoscale unlike in micro- or macroscales. Especially, the discreteness becomes a significant factor to describe core region of dislocation so that it contributes to nonlinear properties of the core. In a sense that the core determines mobility of dislocations and concerns interactions among them, the discrete approach must be carefully considered in nanoscale dislocation dynamics. To reflect the discrete characteristics in nanoscale, computer simulations and discrete lattice dynamics approach have been used to quantify properties of the dislocation core.

In our work, we carried out molecular dynamics simulation to study motion of the dislocation in nanoscale and found surprising behavior that internal stress of system where dislocation is inserted is dropped when the dislocation is in motion by externally applied stress. By using discrete lattice dynamics, we proved that this behavior occurs due to scattering of the wave emitted from breaking of atomic bond in the core [1].

Furthermore, we extended our approach to grain boundary since it can be assumed as a collection of dislocations if its misorientation angle is small enough. We simulated the grain boundaries for various misorentation angles under external stress. As a result, dropping of internal stress is also observed as in dislocation case. Not only the stress-drop, but the grain boundaries were curved during their motion and magnitude of the curvature and speed were inversely proportional to the misorientation angle. We analyzed these behaviors by using the discrete lattice dynamics and concluded that these are able to be appeared only in nanoscale materials.

References

[1] S. Kim, D. T. Ho, K. Kang, and S. Y. Kim, *Acta. Mater*, **115** (2016), p143-154.

(Thu. Nov 1, 2018 9:45 AM - 11:00 AM Room4)

[SY-G5] Investigation on 1/2<11-1>{112} and 1/2<11-1>{123} mixed dislocations in BCC iron by classical molecular dynamics

○Tomohisa Kumagai[1], Akiyoshi Nomoto[1], Akiyuki Takahashi[2] （1.Central Research Institute of Electric Power Industory, Japan, 2.Tokyo University of Science, Japan）

Mixed dislocation motion of 1/2<11-1>{112} and 1/2<11-1>{123} slip systems in pure BCC iron was observed by using classical molecular dynamics (MD). Angles between Burgers vector and dislocation line, which is referred as mixed dislocation angle, were between 0 degree and 180 degree (i.e., 0 degree and 180 degree correspond to screw dislocation and 90 degree corresponds to edge dislocation). As an initial configuration, one mixed dislocation was introduced in the MD box. Then, shear strain parallel to the slip plane with constant strain rate was applied to glide the dislocation to calculate Peierls stress, or shear stress was applied to calculate mobility and friction stress.The directions of dislocation motion were both twinning and anti-twinning directions. Dislocation mobility and friction stress at 100K and 300K were evaluated as well as Peierls stress. High Peierls stress was observed on a mixed dislocation whose core structure was straight (i.e., it does not contain kinks) since all of the dislocation had to jump to the next position at the same time. On the other hand, low Peierls stress was observed on a mixed dislocation whose core structure contains kinks since it could gradually move through kink movement along with the dislocation line. There seemed that the friction stress and the mobility of the mixed dislocations were affected by the dislocation core structure at 100K; the friction stress was high and the mobility was low at the mixed dislocation angles where Peierls stress was high. On the other hand, there seemed to be less effect of the core structure on the friction stress nor the mobility at 300K. It is found that directions of dislocation motion have almost no effects on the Peierls stress, mobility and friction stress as a whole.

Symposium | G. Modeling Mechanical Behavior of Materials under Harsh Environments

[SY-G6] Symposium G-6

Chairs: Akiyuki Takahashi(Tokyo University of Science, Japan), Keonwook Kang(Yonsei University, Korea)
Thu. Nov 1, 2018 11:15 AM - 12:15 PM Room4

[SY-G6] Repulsive Correction in Tersoff Potential for Irradiated Si

○Youhwan Jo, Taeyeon Kim, Byeongchan Lee （Kyung Hee University, Korea）

[SY-G6] Phase-field modeling of microstructural evolution of Fe-Cr-Al system

○Kunok Chang （Kyung Hee Univ., Korea）

[SY-G6] Dissolution kinetics of ejecta in hydrogen at megabar pressure

○Arslan B. Mazitov[1,2], Artem R. Oganov[3,1,4], Alexey V. Yanilkin[1,2] （1.Dukhov Research Institute of Automatics (VNIIA), Moscow, Russian Federation, Russia, 2.Moscow Institute of Physics and Technology, Dolgoprudny, Russian Federation, Russia, 3.Skolkovo Institute of Science and Technology, Skolkovo Innovation Center, Moscow, Russian Federation, Russia, 4.International Center for Materials Discovery, Northwestern Polytechnical University, Xi’ an, China）

[SY-G6] MD simulation study of displacement damage in bulk wurtzite GaN by proton irradiation

○SangHyuk Yoo, Yongwoo Kim, Keonwook Kang （Dept. of Mechanical Engineering, Yonsei Univ., Korea）

(Thu. Nov 1, 2018 11:15 AM - 12:15 PM Room4)

[SY-G6] Repulsive Correction in Tersoff Potential for Irradiated Si

○Youhwan Jo, Taeyeon Kim, Byeongchan Lee （Kyung Hee University, Korea）

Engineering applications for nuclear fussion/fission facilities usually require a material with exceptional properties. Silicon carbide (SiC) and its composites are prospective materials for such usage due to low degradation of mechanical properties at high temperature as well as high resistance to irradiation. There are ongoing attempts to employ SiC/SiC composites like flow channel inserts (FCI) in dual coolant lead lithium (DCLL) blankets and fuel claddings for the Generation IV nuclear reactors. SiC/SiC composites are yet to be examined further before confirmed to be the best option. As an example, irradiation damages in SiC/SiC composites may cause a serious problem by interacting with various elements in nuclear operations.

Understanding the microstructural evolution under irradiation is critical to validate SiC/SiC composites and the resulting safety under irradiation, and Molecular dynamics (MD) is a viable option for that purpose. Nevertheless the reliability of MD simulations heavily depends on the accuracy of an interatomic potential. The Tersoff potential is a good candidate, but not particularly optimized for high-energy environment, resulting in a few pathological behaviors.

In this talk we propose a correction function that minimizes the problems of the Tersoff potential developed for bulk equilibrium. In particular, the correction function replaces the repulsive part of Tersoff within a threshold interatomic spacing. The function behaves monotonically and is continuous with the original repulsive part up to the third derivative at the threshold, and moreover, complexity does not increase significantly because the correction function introduces only two additional free parameters. By primary knock-on atom (PKA) simulations, the effect of the correction is examined. We evaluate a maximum penetration length and the number of Frenkel pairs and discuss a benefit from the correction.

(Thu. Nov 1, 2018 11:15 AM - 12:15 PM Room4)

[SY-G6] Phase-field modeling of microstructural evolution of Fe-Cr-Al system

○Kunok Chang （Kyung Hee Univ., Korea）

After Fukushima nuclear power plant accident, the Accident Tolerant Fuel Cladding (ATFC) has attracted a great deal of attention. The Fe-Cr-Al system has been studied for a long time as a potential candidate for ATFC due to its excellent high-temperature oxidation resistance. To optimize the microstructure has been performed for a long period of time in order to enhance the mechanical stability of the Fe-Cr-Al alloy in the neutron irradiation environment. The spinodal decomposition generally takes place at nuclear power plants operation temperature, 290 Celsius degree and it is generally have negative effect on their performace. Therefore, we performed the phase-field modeling to predict the phase separation behavior in Fe-Cr-Al system to investigate a role of Cr and Al compositions on decomposition behavior. To obtain large-scale 3D microstructure, we applied CUDA parallelizing computing technique. I will also present comparative analysis

results with the microstructure obtained experimentally.

(Thu. Nov 1, 2018 11:15 AM - 12:15 PM Room4)

[SY-G6] Dissolution kinetics of ejecta in hydrogen at megabar pressure

○Arslan B. Mazitov[1,2], Artem R. Oganov[3,1,4], Alexey V. Yanilkin[1,2] （1.Dukhov Research Institute of Automatics (VNIIA), Moscow, Russian Federation, Russia, 2.Moscow Institute of Physics and Technology, Dolgoprudny, Russian Federation, Russia, 3.Skolkovo Institute of Science and Technology, Skolkovo Innovation Center, Moscow, Russian Federation, Russia, 4.International Center for Materials Discovery, Northwestern Polytechnical University, Xi’ an, China）

A process of metal particles, *ejecta*, transport in gases is the subject of recent researches in the field of nuclear energetics. Practical necessity of the study arises from the processes of inertial thermonuclear fusion, which are often accompanied by separation of ejecta particles from the interior surface of the fuel container. At the pressure of approximately 1 megabar, saturation of the ejecta with hydrogen adversely affect a fraction of pure fuel in the system. In this work, we studied a solution process of titanium ejecta in warm dense hydrogen at megabar pressure. Thermodynamic and kinetic properties of the process were investigated using classical and quantum molecular dynamics. We estimated such features as a solution time of ejecta, a degree of saturation of titanium atoms with hydrogen as well as a heat effect of the solution. It was found that particles with a radius of 1-10 mkm dissolve in hydrogen within a time of 10^{-1}-10^{-2} mks, while a mixing process can be described by diffusion law at discussed the conditions. Presented approach demonstrates the final state of the titanium-hydrogen system as a homogenized fluid with completely dissolved titanium particles. This result can be generalized to all external conditions under which titanium and hydrogen are an atomic fluids.

(Thu. Nov 1, 2018 11:15 AM - 12:15 PM Room4)

[SY-G6] MD simulation study of displacement damage in bulk wurtzite GaN by proton irradiation

○SangHyuk Yoo, Yongwoo Kim, Keonwook Kang （Dept. of Mechanical Engineering, Yonsei Univ., Korea）

Gallium nitride (GaN) based optoelectronic devices including LED and HEMT (High Electron Mobility Transistor) are widely used in aerospace industry because of large, direct band gap, high breakdown voltage and high electron mobility. Those applications loaded in satellites will be damaged during operating on the low earth orbit by radiation, which is mostly consisted of protons. Previous experimental research showed the decrements of the electron mobility and LED light intensity according to the proton fluence [1, 2]. However, it is difficult to show which kind of point defects are created and affected to the device. In this study, authors conduct Primary Knock-on Atom simulations in order to predict displacement damage on bulk wurtzite GaN by proton irradiation. PKA energy used in the MD simulation are obtained from GEANT4 simulation and experimental results. And author will show favorable type of point defects induced by displacement damage.

Reference

1. Xinwen, H., et al., *Proton-irradiation effects on AlGaN/AlN/GaN high electron mobility transistors.* IEEE Transactions on Nuclear Science, 2003. **50**(6): p. 1791-1796.

2. Khanna, S.M., et al., *Proton energy dependence of the light output in gallium nitride light-emitting diodes.* IEEE Transactions on Nuclear Science, 2004. **51**(5): p. 2729-2735.

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Symposium | N. Towards Experimentally Relevant Time Scales: Methods for Extending Atomistic Simulation Times and Their Applications in Material Science

[SY-N5] Symposium N-5

Chair: Jutta Rogal(ICAMS Ruhr University Bochum, Germany)

Thu. Nov 1, 2018 2:00 PM - 3:30 PM Room4

[SY-N5] Understanding the impact of extended defects on the behaviour of C atoms: a multi technique approach

○Christophe Domain[1], charlotte S becquart[2] （1.EDF, France, 2. Univ.Lille, CNRS, INRA, ENSCL, UMR 8207, UMET, Unité Matériaux et Transformations, France）

[SY-N5] Localised on-the-fly Kinetic Monte Carlo

○Johannes Bulin （Fraunhofer-Institut SCAI, Germany）

[SY-N5] A Preconditioning scheme for Minimum Energy Path finding methods

○Stela Makri, James Kermode, Christoph Ortner （University of Warwick, UK）

[SY-N5] Temperature Programmed Molecular Dynamics - Accessing rare events using a combination of finite time sampling and bias potentials

○Abhijit Chatterjee （Dept. of Chemical Engineering, Indian Institute of Technology Bombay, India）

(Thu. Nov 1, 2018 2:00 PM - 3:30 PM Room4)

[SY-N5] Understanding the impact of extended defects on the behaviour of C atoms: a multi technique approach

Invited

○Christophe Domain[1], charlotte S becquart[2] (1.EDF, France, 2. Univ.Lille, CNRS, INRA, ENSCL, UMR 8207, UMET, Unité Matériaux et Transformations, France)

The interaction at the atomistic scale of interstitial solutes such as carbon or nitrogen with extended point defects has consequences at the macroscopic level. Typical examples are the yield peak and Lü ders plateau, related to static strain aging or the Portevin-Le Chatelier effect (the presence of serrations on the plastic part of the stress-strain curve during tensile test) due to dynamic strain aging. In ferritic steels, these atypical behaviors are due to the interaction between dislocations and solute atoms (mainly C). Depending on aging time and temperature, solute atoms diffuse towards dislocations, forming Cottrell atmospheres, and reduce their mobility. Because of the time scale of C diffusion and the stresses created near the extended defects, typical atomistic approaches such as molecular dynamics (MD) or on-lattice atomistic kinetic Monte Carlo (on-lattice AKMC) approaches are not appropriate to investigate, at the atomistic level, these phenomena. In this talk, we will thus present the approach we have pursued to investigate the behavior of C atoms in the vicinity of extended defects (dislocations, dislocation loops …) in Fe. We have applied different complementary techniques. Calculations based on the density functional theory (DFT) as well as with an empirical FeC atomistic potential have been used extensively to determine the strength of the interaction between carbon atoms and the various defects in stable or metastable configurations. On-lattice static Monte Carlo as well as off-lattice kinetic Monte Carlo approaches have been applied to build Cottrell atmospheres and study dynamically the behavior of C atoms in the vicinity of extended defects (dislocations, …). Finally molecular dynamics (MD) simulations have been deployed to estimate the stress necessary to release the dislocations from the C atmospheres.

(Thu. Nov 1, 2018 2:00 PM - 3:30 PM Room4)

[SY-N5] Localised on-the-fly Kinetic Monte Carlo

○Johannes Bulin (Fraunhofer-Institut SCAI, Germany)

Various on-the-fly Kinetic Monte Carlo algorithms have been used to simulate the long-term evolution of atomistic systems. Unlike classical Kinetic Monte Carlo methods, these algorithms search for possible transitions/reactions only when necessary (hence on-the-fly), rather than relying on a previously-known set of transitions. Unfortunately, their performance deteriorates when large systems or systems with many similar transition mechanisms are investigated.

We will present a localised on-the-fly Kinetic Monte Carlo variant that is based on the k-ART algorithm by El-Mellouhi, Lewis, and Mousseau. This algorithm is capable of localising transition searches, enabling the simulation of significantly larger systems, and can also recycle known transition mechanisms. Unlike k-ART, which uses a graph-based technique to identify similar local environments, we use an RMSD (root mean square deviation) measure that is invariant under index permutations and rotations of local environments. This allows our algorithm to deal not only with highly-structured materials like crystals, but also with amorphous materials, which are difficult to classify with graphs.

We will conclude by demonstrating computational results of our algorithm, and discuss potential areas of application.

(Thu. Nov 1, 2018 2:00 PM - 3:30 PM Room4)

[SY-N5] A Preconditioning scheme for Minimum Energy Path finding methods

○Stela Makri, James Kermode, Christoph Ortner （University of Warwick, UK）

In transition state theory, the study of thermally activated transitions between energy minima is achieved by finding transition paths connecting the minima. These paths provide information on the energy barrier and reaction rates of the system without going through long and expensive simulations. To find them, current techniques use steepest descent-like minimisation to relax a discretised initial guess. However, steepest descent typically gives slow convergence rates in the presence of ill-conditioned potentials. In this talk I will be discussing how to reduce the condition number of the potential of an arbitrary system and improve the convergence speed and robustness of transition path finding methods, using a preconditioning scheme. Our key assumption is that the cost of constructing a preconditioner is much smaller than the cost of computing the potential; for density functional theory the cost of single point evaluations is much more expensive than the computation of a preconditioner and thus the proposed approach improves computing times significantly. We have developed a preconditioning scheme, where the preconditioner acts as a coordinate transformation of the discrete images along the path to aid the ill-conditioning in the transverse direction and a preconditioning scheme that considers the interactions between the images is currently in development. Finally, we are working towards a preconditioning scheme for finding energy barriers in hybrid quantum mechanical - molecular mechanical models.

(Thu. Nov 1, 2018 2:00 PM - 3:30 PM Room4)

[SY-N5] Temperature Programmed Molecular Dynamics - Accessing rare events using a combination of finite time sampling and bias potentials

Invited

○Abhijit Chatterjee （Dept. of Chemical Engineering, Indian Institute of Technology Bombay, India）

Rates of physical and chemical processes often obey Arrhenius law. Recently, we developed the temperature-programmed molecular dynamics (TPMD) method[1,2,3] that provides a convenient way of estimating the Arrhenius parameters of kinetic pathways even in situations where the underlying landscape is rugged. The TPMD method employs a temperature program with finite temperature MD in order to accelerate thermally activated events from a particular state of the system. Kinetic pathways are sought from a collection of states without any prior knowledge of these pathways. Since kinetic pathways are selected with a probability that is proportional to their rate constants, we find that slow pathways with small pre-exponential factors and large activation barriers are rarely sampled with TPMD. We introduce a procedure to overcome this limitation by bias potentials. This additional feature in the TPMD method dramatically improves its ability to estimate Arrhenius parameters. Examples of the variation of the TPMD method are provided for metal surface diffusion

in presence of solvent.

1. V Imandi, A Chatterjee, Estimating Arrhenius parameters using temperature programmed molecular dynamics, The Journal of Chemical Physics 145, 034104, 2016.

2. S Divi, A Chatterjee, Accelerating rare events while overcoming the low-barrier problem using a temperature program, The Journal of Chemical Physics 140 (18), 184116, 2014

3. A Chatterjee, Accelerating Rare Events and Building Kinetic Monte Carlo Models Using Temperature Programmed Molecular Dynamics, Journal of Materials Research, http://dx.doi.org/10.1557/jmr.2017.460

Symposium | N. Towards Experimentally Relevant Time Scales: Methods for Extending Atomistic Simulation Times and Their Applications in Material Science

[SY-N6] Symposium N-6

Chair: Chad W Sinclair(Dept. of Materials Engineering, University of British Columbia, Canada)
Thu. Nov 1, 2018 4:00 PM - 5:30 PM Room4

[SY-N6] Modelling metals, alloys and cement paste across length and time scales

○Laurent Karim Beland[1], Roger E Stoller[3], Yuri N Osetsky[3], Tingtao Zhou[2], Katerina Katerina Ioannidou[2], Franz-Josef Ulm[2], Roland Pellenq[2] （1.Queen's University, Canada, 2.Massachusetts Institute of Technology, United States of America, 3.Oak Ridge National Laboratory, United States of America）

[SY-N6] BCA-MD-KMC hybrid simulation for long time helium plasma irradiation inducing fuzzy nanostructure on tungsten

○Atsushi M Ito[1,2], Arimichi Takayama[1], Hiroaki Nakamura[1,3] （1.National Institute for Fusion Science, National Institutes of Natural Sciences, Japan, 2.The Graduate University for Advanced Studies, Japan, 3.Department of Electrical Engineering, Graduate School of Engineering, Nagoya University, Japan）

[SY-N6] Atomistic Modelling of Pipe Diffusion: a Direct Comparison of MD, KMC, aKMC and DMD

Frederic Houlle[1], Jutta Rogal[2], ○Erik Bitzek[1] （1.FAU Erlangen-Nuernberg, Germany, 2.ICAMS Ruhr University Bochum, Germany）

[SY-N6] Strategies for optimal construction of Markov chain representations of atomistic dynamics

○Danny Perez, Thomas Swinburne （Los Alamos National Laboratory, United States of America）

[SY-N6] Simulating the collective diffusion mechanism of amorphous solids at experimentally relevant time scales

○Yunjiang Wang[1,2], Shigenobu Ogata[3] （1.Institute of Mechanics, Chinese Academy of Sciences, China, 2.School of Engineering Science, University of Chinese Academy of Sciences, China, 3.Graduate School of Engineering Science, Osaka University, Japan）

(Thu. Nov 1, 2018 4:00 PM - 5:30 PM Room4)

[SY-N6] Modelling metals, alloys and cement paste across length and time scales

Invited

○Laurent Karim Beland[1], Roger E Stoller[3], Yuri N Osetsky[3], Tingtao Zhou[2], Katerina Katerina Ioannidou[2], Franz-Josef Ulm[2], Roland Pellenq[2] （1.Queen's University, Canada, 2.Massachusetts Institute of Technology, United States of America, 3.Oak Ridge National Laboratory, United States of America）

Fundamentally, structural materials are bound by atomistic cohesive interactions, while our societies use these to design systems at scales of meters—or more. Likewise, the material’s microstructural evolution takes place on scales as short as nanoseconds—e.g. diffusion of radiation-induced defects clusters in metallic alloys—all the way up to decades—e.g. creep of concrete under load.

This presentation will focus on applying multi-scale methods to address these challenges for two classes of systems: (1) metals and alloys under irradiation, and (2) calcium silicate hydrates (C-S-H), the main binding phase of cement paste.

In metals and alloys, the kinetics of collision cascade induced defects was modelled using adaptive kinetic Monte Carlo. Namely, the kinetic Activation Relaxation Technique —a self-learning, fully atomistic algorithm able to handle off-lattice defects and handle long-range elastic interactions—was used to capture the time-evolution of cascade debris after neutron or ion irradiation. Furthermore, a detailed investigation of point-defect diffusion in $Ni_xFe_{(1-x)}$ concentrated alloys revealed a non-monotonic dependence of diffusion coefficients as a function of Fe concentration. This was explained by coupling percolation effects with the composition dependence of point-defect vacancy migration energies.

In C-S-H, the adsorption of alkali ions—Na, K, and Cs—was studied, in the context of the alkali-silica reaction and spent fuel storage. By applying molecular dynamics, semi-grand canonical Monte Carlo, and the Activation Relaxation Technique *nouveau*, adsorption of alkali ions in the hydrated layer of C-S-H was characterized. The effect of alkali uptake on mesoscale mechanical properties was calculated using a coarse-grained model of C-S-H. While alkali uptake leads to significant expansion of individual C-S-H grains, it leads to modest—less than 5 MPa—mesoscopic expansive pressure, well within the elastic regime of concrete.

(Thu. Nov 1, 2018 4:00 PM - 5:30 PM Room4)

[SY-N6] BCA-MD-KMC hybrid simulation for long time helium plasma irradiation inducing fuzzy nanostructure on tungsten

○Atsushi M Ito[1,2], Arimichi Takayama[1], Hiroaki Nakamura[1,3] （1.National Institute for Fusion Science, National Institutes of Natural Sciences, Japan, 2.The Graduate University for Advanced Studies, Japan, 3.Department of Electrical Engineering, Graduate School of Engineering, Nagoya University, Japan）

In this paper, we developed the triple hybrid simulation method for plasma-material interaction (PMI). Although the present method is composed only of atomistic simulations, an elapse time achieved experimentally relevant time scale.
PMI occurs in the processing of semiconductors, thin film depositions, applications into nanomaterial formations, and the inside wall of magnetic confinement nuclear fusion reactors. In atomistic viewpoint, PMI is the surface reaction of a target material due to ion particles continuously injected from plasma. The PMI, which is not an exception, follows the multi-scale multi-physics mechanisms.
Moreover, an important factor in PMI is competition between an irradiation flux and the diffusion speed of the injected particles in the target material. The irradiation flux in laboratory experiments is 10^{20} to 10^{24} $m^{-2}s^{-1}$, and irradiation time is 10^{2} s to 10^{4} s. Although molecular dynamics (MD) is often used for PMI, the experimental irradiation time is too long for MD. Therefore, the irradiation flux was generally set 10^{4} to 10^{8} times of the experimental flux. However, since the diffusion speed in MD becomes realistic, the competition between the irradiation flux and the diffusion speed becomes unrealistic. Thus, the expansion of time scale is necessary for PMI simulation.
Here, the present target phenomenon is fuzzy nanostructure formation on the tungsten surface by exposure to helium plasma. Injected helium atoms agglomerated in the tungsten material, and the nanoscale helium bubbles are formed. After that, the fuzzy nanostructure of tungsten measuring several ten nanometers in width is grown on a surface. To represent the fuzzy nanostructure, we developed the BCA-MD-KMC hybrid simulation method. In this method, the injection process of helium ions is solved by binary collision approximation (BCA), the deformation process of a target material due to the pressure from the helium bubbles is solved by MD, and the diffusion process of the helium atoms in a tungsten material is solved by kinetic Monte-Carlo (KMC). In the hybrid simulation, the injection flux is kept at 10^{22} $m^{-2}s^{-1}$ same as an experimental flux and then the irradiation time achieved 100 s. As a result, the fuzzy nanostructure growth was successfully represented.

(Thu. Nov 1, 2018 4:00 PM - 5:30 PM Room4)

[SY-N6] Atomistic Modelling of Pipe Diffusion: a Direct Comparison of MD, KMC, aKMC and DMD

Frederic Houlle[1], Jutta Rogal[2], ○Erik Bitzek[1] (1.FAU Erlangen-Nuernberg, Germany, 2.ICAMS Ruhr University Bochum, Germany)

Understanding and influencing self-diffusion in complex microstructures is of fundamental importance for improving the high-temperature mechanical properties of materials. Modelling diffusion in a quantitatively predictive way requires information about the underlying atomic-scale processes and corresponding activation energies. While various atomic-scale simulation approaches are routinely employed to study diffusion in homogeneous environments, the presence of strain gradients and defects still poses significant challenges to predictive atomic-scale models. In particular, currently only few detailed studies that compare the application of different simulation methods to diffusion at extended defects exist.

Here we present our recent atomistic simulations results of vacancy-mediated diffusion in the vicinity of an edge dislocations in aluminum modelled by an EAM potential. The direct high-temperature molecular dynamics (MD), adaptive kinetic Monte Carlo (aKMC) and diffusive molecular dynamics (DMD) simulations all use the identical atomistic starting configuration. The activation energies of all nearest-neighbor vacancy jumps in this configuration were determined by the nudged elastic band (NEB) method and used to build the

event catalogue for the kinetic Monte Carlo (KMC) simulations and to parametrize the DMD model. Significant differences between the direct MD simulations and the (a)KMC simulations are observed, which could be attributed to the coupling of the diffusive vacancy motion with the thermally-induced fluctuations of the dislocation.

(Thu. Nov 1, 2018 4:00 PM - 5:30 PM Room4)

[SY-N6] Strategies for optimal construction of Markov chain representations of atomistic dynamics

○Danny Perez, Thomas Swinburne （Los Alamos National Laboratory, United States of America）

A common way of representing the long-time dynamics of materials is in terms of a Markov chain that specifies the transition rates for transitions between metastable states. This chain can either be used to generate trajectories using kinetic Monte Carlo, or analyzed directly, e.g., in terms of first passage times between distant states. While a number of approaches have been proposed to infer such a representation from direct molecular dynamics (MD) simulations, challenges remain. For example, as chains inferred from a finite amount of MD will in general be incomplete, quantifying their completeness is extremely desirable. In addition, making the construction of the chain as computationally affordable as possible is paramount. In this work, we simultaneously address these two questions. We first quantify the local completeness of the chain in terms of Bayesian estimators of the yet-unobserved rate, and its global completeness in terms of the residence time of trajectories within the explored subspace. We then systematically reduce the cost of creating the chain by maximizing the increase in residence time against the distribution of states in which additional MD is carried out and the temperature at which these are respectively carried out. Using as example the behavior of vacancy and interstitial clusters in materials, we demonstrate that this is an efficient, fully automated, and massively-parallel scheme to efficiently explore the long-time behavior of materials.

(Thu. Nov 1, 2018 4:00 PM - 5:30 PM Room4)

[SY-N6] Simulating the collective diffusion mechanism of amorphous solids at experimentally relevant time scales

○Yunjiang Wang[1,2], Shigenobu Ogata[3] （1.Institute of Mechanics, Chinese Academy of Sciences, China, 2.School of Engineering Science, University of Chinese Academy of Sciences, China, 3.Graduate School of Engineering Science, Osaka University, Japan）

The nature of collective diffusion in amorphous solids is in strong contrast with diffusion in crystals. However, the atomic-scale mechanism and physics of collective motion remains elusive in disorder materials. Here the free energy landscape of collective diffusion triggered by single atom jump in a prototypical CuZr model metallic glass is explored with the recently advanced well-tempered metadynamics which significantly expands the observation time-scale of diffusion process at atomic-scale. Metadynamics samplings clarify a long-standing experimentally suggested collective diffusion mechanism in the deep glassy state. The collective nature is strongly temperature-dependent. It evolves from string-like motion with participation of only several atoms to be large size collective diffusion at high temperature, which would remarkably promote the atomic transport upon glass transition. The temperature and pressure dependence of collective diffusion are further quantified with big activation entropy and small activation volume of half atom volume, which

both agree quantitatively with experiments. Direct atomic-scale simulations of diffusion at laboratory time-scale brings several physical insights into the nature of collective diffusion in amorphous solids which is beyond the knowledge established in diffusion of crystals.

Symposium | K. Multiscale Simulations of Catastrophic Phenomena: Toward Bridging between Materials Fracture and Earthquake

[SY-K1] Symposium K-1

Chairs: Momoji Kubo(Institute for Materials Research, Tohoku University, Japan), Tomoaki Niiyama(Kanazawa Univ., Japan)

Thu. Nov 1, 2018 11:15 AM - 12:30 PM Room5

[SY-K1] Supercomputer Post-K Project “ Challenge of Basic Science - Exploring Extremes through Multi-Physics and Multi-Scale Simulations”

○Momoji Kubo （Tohoku Univ., Japan）

[SY-K1] Universal avalanche statistics across 16 decades in length: From nanocrystals (and neurons) to earthquakes and stars?

○Karin Dahmen （University of Illinois at Urbana Champaign, United States of America）

[SY-K1] Predicting avalanches and failure: wood and paper

○Mikko Alava, Juha Koivisto, Tero Mäkinen, Leevi Viitanen （Aalto University, Finland）

[SY-K1] System-spanning shear avalanches induced by thermal structural relaxation in metallic glasses

○Tomoaki Niiyama[1], Masato Wakeda[2], Tomotsugu Shimokawa[4], Shigenobu Ogata[3] （1.College of Science and Engineering, Kanazawa Univ., Japan, 2.Research Center for Structural Materials, National Institute for Materials Science, Japan, 3.Department of Mechanical Science and Bioengineering, Osaka University, Japan, 4.Faculty of Mechanical Engineering, Kanazawa University, Japan）

(Thu. Nov 1, 2018 11:15 AM - 12:30 PM Room5)

[SY-K1] Supercomputer Post-K Project “Challenge of Basic Science - Exploring Extremes through Multi-Physics and Multi-Scale Simulations”

○Momoji Kubo (Tohoku Univ., Japan)

Japanese government plans to construct a supercomputer Post-K at 2021, which is expected to have over 10^{18} flops. This calculation speed is 100 times faster than the present supercomputer K in Kobe, Japan. Japanese government started 13 projects (9 priority issues and 4 exploratory challenges) to develop original simulators for the supercomputer Post-K. Our Post-K project “Challenge of Basic Science - Exploring Extremes through Multi-Physics and Multi-Scale Simulations” (Leader: Prof. Momoji Kubo, Institute for Materials Research, Tohoku University) was selected as one of four exploratory challenges at June, 2016 and started at August, 2016. The summary of our Post-K project is as follows.

Supercomputer K significantly advanced individual sciences on exploring extremes such as fracture of materials, earthquake, atmospheric flow, ocean flow, volcanic eruption, magma, and extreme properties. On the basis of the above individual understanding obtained by supercomputer K, our Post-K project aims to solve multi-physics and multi-scale problems for exploring extremes by developing new calculation methods beyond the limits of calculation accuracy and possibility and by bridging the different physics and scales. Our Post-K project consists of four sub-challenges.

Sub-Challenge A: Fracture and Catastrophe

(Sub-Leader: Prof. Momoji Kubo, Tohoku University)

Sub-Challenge B: Phase Transitions and Flows

(Sub-Leader: Prof. Toshihiro Kawakatsu, Tohoku University)

Sub-Challenge C: Structures and Properties of Materials in Deep Earth and Planets

(Sub-Leader: Dr. Toshiaki Iitaka, RIKEN)

Sub-Challenge D: Fundamental Quantum Mechanics and Informatics

(Sub-Leader: Prof. Naoki Kawashima, The University of Tokyo)

In the supercomputer Post-K project, our group is focusing on the fracture and catastrophe of materials. Our recent outcomes on the following three topics will be presented in the conference.
Friction and wear processes of diamond-like carbon thin films.Stacking fault generation processes of polycrystalline ceramics.Sintering processes of Ni/YSZ electrode in solid oxide fuel cell.

(Thu. Nov 1, 2018 11:15 AM - 12:30 PM Room5)

[SY-K1] Universal avalanche statistics across 16 decades in length: From nanocrystals (and neurons) to earthquakes and stars?

Invited

○Karin Dahmen （University of Illinois at Urbana Champaign, United States of America）

Slowly-compressed nano-crystals, bulk metallic glasses, rocks, granular materials, and the earth all deform via intermittent slips or “quakes”. We find that although these systems span 12 decades in length scale, they all show the same scaling behavior for their slip size distributions and other statistical properties. Remarkably, the size distributions follow the same power law multiplied with the same exponential cutoff. The cutoff grows with applied force for materials spanning length scales from nanometers to kilometers, indicating an underlying nonequilibrium phase transition. A simple mean field model for avalanches of slipping weak spots explains the agreement across scales. It predicts the observed slip-size distributions and the observed stress-dependent cutoff function. The analysis draws on tools from statistical physics and the renormalization group. The results enable extrapolations from one scale to another, and from one force to another, across different materials and structures, from nanocrystals to earthquakes. Connections to neuron avalanches in the brain and recent observations on stars will also be discussed, extending the range of scales to 16 decades in length.

References:

[1] J.T. Uhl, S. Pathak, D. Schorlemmer, X. Liu, R. Swindeman, B.A.W. Brinkman, M. LeBlanc, G. Tsekenis, N. Friedman, R. Behringer, D. Denisov, P. Schall, X. Gu, W.J. Wright, T. Hufnagel, A. Jennings, J.R. Greer, P.K. Liaw, T. Becker, G. Dresen, and K.A. Dahmen, Scientific Reports 5, 16493 (2015).
[2] N. Friedman, A. T. Jennings, G. Tsekenis, J.-Y. Kim, J. T. Uhl, J. R. Greer, and K. A. Dahmen, Phys. Rev. Lett. 109, 095507 (2012).
[3] J. Antonaglia, W.J. Wright, X. Gu, R.R. Byer, T.C. Hufnagel, M. LeBlanc, J.T. Uhl, and K.A. Dahmen, Physical Review Letters 112, 155501 (2014).
[4] J. Antonaglia, X.Xie, M. Wraith, J.Qiao, Y. Zhang, P.K. Liaw, J.T. Uhl, and K.A. Dahmen, Nature Scientific Reports 4, 4382 (2014).
[5] N. Friedman, S. Ito, B.A.W. Brinkman, L. DeVille, K. Dahmen, J. Beggs, and T. Butler, Phys. Rev. Lett. 108, 208102 (2012).
[6] M.A. Sheikh, R.L. Weaver, and K. A. Dahmen, Phys. Rev. Lett. 117, 261101 (2016).

(Thu. Nov 1, 2018 11:15 AM - 12:30 PM Room5)

[SY-K1] Predicting avalanches and failure: wood and paper

○Mikko Alava, Juha Koivisto, Tero Mäkinen, Leevi Viitanen （Aalto University, Finland）

Natural and man-made structured materials like wood and paper exhibit complex response to external loading. We have demonstrated the presence of deformation avalanches in wood compression in analogy to other laboratory-scale experiments mimicking earthquakes. I will review this and the subsequent predictability of large events and discuss the relation of this to the wood microstructure, based on deformation analyses and tomographic studies [1-3]. Fiber networks - paper - exhibit a very complex creep response in, again, analogy to most other materials. The predictability of sample failure with or without an initial defect/notch depends on the presence of regularities in the rheological response, such as the localization of creep strain or the formation of a large Fracture Process Zone [4-6]. I will discuss the

experimental signatures that are of relevance for predictability, and what coarse-grained models teach us.

[1] T. Mäkinen et al., Phys. Rev. Lett. 115 (055501).
[2] L. Viitanen et al., J. Stat. Mech. 053401 (2017).
[3] T. Mäkinen et al., unpublished.
[4] J. Rosti et al., Phys. Rev. Lett. 105, 100601 (2010).
[5] J. Koivisto et al. Phys. Rev. E 94, 023002 (2016).
[6] L. Viitanen et al., submitted, Physical Review Applied.

(Thu. Nov 1, 2018 11:15 AM - 12:30 PM Room5)

[SY-K1] System-spanning shear avalanches induced by thermal structural relaxation in metallic glasses

○Tomoaki Niiyama[1], Masato Wakeda[2], Tomotsugu Shimokawa[4], Shigenobu Ogata[3] (1.College of Science and Engineering, Kanazawa Univ., Japan, 2.Research Center for Structural Materials, National Institute for Materials Science, Japan, 3.Department of Mechanical Science and Bioengineering, Osaka University, Japan, 4.Faculty of Mechanical Engineering, Kanazawa University, Japan)

Metallic glasses (MGs) are one of the most attractive materials because of their excellent properties [1]. However, brittle fractures are an obstacle for MGs to be applied as structural materials. This brittleness originating from shear band nucleation is determined by structural relaxation using thermal annealing [2]. Thus, the influence of structural relaxation upon the nucleation of shear banding that can induce catastrophic failure in MGs is a significant challenge in material science.
For this challenge, we focus on the avalanche behavior that provides sudden massive deformations and spatiotemporal correlation in solid plasticity [3]. Thus, this avalanche behavior is deeply connected to the localization of plastic deformation and catastrophic failure in MGs.
In this study [4], we investigate the geometry of the shear transformation avalanches that exhibit the power-law statistics using molecular dynamics simulations of shear deformation in two thermally processed MG models that are based on a less-relaxed glass and a well-relaxed glass. The simulation showed a shear-band like heterogeneous pattern in the well-relaxed glass model, whereas the less-relaxed model exhibits homogeneous deformation patterns. Considering the spatial correlation functions of the non-affine least square displacements of atoms during each each avalanche event, we reveal that the regions an avalanche developed in well-relaxed glasses tend to be anisotropic whereas those in less-relaxed glasses are isotropic. Moreover, a temporal clustering feature of the direction of avalanche propagations and a considerable correlation between the anisotropy and size of an avalanche in the well-relaxed glass model are demonstrated.

[1] A. L. Greer, Science 267, 1947 (1995).
[2] G. Kumar, et al., Acta Mater. 57, 3572 (2009).
[3] M. C. Miguel, et al., Nature 410, 667 (2001).
[4] T. Niiyama, et al., arXiv:1804.00852 (2108).

Symposium | K. Multiscale Simulations of Catastrophic Phenomena: Toward Bridging between Materials Fracture and Earthquake

[SY-K2] Symposium K-2

Chairs: Ferenc Kun(University of Debrecen, Hungary), Ian Main(University of Edinburgh, UK)
Thu. Nov 1, 2018 2:00 PM - 3:30 PM Room5

[SY-K2] Predictability of catastrophic failure in porous media

○Ian Main[1], Ferenc Kun[2], Jeremie Vasseur[3], Andrew Bell[1] （1.University of Edinburgh, UK, 2.University of Debrecen, Hungary, 3.Ludwig Maximilian University, Munich, Germany）

[SY-K2] Deciphering the dynamics of precursors to failure in quasi-brittle solids: an inspiration for understanding the statistics of earthquakes ?

○Laurent Ponson[1], Estelle Berthier[1], Vincent Démery[2] （1.Institut Jean le Rond d'Alembert, CNRS - Sorbonne University, Paris, France, 2.Gulliver, CNRS - ESPCI, Paris, France）

[SY-K2] Avalanche precursors and fracture strength in the limit of high disorder

○Ferenc Kun[1,2], Viktória Kádár[1] （1.Department of Theoretical Physics, University of Debrecen, Hungary, 2.Institute for Nuclear Research (Atomki), Debrecen, Hungary）

[SY-K2] Jump statistics of epicenters in thermally induced cracking of fiber bundles

○Naoki Yoshioka[1], Ferenc Kun[2], Nobuyasu Ito[1,3] （1.RIKEN Center for Computational Science, Japan, 2.Department of Theoretical Physics, University of Debrecen, Hungary, 3.Department of Applied Physics, Graduate Schoold of Engineering, The University of Tokyo, Japan）

[SY-K2] Time dependent fracture under unloading in a fiber bundle model

○Reka Korei, Ferenc Kun （Department of Theoretical Physics, University of Debrecen, Hungary）

(Thu. Nov 1, 2018 2:00 PM - 3:30 PM Room5)

[SY-K2] Predictability of catastrophic failure in porous media

Invited

○Ian Main[1], Ferenc Kun[2], Jeremie Vasseur[3], Andrew Bell[1] (1.University of Edinburgh, UK, 2.University of Debrecen, Hungary, 3.Ludwig Maximilian University, Munich, Germany)

Recent discrete element models for the processes leading up to material failure provide a very close match to experiment in the case of high porosity, highly disordered materials. On approach to catastrophic, system-sized failure the number of micro-cracks and their associated acoustic emissions (AE) increase at a rate marked by a smooth inverse power law, defining a failure time at the singularity in AE rate. This behaviour is reminiscent of a second-order phase transition. At the same time the deformation becomes progressively more localised on an incipient optimally oriented fault plane, and the scaling exponent *b* for the frequency-magnitude distribution of the acoustic emissions decreases to a minimum near the failure time. On the other hand, a simple elastic fracture mechanics for an ideal ordered, uniform solid with a single pre-existing crack provides no warning of incipient failure. In between these limits there are clear precursors, but failure occurs suddenly, and earlier than predicted by the inverse power-law model, more reminiscent of a first-order phase transition. We develop a mean field model for a population of cracks emanating from pores in an otherwise uniform medium to explain this systematic error in the predicted failure time. The correction depends non-linearly on the porosity, specifically the distance between pores in the starting model, and tends to zero in the limiting case of high-porosity materials. It provides a good match to aggregate data obtained from experiments on a range of materials, both natural and synthetic. We show the behaviour scales very well to a range of data from earthquakes prior to volcanic eruptions, including quasi-periodic 'drumbeat' long-period earthquake signals preceding a recent large vulcanian explosion at Tungurahua volcano, Ecuador. Unfortunately, such signals are not yet detectable prior to large earthquakes above a null hypothesis of conventional epidemic-type earthquake triggering models.

(Thu. Nov 1, 2018 2:00 PM - 3:30 PM Room5)

[SY-K2] Deciphering the dynamics of precursors to failure in quasi-brittle solids: an inspiration for understanding the statistics of earthquakes ?

○Laurent Ponson[1], Estelle Berthier[1], Vincent Démery[2] (1.Institut Jean le Rond d'Alembert, CNRS - Sorbonne University, Paris, France, 2.Gulliver, CNRS - ESPCI, Paris, France)

Quasi-brittle failure results from the evolution of a large number of interacting microcracks growing through the material microstructural disorder. Despite this complexity, quasi-brittle materials under slowly increasing compressive load exhibit a remarkably robust failure behavior: During a first stage, damage grows and accumulates through bursts of failure events that are localized both in space and time. This earthquake-like dynamic is characterized by scale free statistics with exponents that vary weakly with the type of materials and the loading conditions. Ultimately, the damage localizes into a macroscopic band that leads to the catastrophic failure of the specimen.
In this study, we investigate theoretically the physical mechanisms underlying intermittency and localization during quasi-brittle failure. Elasticity is shown to promote long-range interactions between the damaging elements constituting the specimen and to drive the collective response of the array of microcracks. To capture this cooperative dynamic, we encapsulate the interactions in an elastic kernel that derives from the

continuum mechanics of elasto-damageable solids. We then show how it can be used to (i) disentangle the statistical properties of precursors to failure and explain their scale-free statistics and (ii) predict the onset of localization and the emerging fracture pattern. Our theoretical predictions are critically compared to experimental and numerical observations made during the compressive failure of disordered quasi-brittle solids.
The relevance of this theoretical framework for unravelling the statistics of earthquakes is finally discussed.

(Thu. Nov 1, 2018 2:00 PM - 3:30 PM Room5)

[SY-K2] Avalanche precursors and fracture strength in the limit of high disorder

○Ferenc Kun[1,2], Viktória Kádár[1] （1.Department of Theoretical Physics, University of Debrecen, Hungary, 2.Institute for Nuclear Research (Atomki), Debrecen, Hungary）

Most of the materials have an inherent disorder which appears at different length scales in the form of dislocations, flaws, microcracks, grain boundaries, or internal frictional interfaces. Under mechanical load, this quenched disorder plays a decisive role in the emerging fracture process: Increasing the extension of samples a size effect emerges, i.e. the ultimate strength of disordered materials is a decreasing function of their size. On the microscale the fracture process is composed of a large number of crack nucleation - propagation - arrest steps which generate a sequence of precursory cracking avalanches. This crackling noise is of ultimate importance to forecast natural catastrophes such as landslides and earthquakes, and the catastrophic failure of engineering constructions.

We investigate how the amount of microscale disorder affects the emerging fracture process focusing on the size scaling of the ultimate fracture strength and on the time series of avalanche precursors. We consider a fiber bundle model where the strength of fibers is described by a power law distribution. Tuning the amount of disorder by varying the power law exponent and the upper cutoff of fibers' strength, in the mean field limit an astonishing size effect is revealed: For small system sizes the bundle strength increases with the number of fibers and the usual decreasing size effect is only restored beyond a characteristic size. We show that the extreme order statistics of the micro-scale disorder is responsible for this peculiar behavior, which can be exploited for materials' design.

In the limit of very high disorder the avalanche activity does not show any acceleration so that no signatures of the imminent catastrophic failure can be identified. Limiting the disorder to a finite range an acceleration period emerges with precursors, however, the predictability of the catastrophic event depends on the details of the tail of the disorder distribution.

[1] V. Kádár, Zs. Danku, and F. Kun, Physical Review E **96**, 033001 (2017).
[2] Zs. Danku and F. Kun, J. Stat. Mech.: Theor. Exp. **2016**, 073211 (2016).

(Thu. Nov 1, 2018 2:00 PM - 3:30 PM Room5)

[SY-K2] Jump statistics of epicenters in thermally induced cracking of fiber bundles

○Naoki Yoshioka[1], Ferenc Kun[2], Nobuyasu Ito[1,3] （1.RIKEN Center for Computational Science, Japan, 2.Department of Theoretical Physics, University of Debrecen, Hungary, 3.Department of Applied Physics, Graduate Schoold of Engineering, The University of Tokyo, Japan）

Based on a fiber-bundle model we investigate epicenters of breaking events in thermally activated creep rupture. Breaking events are initiated by thermal fluctuation of load followed by load redistribution which leads to an avalanche of breakings. Using recently introduced kinetic Monte Carlo algorithm for a thermally activated fiber-bundle model, it is shown that jump distance between epicenters of consecutive breaking events has a power-law distribution with a non-trivial exponent. We also discuss relations between burst size and other quantities such as jump distance of epicenters and waiting time of breaking events.

(Thu. Nov 1, 2018 2:00 PM - 3:30 PM Room5)

[SY-K2] Time dependent fracture under unloading in a fiber bundle model

○Reka Korei, Ferenc Kun （Department of Theoretical Physics, University of Debrecen, Hungary）

Failure of materials can also occur due to unloading from a previously applied stress level. Excavation during underground engineering rapidly releases stress which can result in rock bursts. Similar conditions may also occur on much larger length and time scales at the emergence of earthquakes: crustal unloading due to near-surface mass redistribution (water, ice or quarried material) can affect the subsurface stress field altering seismic activity and being also responsible for rupture activation and induced earthquakes. Fracture processes under unloading present a high degree of complexity which makes it difficult to achieve a general understanding.

To consider this problem, we investigate the process of sub-critical fracture which occurs when unloading from an initial load. We use a fiber bundle model of time dependent deformation and rupture which captures the slow damaging of loaded fibers and their immediate breaking when the local load exceeds the fibers' fracture strength. We focus on the case when a constant sub-critical load gives rise to failure in a finite time so that unloading may prevent the final breakdown. We show that the system has two phases: at rapid unloading only partial failure occurs and the sample has an infinite lifetime, however, slow unloading results in global failure in a finite time. We demonstrate that the transition between the phases of finite and infinite lifetime occurs as a continuous phase transition.

The unloading process is accompanied by breaking bursts of fibers with a varying rate. We show by computer simulations that in the regime of finite lifetime the initial relaxation is followed by a short acceleration period of bursting activity towards failure which is described by the Omori law. Based on the pattern of the time varying burst rate we propose a method to forecast the impending failure under unloading.

Symposium | K. Multiscale Simulations of Catastrophic Phenomena: Toward Bridging between Materials Fracture and Earthquake

[SY-K3] Symposium K-3

Chairs: Takahiro Hatano(University of Tokyo, Japan), Akio Nakahara(Nihon Univ., Japan)
Thu. Nov 1, 2018 4:00 PM - 5:30 PM Room5

[SY-K3] Creep of strongly disordered materials: Plasticity, damage and approach to failure

○Michael Zaiser, David Fernandez Castellanos （Inst,. of Materials Simulation, Dept of Materials Science, FAU University of Erlangen-Nuremberg, Germany）

[SY-K3] Creep rupture and Omori-Utsu law: Fiber bundle model approach

○Takahiro Hatano[1], Subhadeep Roy[2] （1.University of Tokyo, Japan, 2.Norwegian University of Science and Technology, Norway）

[SY-K3] Temperature dependent shear friction in metallic glass

○Akio Ishii[1], Tomoaki Niiyama[2], Takahiro Hatano[3], Tomotsugu Shimokawa[2], Shigenobu Ogata[1] （1.Osaka Univ., Japan, 2.Kanazawa Univ., Japan, 3.Tokyo Univ., Japan）

[SY-K3] Mechanism of controlled crack formation induced by memory effect of clay paste

○Akio Nakahara[1], Rokuya Hayashi[1], Tomoki Hiraoka[1], Yousuke Matsuo[1], So Kitsunezaki[2] （1.Nihon Univ., Japan, 2.Nara Women's University, Japan）

[SY-K3] Effects of Shockwave-Induced Nanobubble Collapse on Precision Polishing : Molecular Dynamics Study

○yoshimasa aoyama[1], Jingxiang Xu[2], Yuske Ootani[1], Nobuki Ozawa[1], Momoji Kubo[1] （1.Dept. of Materials Science, Tohoku Univ., Japan, 2.Dept. of Mechanical Engineering, Shanghai Ocean Univ., China）

(Thu. Nov 1, 2018 4:00 PM - 5:30 PM Room5)

[SY-K3] Creep of strongly disordered materials: Plasticity, damage and approach to failure

Invited

○Michael Zaiser, David Fernandez Castellanos （Inst,. of Materials Simulation, Dept of Materials Science, FAU University of Erlangen-Nuremberg, Germany）

Stochastic plasticity models have recently become popular for modelling the deformation behavior of structually disordered materials, from amorphous solids over crystals with disordered microstructure to geomaterials. We generalize such models to account for thermally activated creep processes in conjunction with structural damage. We show that the thus modified models exhibit three-stage creep curves where failure occurs as a finite-time singularity of the creep rate in conjunction with strong localization of deformation in a catastrophic shear band. Deformation occurs as a stochastic sequence of discrete avalanches with a rate that accelerates towards failure in the form of an inverse Omori law. Immediately before failure, the system switches to a regime of mechanical activation where the avalanche statistics exhibits universal features. We compare our findings with experimental data on failure of rock samples and discuss relations with other stochastic models of plasticity and fracture.

(Thu. Nov 1, 2018 4:00 PM - 5:30 PM Room5)

[SY-K3] Creep rupture and Omori-Utsu law: Fiber bundle model approach

○Takahiro Hatano[1], Subhadeep Roy[2] （1.University of Tokyo, Japan, 2.Norwegian University of Science and Technology, Norway）

We study the dynamical aspects of a statistical-mechanical model for fracture of heterogeneous media: the fiber bundle model with various interaction range. Although the model does not include any nontrivial elementary processes such as nonlinear rheology or stochasticity, the system exhibits creep-like behaviors under a constant load being slightly above the critical value. These creep-like behaviors comprise three stages: in the primary and tertiary stages, the strain rate exhibits power-law behaviors with time, which are well described by the Omori-Utsu and the inverse Omori laws, respectively, although the exponents are larger than those typically observed in experiments. A characteristic time that defines the onset of power-law behavior in the Omori-Utsu law is found to decrease with the strength of disorder in the system. The analytical solution, which agrees with the above numerical results, is obtained for the mean-field limit. Beyond the mean-field limit, the exponent for the Omori-Utsu law tends to be even larger but decreases with the disorder in the system. Increasing the spatial range of interactions, this exponent is found to be independent of disorder and to converge to the mean-field value. In contrast, the inverse Omori law remains independent of the spatial range of interaction and the disorder strength.

(Thu. Nov 1, 2018 4:00 PM - 5:30 PM Room5)

[SY-K3] Temperature dependent shear friction in metallic glass

○Akio Ishii[1], Tomoaki Niiyama[2], Takahiro Hatano[3], Tomotsugu Shimokawa[2], Shigenobu Ogata[1] （1.Osaka Univ., Japan, 2.Kanazawa Univ., Japan, 3.Tokyo Univ., Japan）

Sharp local sliding such as shear band is frequently observed in bulk metallic glass subject to mechanical loading, and it usually leads to a global mechanical instability and then a catastrophic failure of metallic glass. Although sliding induced frictional force is a key to understand the stability of metallic glass, the details has not been fully clarified yet. Using a micromechanics-based kinetic Monte Carlo tensile test simulation of metallic glass [1], we computed a temperature and velocity dependent shear frictional force in metallic glass in experimental time scale. We found a negative velocity dependency (velocity weakening) within certain temperature range and thus a velocity dependency transition from negative to positive (velocity hardening) at a transition temperature as the temperature increases. The similar trend has been observed in rock as well [2].

[1] P. Zhao, et al., International Journal of Plasticity, 40 pp.1-22 (2013).

[2] C H. Scholz, nature, 391 pp.37-42 (1998).

(Thu. Nov 1, 2018 4:00 PM - 5:30 PM Room5)

[SY-K3] Mechanism of controlled crack formation induced by memory effect of clay paste

○Akio Nakahara[1], Rokuya Hayashi[1], Tomoki Hiraoka[1], Yousuke Matsuo[1], So Kitsunezaki[2] （1.Nihon Univ., Japan, 2.Nara Women's University, Japan）

Wet clay paste remembers the direction of vibration and flow it has experienced and, when the paste is dried, the direction of desiccation cracks strongly depends on the memory of such motions. To find out the mechanism of memory effect of vibration, we perform experiments to rewite memory in paste by applying additional vibration to the paste along different direction. Experimental results are found to be consistent with theoretical models which are based on residual stress theory.

(Thu. Nov 1, 2018 4:00 PM - 5:30 PM Room5)

[SY-K3] Effects of Shockwave-Induced Nanobubble Collapse on Precision Polishing : Molecular Dynamics Study

○yoshimasa aoyama[1], Jingxiang Xu[2], Yuske Ootani[1], Nobuki Ozawa[1], Momoji Kubo[1] （1.Dept. of Materials Science, Tohoku Univ., Japan, 2.Dept. of Mechanical Engineering, Shanghai Ocean Univ., China）

Chemical mechanical polishing (CMP) is used for the planarization of semiconductor materials. However, some of them are much hard. Therefore, the designing of efficient CMP process of hard materials is required. In order to achieve an efficient CMP process, we focused on a nanobubble. When the nanobubble collapses, the liquid around the bubble forms a jet which creates a water hammer shock. Therefore, we suggested that applying the jet increases the efficiency of CMP process. To establish the efficient CMP, revealing the effects of the nanobubble collapse on precise polishing is required. In order to reveal the effects of the nanobubble collapse on a solid surface, we performed nanobubble collapse simulation on a solid surface by molecular

dynamics method. First, we made the nanobubble in water solvent by removing the solvent molecules spherically. Next, we applied shockwave and performed nanobubble collapse simulation on the solid surface. In order to clarify the effects of one nanobubble collapse, we compared the nanobubble collapse simulations and only shockwave simulation. In the nanobubble collapse simulation, a jet was generated by the nanobubble collapse and the structural change in the solid surface was larger compared with the shockwave simulation. This suggests that a nanobubble would be useful to increase the removal rate of a solid surface. Next, in order to clarify the effects of different number of nanobubbles, we compared the nanobubble collapse simulations with one and two nanobubbles. We found that the structural change by the two nanobubbles simulation was larger than that by the one nanobubble simulation. When the jet passes the water solvent, the stream of the jet decays. However, when the generated jet passes another nanobubble, the stream of the jet does not decay, because there are no water molecules in the nanobubble. Therefore, increasing the number of nanobubbles would be useful to improve the removal rate.

Symposium | O. Tribology and Interface: Multi-Scale, Multi-Physics, and Multi-Chemistry Phenomena in Friction, Lubrication, Wear, and Adhesion

[SY-O9] Symposium O-9

Chairs: Yusuke Ootani(Tohoku University, Japan), Shuichi Uehara(Tohoku University, Japan)
Thu. Nov 1, 2018 9:45 AM - 11:00 AM Room5

[SY-O9] **Combined experimental and computational study on the superlubricity mechanism of 2D Materials at the microscale**

○Tianbao Ma （Tsinghua University, China）

[SY-O9] Quantum chemistry vs. rheology of some EMIM-based ionic liquids

Szerena Kisztina Ujvari[1,2], Konstantinos Gkagkas[1], ○Andras Vernes[2,3] （1.Advanced Material Research Division, Toyota Motor Europe NV/SA, Technical Center, Hoge Wei 33B, 1930 Zaventem, Belgium, 2.AC2T research GmbH, Viktor-Kaplan-Str. 2/C, 2700 Wiener Neustadt, Austria, 3.Institute of Applied Physics, TU Wien, Wiedner Hauptstr. 8-10/134, 1040 Vienna, Austria）

[SY-O9] Lubrication with a refrigerant : a challenge made possible thanks to fluid/surface chemistry

Stéphane TROMP[1], Laurent JOLY[2], Manuel COBIAN[3], ○Nicolas FILLOT[1] （1.Univ Lyon, INSA-Lyon, , CNRS UMR5259, LaMCoS, F-69621 Villeurbanne, France, 2.Univ Lyon, Universite Claude Bernard Lyon 1, CNRS, Institut Lumiere Matiere, F-69622 Villeurbanne, France, 3.Univ Lyon, Ecole Centrale de Lyon, ENISE, ENTPE, CNRS UMR5513, Laboratory of Tribology and System Dynamics, F-69134 Ecully, France）

[SY-O9] Meso-scale SPH simulation for friction and wear between elastic-plastic solids with various asperities

○Natsuko Nakagawa Sugimura[1,2], Le Van Sang[2], Yuji Mihara[1], Hitoshi Washizu[2] （1.Dept. of Mechanical Engineering, Tokyo City Univ., Japan, 2.Grad. Sch. of Simulation Studies, Univ. of Hyogo,, Japan）

(Thu. Nov 1, 2018 9:45 AM - 11:00 AM Room5)

[SY-O9] Combined experimental and computational study on the superlubricity mechanism of 2D Materials at the microscale

Invited

○Tianbao Ma （Tsinghua University, China）

With chemical inertness, atomically flatness and interlayer van der Waals interaction, graphene and other 2D materials could act as potential ultra-thin protective coating to reduce adhesion, friction and wear.
Firstly, we predict a stable superlubricity state with vanishing friction between graphene and MoS_2 heterostructure. This is attributed to the perpetual interfacial incommensurability with the large intrinsic lattice mismatch, which leads to near-zero sliding-induced interfacial charge density fluctuation and ultrasmooth potential energy surface. Theoretical prediction has found preliminary evidence by the measurement of interlayer lateral force constant of 2D materials.
Secondly, we report a direct AFM measurement of sliding friction between graphene-coated microsphere (GMS) and graphene, and between GMS and hexagonal boron nitride (h-BN) hetero 2D layers. The exceptionally low and robust friction coefficient of 0.003 is obtained in ambient atmosphere, under high local contact pressure. This sustainable ultralow friction is attributed to the overall incommensurability of the multi-asperity contact covered with randomly oriented graphene nanograins. Furthermore, the local contact pressure fluctuations induced by the atomic roughness could be markedly suppressed by coating few-layer graphene (layer number >3) on the contacting asperities.
Thirdly, we report the preservation of ultra-low-friction state on graphene even under harsh chemical modifications. By proper alignment of graphene on a Ge(111) substrate, friction of graphene could be well preserved at an ultra-low level even after fluorination or oxidation. This behavior is experimentally found to be closely related to the suppression of molecular-level deformation of graphene within the moiré superlattice structure. Furthermore, friction modulation with dual-scale stick-slip behavior is observed on graphene/Ru(0001) substrate. The moiré superlattice-level slip instability could be attributed to the large sliding energy barrier, which arises from the morphological corrugation of graphene on Ru(0 0 0 1) surface.

(Thu. Nov 1, 2018 9:45 AM - 11:00 AM Room5)

[SY-O9] Quantum chemistry vs. rheology of some EMIM-based ionic liquids

Szerena Kisztina Ujvari[1,2], Konstantinos Gkagkas[1], ○Andras Vernes[2,3] （1.Advanced Material Research Division, Toyota Motor Europe NV/SA, Technical Center, Hoge Wei 33B, 1930 Zaventem, Belgium, 2.AC2T research GmbH, Viktor-Kaplan-Str. 2/C, 2700 Wiener Neustadt, Austria, 3.Institute of Applied Physics, TU Wien, Wiedner Hauptstr. 8-10/134, 1040 Vienna, Austria）

Ab-initio tribology is the part of computational tribology mainly dealing with tribological phenomena where electrons matter. In a previous work, [1] for example, the electronic contribution to the real contact area has been estimated by applying Bader’s quantum theory of atoms in molecules (AIM). [2]

In this contribution, AIM is used in combination with the density-functional theory (DFT), i.e., for the accordingly determined ab-initio electronic charge density in case of some 1-ethyl-3-methyl-imidazolium-based ionic liquids (ILs) to topologically characterize the involved ions also when the selected EMIM-based ILs are confined. Considering the calculated Bader’s manifolds for both the free-standing and confined

ions, and the separation area between the ions, an attempt will be made (i) to explain for ILs both experimentally [3] and computationally [4] observed layered structures, and (ii) to evaluate the relaxation time of ions. The latter will also be compared with that derived from the measured viscosities, and in addition the measured viscosities will be correlated with some DFT-determined quantum chemical indices [5].

1. M. Wolloch, G. Feldbauer, P. Mohn, J. Redinger, and A. Vernes, *Ab-initio calculation of the real contact area on the atomic scale*, Phys. Rev. B 91, 195436 (2015)
2. Richard F. W. Bader, *The density in density-functional theory*, J. Mol. Struc - TheoChem 943 (1-3), 2 (2010)
3. A. M. Smith, K. R. J. Lovelock, N. N. Gosvami, Peter Licence, A. Dolan, T. Welton, and S. Perkin, *Monolayer to bilayer structural transition in confined pyrrolidinium-based ionic liquids*, J. Phys. Chem. Lett. 4, 378 (2013)
4. K. Gkagkas, and V. Ponnuchamy, *The impact of coulombic interactions among polar molecules and metal substrates on flow and lubrication properties*, Model. Simul. Mater. Sci. Eng. 25 (6), 064004 (2017)
5. M. Karelson, V. S. Lobanov, and A. R. Katritzky, *Quantum chemical descriptors in QSAR/QSPR studies*, Chem. Rev. 96, 1017 (1996)

(Thu. Nov 1, 2018 9:45 AM - 11:00 AM Room5)

[SY-O9] Lubrication with a refrigerant : a challenge made possible thanks to fluid/surface chemistry

Stéphane TROMP[1], Laurent JOLY[2], Manuel COBIAN[3], ○Nicolas FILLOT[1] (1.Univ Lyon, INSA-Lyon, , CNRS UMR5259, LaMCoS, F-69621 Villeurbanne, France, 2.Univ Lyon, Universite Claude Bernard Lyon 1, CNRS, Institut Lumiere Matiere, F-69622 Villeurbanne, France, 3.Univ Lyon, Ecole Centrale de Lyon, ENISE, ENTPE, CNRS UMR5513, Laboratory of Tribology and System Dynamics, F-69134 Ecully, France)

Lubrication is often seen as the major solution to avoid wear and high friction due to the relative motion of solids in contact. But this sometimes requires a heavy design (e.g. addition of lubricant pumps) while the actual trend goes for weight reduction of mechanical systems. The use of working fluids (e.g. refrigerant, gasoline) instead of classical lubricants (oil) allow to bypass this problem. Nonetheless, tribological contacts have to work with ultra low viscosity fluids (not designed to be good lubricants). The major consequence is that the film thickness separating the surfaces reaches the same order of magnitude as surface roughness. At this stage, a minimum quantity of fluid needs to be trapped between apserities to avoid direct contact. This is made possible if fluid molecules are adsorbed onto the surfaces.
The work presented here aims at explaining experimental observations of R-1233zd refrigerant ability to lubricate a highly loaded contact. Starting from a dedicated force field parametrization for the refrigerant-hematite interaction (from DFT calculations [1]), Large-Scale Molecular Dynamics simulations of extreme compression and shearing of R-1233zd show the resistance of the refrigerant adsorption, and its capability to undergo normal and tangential stresses.

[1] S. Tromp, L. Joly, M. Cobian, N. Fillot, Chemical Physics at Interfaces within a Refrigerant-Lubricated Contact: From Electronic Structure to Large-Scale Molecular Dynamics Simulations. J. Phys. Chem. C, 2018, DOI: 10.1021/acs.jpcc.7b11267

(Thu. Nov 1, 2018 9:45 AM - 11:00 AM Room5)

[SY-O9] Meso-scale SPH simulation for friction and wear between elastic-plastic solids with various asperities

○Natsuko Nakagawa Sugimura[1,2], Le Van Sang[2], Yuji Mihara[1], Hitoshi Washizu[2] (1.Dept. of Mechanical Engineering, Tokyo City Univ., Japan, 2.Grad. Sch. of Simulation Studies, Univ. of Hyogo,, Japan)

We made the meso(micron-oder) scale model to simulate friction, wear and adsorption with heating between elastic-plasic bodies. Constitutive equation is based on the continuum equation and calculated with SPH(Smoothed Particle Hydrodynamics). SPH is one of particle methods to solve continuum equation with mesh free. SPH was initially developed for the hydrodynamics by Lucy et al., but it was applied to calculation of solids afterwards by Swegle et al. and has gained good results. In SPH, the physical variables of the particles are reconstructed by the adding the physical variables of the surrounding particles by an appropriate weighting called kernel. SPH particles are not truly particles like molecules but only physical fields. However, we regard the particles on the friction surfaces as also coarse grained molecules and add the interaction forces directly between such “particles”, which is mimicking the particle approach. That is, our model is what continuum calculation and particle calculation are mixed. It is just meso-scale that is situated in between the macro scale to demand continuum approach and the nano scale to demand particle approach. Although its physical discontinuity is not yet resolved, if the using both approaches confirm the reproducing valid frictional phenomena, the mechanism of its discontinuity may also be resolved. At this time, for the purpose to efficiently realize the calculation of the great amount of particles with parallel code, we use the FDPS open platform by Iwasawa &Makino et al. to create our simulation code.

We set the tens of micron system in which elastic-plastic bodies with various asperities are faced and one body is sliding under the vertical load to cause shear friction. So far, in the system with interface with regular asperities, the elasticity, plasticity, friction cure, heat generation and conduction were to some extent qualitatively expressed, although the frictional results depend on the several parameters and SPH boundary processing. Then, we will firstly show the characteristics of our model with regular asperity system in detail. Moreover, we will discuss the frictional properties changing the shape of asperities, i.e. with realistic asperities.

Symposium | A. Advances in Materials Theory for Multiscale Modeling

[SY-A9] Symposium A-9

Chair: Eliot Fried(Okinawa Institute of Science and Technology, Japan)

Thu. Nov 1, 2018 9:45 AM - 11:00 AM Room6

[SY-A9] Group-theoretical construction for constitutive equation of the first strain gradient elasticity

○Ryuichi Tarumi[1], Shunsuke Kobayashi[2], Yoji Shibutani[2] （1.Graduate School of Engineering Science, Osaka Univ., Japan, 2.Dept. of Mechanical Engineering, Osaka Univ., Japan）

[SY-A9] Physically based strain gradient plasticity model for length scale dependent yield strength

○Peter Gudmundson （Department of Solid Mechanics, KTH Royal Institute of Technology, Sweden）

[SY-A9] FTMP-based Seamless Description of Deformation-Fracture Transitions

○Tadashi Hasebe （Kobe Univ., Japan）

[SY-A9] On the crucial role played by instantaneous and hidden multifield features of lattice dynamics in their nonlocal pseudocontinuum modeling

○Miguel Charlotte （University of Toulouse, Institute Clement Ader, CNRS -- UMR 5312 INSA/UPS/ISAE-SupAero/Mines Albi, France）

(Thu. Nov 1, 2018 9:45 AM - 11:00 AM Room6)

[SY-A9] Group-theoretical construction for constitutive equation of the first strain gradient elasticity

○Ryuichi Tarumi[1], Shunsuke Kobayashi[2], Yoji Shibutani[2] （1.Graduate School of Engineering Science, Osaka Univ., Japan, 2.Dept. of Mechanical Engineering, Osaka Univ., Japan）

Development of the theory of continuum mechanics is one of the central issues for quantitative understanding of multiscale phenomena. The first strain gradient elasticity (FSGE) is an attractive framework as it includes *non-locality* in the constitutive equation. Application of the theory for multiscale material modeling is however still limited due to the large number of independent strain gradient elastic constants. This study aims to overcome the difficulty by using the group theory. We conduct the irreducible decomposition for the 5th and 6th-rank strain gradient elastic constants, $\boldsymbol{M}$ and $\boldsymbol{A}$, under general linear group GL(3). The decomposition is based on the Schur-Weyl duality principle and Young symmetrizer technique in Frobenius algebra. For the isotropic and centro-symmetric case, the 6th-rank tensor is decomposed into three sub-tensors, $\boldsymbol{A} = \boldsymbol{A}^{\{6\}}+\boldsymbol{A}^{\{4,2\}}+\boldsymbol{A}^{\{3,2,1\}}$, whereas the 5th-rank tensor $\boldsymbol{M}$ vanishes identically. Here, the one-dimensional sub-tensor $\boldsymbol{A}^{\{6\}}$ is called the primitive symmetry class and satisfies the generalized Cauchy solid condition. The corresponding stress equilibrium equation yields a simplified 4th-order partial differential equation that is different from Aifantis' Laplacian-type gradient theory. Another one-dimensional sub-tensor $\boldsymbol{A}^{\{3,2,1\}}$ denotes the elastic null-Lagrangian which is absent in the classical elasticity. The remaining three-dimensional sub-tensor $\boldsymbol{A}^{\{4,2\}}$ has two characteristic length scales and one of which has an imaginary value. We also revealed that the combined sub-tensors, $\boldsymbol{A}^{\{4,2\}}+\boldsymbol{A}^{\{3,2,1\}}$, with a proper kinematic constrain condition, reduces the well-known couple stress elasticity. Implementation of the Cauchy-type FSGE for NURBS-based isogeometric analysis (IGA) demonstrates that stress field around a point defect is regularized due to the non-locality included in $\boldsymbol{A}^{\{6\}}$.

(Thu. Nov 1, 2018 9:45 AM - 11:00 AM Room6)

[SY-A9] Physically based strain gradient plasticity model for length scale dependent yield strength

○Peter Gudmundson （Department of Solid Mechanics, KTH Royal Institute of Technology, Sweden）

Many experimental studies have shown a plastic strengthening effect for structural length scales approaching microstructural dimensions. Both increases in initial yield strength and strain hardening have been observed. Over the last 30 years different strain gradient plasticity (SGP) theories have been developed in order to capture these length scale dependences. However, up to now no generally accepted theory has emerged. In the present paper, focus is directed into a physically based SGP model for initiation of plastic deformation. The plastic behavior is governed by a dissipative part that primarily controls the hardening at moderate plastic strains and an energetic part that is of importance for the initiation of plastic flow. It is shown that a model based on the self-energies of dislocations can be translated into an internal free energy in terms of plastic strain gradients. In this way a physical connection is made between the SGP framework and dislocation mechanics. A microstructural length scale can then be defined as the Burgers vector divided by the strain for initiation of plastic deformation. When structural length scales approach this microstructural length scale, strengthening effects result. It the Taylor model is used for the dissipative part, the same microstructural length scale appears. The so developed three-dimensional SGP model is specialized to the simple load cases of tensile tension with a passivation layer that prohibits plastic deformation on surfaces as

well as pure bending with free and fixed boundary conditions for plastic strain. Simulations for varying thicknesses are compared to experimental observations reported in the literature. It is shown that the model in a good way can capture the length scale dependences. Suggestions for improvement of the dislocation theory based model for the internal free energy are discussed.

(Thu. Nov 1, 2018 9:45 AM - 11:00 AM Room6)

[SY-A9] FTMP-based Seamless Description of Deformation-Fracture Transitions

○Tadashi Hasebe （Kobe Univ., Japan）

This study attempts to tackle one of the ultimate problems in mechanics of materials based on FTMP (Field Theory of Multiscale Plasticity), i.e., modeling deformation-fracture transitions. Three typical fracture modes are targeted: (1) ductile fracture, (2) creep rupture and (3) fatigue crack initiation, whose evolutions are respectively triggered or promoted by deformation-induced substructures. For (1), critical conditions governing the outsets of macro/micro instabilities are extensively discussed, while (2) is concerned with localized recovery-induced rupture in packet models for lath martensite structures, in connection with the interaction fields. The mode (3), on the other hand, is successfully reproduced via evolving PSB ladder structure and attendant vacancy formation/diffusion processes. A noteworthy output here is that the use of the corresponding duality diagram representations enables us to “visualize” these complex processes, manifested as dynamic energy conversion between fluctuating elastic strain

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(Thu. Nov 1, 2018 9:45 AM - 11:00 AM Room6)

[SY-A9] On the crucial role played by instantaneous and hidden multifield features of lattice dynamics in their nonlocal pseudocontinuum modeling

○Miguel Charlotte （University of Toulouse, Institute Clement Ader, CNRS -- UMR 5312 INSA/UPS/ISAE-SupAero/Mines Albi, France）

In the past, a very large number of investigations has been interested in building various continuum descriptions of periodical mass-spring lattices which are capable of capturing at least some microscopically fast and microscopically localized phenomena that cannot be handled correctly by the classical continuum theories relying on a single displacement field. Very few of these works have however tried to illuminate some of the less well-known aspect of the concept of “action-at-a distance” involved in periodical mass-spring lattices, namely the “instantaneous propagation of disturbances”,
and its nonlocal effects in finite material systems. These instantaneous features, that are developed in the present work, have notably been discussed formerly partly by Lord Rayleigh and T.H. Havelock for other dispersive media and more recently evoked by M. Charlotte and L. Truskinovsky. Such features have although been ignored or minimized up to now in most derivations of pseudocontinuum hamiltonian models of elasticity. In order to account for these features, the alternative viewpoint developed here uses on an implicit but somewhat standard multi-displacement

field description of the periodical mass-spring lattice motions and their (spatially nonlocal) pseudocontinuum wave mechanic representations which allow to deal in the same framework with both quasi-continuum (atomically diffuse) and anti-continuum (atomically localized) phenomena in finite material systems. In particular, the focus is put on the lattice motions of a simple finite particle chain with nearest neighbor interactions owing to its simplicity, complete analyticity, and physical clearness. The current analysis also explores an alternative standpoint, including both bulk- and boundary-dependent multi-field or multi-modal continuum descriptions, and that may constitute a new direction in which the continuum modeling theory could be fundamentally generalized. Thus, the outcome of the present multi-field approach is merely another non-classical quasi-continuum elastodynamics with both non-trivial nonlocal inertia and elasticity whose complexity depends naturally on the non-trivial interplay between the atomic bulk interactions and the boundary conditions.

Symposium | A. Advances in Materials Theory for Multiscale Modeling

[SY-A10] Symposium A-10

Chair: Steve Fitzgerald(University of Leeds, UK)

Thu. Nov 1, 2018 11:15 AM - 12:30 PM Room6

[SY-A10] Interdiffusion and atomic mobilities in fcc Ag-Mg, Ag-Mn and Ag-Mg-Mn alloy

○Qianhui Min[1], Yuling Liu[1], Yong Du[1], Huixin Liu[1], Li Chen[1], Biao Hu[3], Changfa Du[2], Zhoushun Zheng[2] （1.Powder Metallurgy Research Institute,Central South University, China, 2.School of mathematics and statistics,Central South University, China, 3.School of Material Science and Engineering, Anhui University Of Science And Technology, China）

[SY-A10] **Stacking and Multilayered Nature of Martensite in Copper Based Shape Memory Alloys**

○Osman ADIGUZEL （Firat University , Turkey）

[SY-A10] Mesoscale understanding of ionic conduction in yttria stabilized zirconia

○Abhijit Chatterjee （Dept. of Chemical Engineering, Indian Institute of Technology Bombay, India）

[SY-A10] cancellation

[SY-A10] Accelerating stochastic simulations with path integrals

○Steve Fitzgerald （University of Leeds, UK）

(Thu. Nov 1, 2018 11:15 AM - 12:30 PM Room6)

[SY-A10] Interdiffusion and atomic mobilities in fcc Ag-Mg, Ag-Mn and Ag-Mg-Mn alloy

○Qianhui Min[1], Yuling Liu[1], Yong Du[1], Huixin Liu[1], Li Chen[1], Biao Hu[3], Changfa Du[2], Zhoushun Zheng[2]
（1.Powder Metallurgy Research Institute,Central South University, China, 2.School of mathematics and statistics,Central South University, China, 3.School of Material Science and Engineering, Anhui University Of Science And Technology, China）

On the basis of Ag/Ag-Mg, Ag/Ag-Mn, Ag-Mg/Ag-Mn, and Ag/Ag-Mg-Mn diffusion couples, the interdiffusion coefficients in face-centered cubic (fcc) phase of the Ag-Mg, Ag-Mn, and Ag-Mg-Mn alloys were messured at the temperature range between 873 and 1173 K by using semi-infinite diffusion couples together with the Sauere-Freise method. A reliable method was applied to evaluate the errors of the identified interdiffusivities in consideration of the propagation of errors. Based on available thermodynamic information, the atomic mobilities for the fcc Ag-Mg, Ag-Mn,and Ag-Mg-Mn syetems are obtained by using the DICTRA software package, and the computed results agree in general with experimental data.

(Thu. Nov 1, 2018 11:15 AM - 12:30 PM Room6)

[SY-A10] Stacking and Multilayered Nature of Martensite in Copper Based Shape Memory Alloys

○Osman ADIGUZEL （Firat University , Turkey）

Shape memory effect is characterized by the recoverability of two certain shapes of material at different temperatures. These materials are often called smart materials due to the functionality and their capacity of responding to changes in the environment. Shape memory is initiated by cooling and stressing material and processed by heating and cooling.

Shape memory effect is a result of successive thermal induced and stress induced martensitic transformations. Thermal induced martensitic transformation occurs as twinned martensite on cooling as martensite variants with cooperative movement of atoms by means of lattice invariant shears on {110} - type planes of austenite matrix. Twinned structures turn into detwinned martensite by means of stress induced martensitic transformation on stressing in martensitic state. Lattice invariant shears occurs in <110 >-type directions on the {110}-type basal planes.

Copper based alloys exhibit this property in metastable β-phase region, which has bcc-based structures at high temperature parent phase field. Twinning and lattice invariant shear is not uniform in these alloys and multilayered martensite with complex stacking structures, like 9R or 18R martensites occur by means of thermal induced martensitic transformation. All of these martensite phases are long-period stacking ordered structures that is the underlying lattice is formed by stacks of close-packed planes.

In the present contribution, x-ray diffraction and transmission electron microscopy studies were carried out on two copper based CuZnAl and CuAlMn alloys. X-ray diffraction profiles and electron diffraction patterns reveal that both alloys exhibit super lattice reflections inherited from parent phase due to the displacive character of martensitic transformation.

(Thu. Nov 1, 2018 11:15 AM - 12:30 PM Room6)

[SY-A10] Mesoscale understanding of ionic conduction in yttria stabilized zirconia

○Abhijit Chatterjee （Dept. of Chemical Engineering, Indian Institute of Technology Bombay, India）

Yttria-stabilized zirconia (YSZ) is widely used as an electrolyte in solid oxide fuel cells (SOFCs). Much of past research on ionic conductivity in YSZ has focused on understanding diffusion process atomistically, e.g., migration barriers for O^{2-} ion movement and vacancy trapping behavior, in an attempt to explain the bulk O^{2-} transport. How the mesoscale structure of YSZ, i.e., structures at length scales lying between the atomic/micro-scale and the macroscale, influences ionic conduction remains poorly understood. An improved understanding of mesoscale factors that affect ionic conduction in YSZ can potentially benefit our efforts to search for new SOFC electrolyte materials.

Two mesoscale aspects will be covered in this talk. The first part of the talk relates to the percolation network structure formed in YSZ. It is well known that Y3+ ions in the YSZ structure block the movement of O2- ions. Other parts of YSZ that locally do not contain the Y3+ ions form a fast ion conducting percolation network. The network topology is determined by the underlying cation arrangement. Insights into the percolation network composition, topology and O^{2-} ion conduction rates are provided using kinetic Monte Carlo simulations. A relationship between the ionic conductivity and the topological details of the network is derived.

The second part relates to free energy of finding O^{2-}-vacancy (O^{2-}-vac) pairs in a local environment, which again is a mesoscale property of the material. Higher probability of O^{2-}-vac pairs in some regions of YSZ can result in greater number of transitions in those regions. O^{2-} ion movement in bulk YSZ is studied using multiple independent short molecular dynamics (MD) trajectories. Analysis of the MD trajectories yields free energy of O^{2-}-vac pairs in 42 different local cation (Y^{3+}/Zr^{4+}) environments, as well as effective O^{2-} hopping rates and Arrhenius parameters. Based on the free energies we conclude that it is possible that ionic movement is hindered in some environments not just because of high migration barriers or vacancy trapping as believed earlier, but also because O^{2-}-vac pairs are destabilized by these environments. Increasing the temperature and/or decreasing the dopant composition stabilizes O^{2-}-vac pairs in these environments, which in turn affects the YSZ conductivity.

(Thu. Nov 1, 2018 11:15 AM - 12:30 PM Room6)

[SY-A10] cancellation

(Thu. Nov 1, 2018 11:15 AM - 12:30 PM Room6)

[SY-A10] Accelerating stochastic simulations with path integrals

○Steve Fitzgerald （University of Leeds, UK）

Monte Carlo-type simulations can extend accessible timescales c.f. atomistic models by many orders of magnitude. However, their efficiency can be significantly reduced when some of the species being simulated have very low migration barriers. This can be addressed by coarse-graining the low-barrier migration into pseudo-free continuum diffusion and, and evolving the system by drawing timesteps and hop lengths from a first passage time distribution [1,2], but this neglects the effects of spatial variation in the potential landscape in which the particles move, i.e. drift. Existing extensions require every step of a random walk to be computed, or a Fokker-Planck equation to be solved numerically [3], thus increasing the computational cost.

In this work I will describe an alternative approach, beginning from the Langevin equation for a particle moving in a general smooth potential V(x). Assuming Gaussian white noise, the stochastic equation of motion can be recast as a path integral, which can be analysed using methods borrowed from quantum field theory. Closed-form solutions for the Green function / propagator P(x,t|0,0) in a general potential are possible when the noise strength (temperature) is less than the energy scale characterising the barriers the particle has to overcome (i.e. the same range of validity as the Arrhenius rate function exp(-E/kT).) Potential applications to material simulations will be discussed.

[1] Opplestrup, Tomas, et al. "First-passage Monte Carlo algorithm: diffusion without all the hops." *Physical review letters* 97.23 (2006): 230602.

[2] Muller, Mervin E. "Some continuous Monte Carlo methods for the Dirichlet problem." *The Annals of Mathematical Statistics*(1956): 569-589.

[3] Mauro, Ava J., et al. "A first-passage kinetic Monte Carlo method for reaction-drift-diffusion processes." *Journal of Computational Physics* 259 (2014): 536-567.

Symposium | I. Multiscale Modeling of Grain Boundary Dynamics, Grain Growth and Polycrystal Plasticity

[SY-I9] Symposium I-9

Chairs: Yuri Mishin(George Mason University, United States of America), Yang Xiang(Hong Kong University of Science and Technology, Hong Kong)

Thu. Nov 1, 2018 9:45 AM - 11:00 AM Room7

[SY-I9] Grain Boundary Microstates Under Irradiation: A Moment in Time?

○Mitra L Taheri （Drexel University, Department of Materials Science &Engineering, United States of America）

[SY-I9] The Role of Grain Boundaries under Long-Time Radiation

○Jing Luo[1], Yichao Zhu[1], Xu Guo[1], Yang Xiang[3], Stephen Jonathan Chapman[2] （1.Dalian University of Technology, China, 2.Mathematical Institute, University of Oxford, UK, 3.Department of Mathematics, The Hong Kong University of Science and Technology, Hong Kong）

[SY-I9] Quantifying point defect fluxes to interfaces and the role of interface structure

○Shen J Dillon （University of Illinois , United States of America）

(Thu. Nov 1, 2018 9:45 AM - 11:00 AM Room7)

[SY-I9] Grain Boundary Microstates Under Irradiation: A Moment in Time?

Invited

○Mitra L Taheri （Drexel University, Department of Materials Science &Engineering, United States of America）

Understanding the sink efficiency of interfaces under irradiation is of paramount importance to tailoring materials for radiation tolerance. Using in situ irradiation coupled with precession electron diffraction analysis, defect absorption was tracked for increasing dose. Denuded zones were found to collapse, but in the absence of any detected changed in macroscopic degrees of freedom of the grain boundaries. Each grain boundary denuded zone experienced changes different doses, indicating a direct observation of the difference in grain boundary “immunity” to irradiation depending on character. Since a change in sink efficiency is likely due to a change in point defect absorption at the boundary, this indicates that something about the structure of these boundaries has changed. The grain boundary macroscopic character remains the same, however, leading to the conclusion that a change in microscopic character has occurred, possibly due to the formation of extrinsic defects on the boundary. To analyze this further, simulations were used to explore grain boundary microstates loaded with defects (mimicking a collision cascade) and assessed for vacancy formation energies. Overall, the results present a foundation for improving sink efficiency descriptions under irradiation, and take a step forward in understanding complex interfacial dependencies. Additionally, results will be shown for studies of grain boundary structure and stability, including faceting, in the context of grain boundaries acting as “phases.” These advances present the possibility that the extent to which a grain boundary is at “equilibrium” controls many of its properties, and that its equilibrium is possible to be tuned.

(Thu. Nov 1, 2018 9:45 AM - 11:00 AM Room7)

[SY-I9] The Role of Grain Boundaries under Long-Time Radiation

○Jing Luo[1], Yichao Zhu[1], Xu Guo[1], Yang Xiang[3], Stephen Jonathan Chapman[2] （1.Dalian University of Technology, China, 2.Mathematical Institute, University of Oxford, UK, 3.Department of Mathematics, The Hong Kong University of Science and Technology, Hong Kong）

Materials containing a high proportion of grain boundaries offer significant potential for the development of radiation-resistent structural materials. However, a proper understanding of the connection between the radiation-induced microstructural grain boundary behaviour and its impact at long natural time scales is still missing. To bridge this gap in time scales, a rigorously coarse-grained formulation describing the coupled evolution of point defects and low-angle tilt grain boundaries is proposed. The derived formulation captures well the radiation-induced climb behaviour of grain boundary dislocations, which leads to asymmetry in grain shape evolution. It also reveals that the presence of point defect sources within a grain further accelerates its shrinking process, and radiation tends to elongate the twin boundary sections. Based on the proposed formulation, it is predicted for the first time that the minimum dimension of a polycrystalline aggregate needed for shielding the point defect concentration to a prescribed level scales with its grain boundary fraction at a sublinear rate.

(Thu. Nov 1, 2018 9:45 AM - 11:00 AM Room7)

[SY-I9] Quantifying point defect fluxes to interfaces and the role of interface structure

Invited

○Shen J Dillon （University of Illinois , United States of America）

Point defect fluxes to and from interfaces can dominate the response of materials exposed to irradiation, their equilibration after thermal perturbation, and their sintering. However, little is known experimentally about how non-equilibrium point defect concentrations equilibrate, how their concentration gradients develop in the lattice, and the role of interface structure in affecting sink efficiency. This talk describes experimental approaches to probing these phenomena using localized tracer diffusion measurements and irradiaiton induced creep in model sample geometries.

Symposium | I. Multiscale Modeling of Grain Boundary Dynamics, Grain Growth and Polycrystal Plasticity

[SY-I10] Symposium I-10

Chair: Saryu Fensin(Los Alamos National Lab, United States of America)

Thu. Nov 1, 2018 11:15 AM - 12:15 PM Room7

[SY-I10] Structure and Mobility of Dissociated Cacancies at Twist Grain Boundaries and Screw Dislocations in Ionic Compounds

○Blas Pedro Uberuaga, Enrique Martinez, Kedarnath Kolluri, Xiang-Yang Liu （Los Alamos National Laboratory, United States of America）

[SY-I10] Reverse engineering the kinetics of grain growth

Mingyan Wang[1], Jules Dake[1], Søren Schmidt[2], ○Carl Krill[1] （1.Institute of Micro and Nanomaterials, Ulm University, Germany, 2.Dept. of Physics, Technical University of Denmark, Denmark）

(Thu. Nov 1, 2018 11:15 AM - 12:15 PM Room7)

[SY-I10] Structure and Mobility of Dissociated Cacancies at Twist Grain Boundaries and Screw Dislocations in Ionic Compounds

Invited

○Blas Pedro Uberuaga, Enrique Martinez, Kedarnath Kolluri, Xiang-Yang Liu （Los Alamos National Laboratory, United States of America）

Interfaces, grain boundaries, and dislocations are known to have significant impact on the transport properties within materials. Even so, it is still not clear how the structure of interfaces influence the mobility and concentration of carriers that are responsible for transport. Using low angle twist grain boundaries in MgO as a model system for semi-coherent interfaces more generally, we examine the structural and kinetic properties of vacancies. These boundaries are characterized by a network of screw dislocations. Vacancies of both types, Mg and O, are strongly attracted to the dislocation network, residing preferentially at the misfit dislocation intersections (MDIs). However, the vacancies can lower their energy by splitting into two parts, which then repel each other along the dislocation line between two MDIs because of electrostatic repulsion, further lowering their energy.

This dissociated structure has important consequences for transport, as the free energy of the dissociated vacancies decreases with decreasing twist angle, leading to an increase in the net migration barrier for diffusion as revealed by molecular dynamics simulations. Similar behavior is observed in BaO and NaCl, highlighting the generality of the behavior. We analyze the structure of the dissociated vacancies as a pair of jogs on the dislocation and construct a model containing electrostatic and elastic contributions that qualitatively describe the energetics of the dissociated vacancy. Finally, we examine the nature of this mechanism in other ionic compounds without a rocksalt structure. Our results represent the first validation of a mechanism for vacancy dissociation on screw dislocations in ionic materials first discussed by Thomson and Balluffi in 1962.

(Thu. Nov 1, 2018 11:15 AM - 12:15 PM Room7)

[SY-I10] Reverse engineering the kinetics of grain growth

Invited

Mingyan Wang[1], Jules Dake[1], Søren Schmidt[2], ○Carl Krill[1] （1.Institute of Micro and Nanomaterials, Ulm University, Germany, 2.Dept. of Physics, Technical University of Denmark, Denmark）

At first glance, the strategy for modeling grain growth seems obvious: simply combine an expression governing the physics of grain boundary (GB) migration with a treatment of the connectivity of the boundary network, such that shrinkage of one grain corresponds to growth of its neighbor. However, 70 years of analytic models and three decades’ worth of computer simulations have left us with seemingly intractable discrepancies between theory and experiment—concerning, for example, the shape of the self-similar grain size distribution; the occurrence of growth stagnation at long annealing times; and, most strikingly, the emergence of a bimodal size distribution during instances of so-called “abnormal” grain growth.

In the world of industry, when repeated attempts to solve a technological challenge end in failure, employees

sometimes try to “reverse engineer” a competitor’s product, dissecting the interplay between the device’s internal parts to uncover its working principle. Afflicted with a similar sense of desperation, we applied this approach to the phenomenon of grain growth! Exploiting three-dimensional x-ray diffraction (3DXRD) microscopy, we investigated thermally induced coarsening in two different Al alloys. From microstructural snapshots interspersed between isothermal annealing steps, we were able to track the morphology, misorientation and migration of thousands of GBs over time, acquiring the basis for a robust statistical analysis of local growth kinetics. The results allow extracting dependencies of reduced mobility (the product of GB mobility and energy) on GB misorientation and inclination. In one specimen, the measured dependency is consistent with expectations for normal grain growth, but, in the other case, we find evidence for boundary kinetics that lie beyond the scope of standard models.

Symposium | I. Multiscale Modeling of Grain Boundary Dynamics, Grain Growth and Polycrystal Plasticity

[SY-I11] Symposium I-11

Chairs: Bob Svendsen(RWTH Aachen University, Germany), Jeremy K Mason(University of California, Davis, United States of America)

Thu. Nov 1, 2018 2:00 PM - 3:30 PM Room7

[SY-I11] Recent advances in the Full-Field modeling of microstructural evolutions using a finite-element level set integrated framework.

○Daniel Pino Munoz, Thomas Toulorge, Charbel Moussa, Nathalie Bozzolo, Marc Bernacki（Mines ParisTech / PSL Research University, France）

[SY-I11] The effect of strong anisotropic grain boundary energy and mobility on microstructure formation and evolution: mesoscale modeling and simulation

○Brandon Runnels[1], Josep Maria Gras Ribot[1], Ian Chesser[2]（1.University of Colorado Colorado Springs, United States of America, 2.Carnegie Mellon University, United States of America）

[SY-I11] A Machine Learning Exploration of Grain Boundary Mobility Mechanisms

Leila Khalili[1], Eric R Homer[2], ○Srikanth Patala[1]（1.North Carolina State University, United States of America, 2.Brigham Young University, United States of America）

(Thu. Nov 1, 2018 2:00 PM - 3:30 PM Room7)

[SY-I11] Recent advances in the Full-Field modeling of microstructural evolutions using a finite-element level set integrated framework.

Invited

○Daniel Pino Munoz, Thomas Toulorge, Charbel Moussa, Nathalie Bozzolo, Marc Bernacki （Mines ParisTech / PSL Research University, France）

Full field modeling of microstructure evolutions at polycrystalline scale is nowadays a very active field of research. Within this context we have been working in tight collaboration with industrial partners in order to be able to predict microstructural evolutions of metallic material due to recrystallization and grain growth phenomena. This collaboration had lead us to the development of a numerical framework based on the Level-Set method that allows to account fro complex microstructural evolution. These complex phenomena includes grain growth, Smith-Zener pinning and, in particular, static, dynamic and post-dynamic recrystallization. In this way the motion of the grain boundaries of microstructures is simulated accurately.

The general numerical framework will be presented along with recent developments that allowed us to significantly improve the performance of our approach. Our on-going developments aim at the enhancement of the existing capabilities of our numerical tools in order to account for high grain boundary energy and mobility. Different examples will the used to illustrate the robustness of the numerical approach as well as its capabilities to accurately simulate microstructural evolutions. Finally, some current challenges for the forthcoming years will be discussed.

(Thu. Nov 1, 2018 2:00 PM - 3:30 PM Room7)

[SY-I11] The effect of strong anisotropic grain boundary energy and mobility on microstructure formation and evolution: mesoscale modeling and simulation

Invited

○Brandon Runnels[1], Josep Maria Gras Ribot[1], Ian Chesser[2] （1.University of Colorado Colorado Springs, United States of America, 2.Carnegie Mellon University, United States of America）

Nanocrystalline materials have exceptional mechanical properties. Because of their small microstructural length scale, their macroscopic properties are dramatically influenced by grain boundaries (GBs). In this work we develop an algorithm for constructing the Allen-Cahn equation for grain boundary migration including an orientation-dependent, nonconvex, anisotropic boundary energy. The energy minimizing morphology for boundaries with nonconvex energy is faceted, but lacks a lengthscale, resulting in unstable solutions in phase field gradient flow. It is therefore necessary to include a second-order regularization to penalize corners To compute the variational derivative of this complex free energy, we simplify by transforming into the eigenbasis of the Hessian. This reduces the computation of principal curvatures to second derivatives with respect to the second and third principal axes, which preserves computational efficiency.To incorporate realistic boundary behavior, the lattice-matching model is used to calculate boundary energy for arbitrary orientations, on-the-fly. Simulations are conducted for microstructure evolution in a real-space implementation using adaptive mesh refinement. Finally, we propose a continuum understanding of GB motion as a shear transformation goverened by compatibility. Optimal boundary transformations are

determined using a systematic process for shear identification, and by computing the minimum energy barrier for each. Such transformations typically require an atomic “shuffle” meaning that they atoms do not transform in the Cauchy-Born sense. The resulting optimal transformation can then be incorporated at the mesoscale by modeling the elastic energy as a multiwell potential. This provides a continuum context for understanding disconnections and faceted boundary migration.

(Thu. Nov 1, 2018 2:00 PM - 3:30 PM Room7)

[SY-I11] A Machine Learning Exploration of Grain Boundary Mobility Mechanisms

Invited

Leila Khalili[1], Eric R Homer[2], ○Srikanth Patala[1] (1.North Carolina State University, United States of America, 2.Brigham Young University, United States of America)

The mobility of grain boundaries plays an important role in governing the kinetics of microstructural evolution in every class of polycrystalline materials. Of particular interest is the role of bicrystallography, characterized by the macroscopic crystallographic degrees of freedom, on the underlying atomistic mechanisms governing grain boundary mobility. In this talk, I will present an algorithm to automatically identify such mechanisms that give rise to mobility of an interface. We use machine-learning methods, inspired by recent work in disordered solids, to correlate local structure with the susceptibility for rearrangement of grain boundary atoms. We show that it is possible to automatically identify mobility mechanisms of grain boundaries with a diverse range of crystallographic character.

Symposium | I. Multiscale Modeling of Grain Boundary Dynamics, Grain Growth and Polycrystal Plasticity

[SY-I12] Symposium I-12

Chairs: Blas Pedro Uberuaga(Los Alamos National Laboratory, United States of America), Chris P Race(University of Manchester, UK)

Thu. Nov 1, 2018 4:00 PM - 5:15 PM Room7

[SY-I12] Formation and shrinkage of grain boundary loops in two-dimensional colloidal crystals

Francois Lavergne, Arran Curran, Dirk Aarts, ○Roel Dullens （University of Oxford, UK）

[SY-I12] Growth and characterization of two-dimensional poly(quasi)crystals

○Petri Hirvonen[1], Gabriel Martine La Boissonière[2], Zheyong Fan[1], Cristian Achim[3], Nikolas Provatas[4], Ken R. Elder[5], Tapio Ala-Nissila[1,6] （1.Dept. of Applied Physics, Aalto Univ., Finland, 2.Dept. of Mathematics and Statistics, McGill Univ., Canada, 3.Dept. of Chemical Engineering, Univ. of Concepción, Chile, 4.Dept. of Physics, McGill Univ., Canada, 5.Dept. of Physics, Oakland Univ., United States of America）

[SY-I12] A Parallel Algorithm for High Resolution 3D Phase Field Simulations of Polycrystalline Solidification

○Pavel Strachota, Aleš Wodecki （Czech Technical University in Prague, Czech Republic）

[SY-I12] Properties of β/ω phase interfaces in Ti and their implications on mechanical properties and ω morphology

○Shuo Cao[1], Qing-Miao Hu[1], Rui Yang[1], Yong Jiang[2] （1.Institute of Metal Research, Chinese Academy of Science , China, 2.Central South University, China）

(Thu. Nov 1, 2018 4:00 PM - 5:15 PM Room7)

[SY-I12] Formation and shrinkage of grain boundary loops in two-dimensional colloidal crystals

Invited

Francois Lavergne, Arran Curran, Dirk Aarts, ○Roel Dullens （University of Oxford, UK）

Understanding the dynamics of grain boundaries in polycrystalline metals and alloys is crucial to enable tuning their mechanical properties. From an experimental point of view, grain boundaries in colloidal crystals are convenient model systems since imaging their dynamics requires only simple optical microscopy and they can be manipulated using optical tweezers. The formation and kinetics of grain boundaries are closely related to the topological constraints imposed on their complex dislocation structure. As such, loop-shaped grain boundaries are unique structures to establish such a link because their overall topological “charge” is zero due to their null net Burgers vector.
Here, we study the formation and shrinkage of such grain boundary loops by creating them on demand via a local rotational deformation of a two-dimensional colloidal crystal using an optical vortex. In particular, we observe that a grain boundary loop only forms if the product of its radius and misorientation exceeds a critical value. In this case, the deformation is plastic and the grain boundary loop spontaneously shrinks at a rate that solely depends on this product while otherwise, the deformation is elastically restored. We show that this elastic-to-plastic crossover is a direct consequence of the unique dislocation structure of grain boundary loops. Our results thus reveal a new general limit on the formation of grain boundary loops in two-dimensional crystals and elucidate the central role of defects in both the onset of plasticity and the kinetics of grain boundaries.

(Thu. Nov 1, 2018 4:00 PM - 5:15 PM Room7)

[SY-I12] Growth and characterization of two-dimensional poly(quasi)crystals

○Petri Hirvonen[1], Gabriel Martine La Boissonière[2], Zheyong Fan[1], Cristian Achim[3], Nikolas Provatas[4], Ken R. Elder[5], Tapio Ala-Nissila[1,6] （1.Dept. of Applied Physics, Aalto Univ., Finland, 2.Dept. of Mathematics and Statistics, McGill Univ., Canada, 3.Dept. of Chemical Engineering, Univ. of Concepción, Chile, 4.Dept. of Physics, McGill Univ., Canada, 5.Dept. of Physics, Oakland Univ., United States of America）

We use a simple two-mode phase field crystal (PFC) model to simulate grain growth in realistic two-dimensional model systems of square and hexagonal, as well as of 10- and 12-fold symmetric quasicrystal lattice symmetries. Modeling the evolution of poly(quasi)crystals had remained a challenge until the arrival of PFC, giving access to long diffusive time scales. We characterize the model systems using a powerful new method for segmenting and analyzing grain structures. This method generalizes effortlessly to all lattice types of even-fold rotational symmetry. To our knowledge, our characterization method is the first of its kind so far for quasicrystals.

The grain structure segmentations produced by the characterization method are found to agree very well with the corresponding human-made segmentations. We observe power-law scaling of the average grain size as a function of the simulation time, and log-normal grain size distributions for all lattice types considered. Similarly, irrespective of the lattice type, grain misorientation distributions appear remarkably flat, indicative of little correlation in the lattice orientations between neighboring grains. Average number of neighboring

grains is between 5 and 6. We are currently working on improving our statistics to cut down the error margins and to verify or to refute the universality of these, and of further related, distributions.

(Thu. Nov 1, 2018 4:00 PM - 5:15 PM Room7)

[SY-I12] A Parallel Algorithm for High Resolution 3D Phase Field Simulations of Polycrystalline Solidification

○Pavel Strachota, Aleš Wodecki （Czech Technical University in Prague, Czech Republic）

We deal with numerical solution of a three-dimensional phase field model of solidification in single component anisotropic materials. In this contribution, we extend the model by crystal orientation transformation. A robust algorithm is then developed to simulate the growth of multiple grains with an arbitrary number of random crystallographic orientations and a fully resolved 3D dendritic geometry. In the first part, the model and the hybrid parallel implementation of the algorithms are explained. The second part is devoted to demonstrating the effect of mesh-related numerical anisotropy, investigation of the parallel efficiency, and the simulations of complex polycrystalline solidification on very fine meshes.

(Thu. Nov 1, 2018 4:00 PM - 5:15 PM Room7)

[SY-I12] Properties of β/ω phase interfaces in Ti and their implications on mechanical properties and ω morphology

○Shuo Cao[1], Qing-Miao Hu[1], Rui Yang[1], Yong Jiang[2] （1.Institute of Metal Research, Chinese Academy of Science , China, 2.Central South University, China）

The ω phase strengthens β-Ti alloys effectively as a precipitate phase but decreases the plasticity with increasing size dramatically. To understand the strengthening and embrittlement mechanism of ω phase in the β-Ti alloys, the property of the β/ω interface is demanded. In this regard, we calculated the interface energies (γ_{int}), cleavage energies (γ_{cl}), and generalized stacking faults energy surfaces of the β/ω interfaces with different orientations using a first-principles method based on density functional theory. The results indicate that the strong anisotropy of the interface energy explains the ellipsoid morphology of the ω phase with its major axis parallel to the $<111>_{\beta}$ direction. The calculated cleavage energies and unstable stacking fault energies γ_{us} are determined. By comparing the γ_{cl}/γ_{us} ratio of both interfaces and those of the bulk ω and β phases, we conclude that the interfaces are prone to crack initiation than the bulk and contribute to the ω-embrittlement of the β-Ti alloy.

Symposium | D. Data-Driven and Physics-Informed Materials Discovery and Design

[SY-D1] Symposium D-1

Chair: Daniel Urban(Fraunhofer IWM, Germany)

Thu. Nov 1, 2018 9:45 AM - 11:00 AM Room8

[SY-D1] **Data-Driven Discovery of new materials**

○Isao Tanaka （Dept. Materials Science and Engineering, Kyoto Univ. , Japan）

[SY-D1] Machine Learning and Materials Discovery*

○Gus Hart （Brigham Young University, United States of America）

[SY-D1] Data-Driven Materials Design in an Industrial Environment

○Thomas Eckl, Lothar Kunz, Benedikt Ziebarth （Robert Bosch GmbH, Germany）

(Thu. Nov 1, 2018 9:45 AM - 11:00 AM Room8)

[SY-D1] Data-Driven Discovery of new materials

Invited

○Isao Tanaka （Dept. Materials Science and Engineering, Kyoto Univ. , Japan）

Challenges for accelerated discovery of materials with the aid of data science have been well demonstrated. One of the approaches uses materials database generated by density functional theory (DFT) calculations. A large number of DFT calculations with the accuracy comparable to experiments can be used for high throughput screening (real screening). Another approach called virtual screening uses machine-learning technique to select predictors for making a model to estimate the target property. The whole library can then be screened. Verification process is generally required to examine the predictive power of the model. Models and the quality of the screening can be improved iteratively through Bayesian optimization. The virtual screening is useful when real screening based upon the DFT data is not practical, i.e. when the computational cost for the descriptors is too high to cover the whole library within the practical time frame. This is the same if one needs to explore too large space to cover exhaustively. Discovery of new low lattice thermal conductivity crystals can be shown as an example of the application of the virtual screening technique [1]. Another approach relies only on inorganic crystal structure database (ICSD) that collects literature data obtained mostly by experiments. We have demonstrated that matrix- and tensor-based recommender systems are very powerful for discovery of currently unknown chemically relevant compositions (CRCs) of inorganic compounds from vast candidates [2]. A Tucker decomposition recommender system shows the best discovery rate of CRCs. For ternary and quaternary compositions, approximately 60 and 50 of the top 100 recommended compositions are found to be CRCs, respectively. The high discovery rate with neither DFT database nor other prior physical/chemical knowledge should be noteworthy.

[1] A. Seko et al, *Phys. Rev. Lett.* 115, 205901 **(2015)**.

[2] A. Seko et al, *Phys. Rev. Mater.* 2, 013805 **(2018)**.

(Thu. Nov 1, 2018 9:45 AM - 11:00 AM Room8)

[SY-D1] Machine Learning and Materials Discovery*

Invited

○Gus Hart （Brigham Young University, United States of America）

The relative accuracy and speed of density functional calculations have transformed computational materials science and enabled the creation of large databases of computed materials properties. But true "materials by design" or in-silico materials discovery has not yet been realized, though there are isolated success stories. It seems likely that into make computational discovery of new materials possible, or to discover materials engineering routes to improve already-deployed materials, a brute force approach will not be practical---some other paradigm will be required. Machine learning, so successful in some other application areas, is an intriguing and promising idea, but there are hurdles to overcome. There are two important differences between the standard machine learning problems of image recognition, voice recognition, etc., and materials prediction. In the first instance, we cannot afford the typical accuracy tradeoff---materials predictions are not useful without meeting a high accuracy target; the energy difference of competing phases is often very small, requiring high fidelity in the models. The second difference is the amount of training data---we don't have

"big data". How do we move forward? In this talk I will review the state of the art in this emerging discipline and show some results from BYU's Materials Simulation Group efforts in this area.

*This work is supported by ONR (MURI N00014-13-1-0635).

(Thu. Nov 1, 2018 9:45 AM - 11:00 AM Room8)

[SY-D1] Data-Driven Materials Design in an Industrial Environment

○Thomas Eckl, Lothar Kunz, Benedikt Ziebarth （Robert Bosch GmbH, Germany）

We will present how a combination of an automated simulation workflow, including high-throughput DFT calculations, textmining, utilization of available data bases and machine learning can be used to design tailored materials with respect to cost efficiency and performance. We will discuss the necessary requirements from an industrial perspective and show first results in the field of battery materials and permanent magnets for electric engines. Possible extensions to go beyond the atomistic description and include the microstructure of materials are also briefly discussed.

Symposium | D. Data-Driven and Physics-Informed Materials Discovery and Design

[SY-D2] Symposium D-2

Chair: Tilmann Hickel(MPIE, Germany)

Thu. Nov 1, 2018 11:15 AM - 12:30 PM Room8

[SY-D2] Using Machine-Learning to Create Predictive Material Property Models

○Chris Wolverton （Northwestern University, United States of America）

[SY-D2] Designing mesoscale structures of Li-ion battery electrode using FIB-SEM image via machine learning

○Yoichi Takagishi, Tatsuya Yamaue （Kobelco Research Institute Inc., Japan）

[SY-D2] **Stability Engineering of Halide Perovskite via Machine Learning**

○Wan-Jian YIN, Wanjian YIN （Soochow University, China）

[SY-D2] Systematic evaluation of ionization potentials of divalent cation binary oxides

○Yoyo Hinuma[1,2,3], Hiroyuki Hayashi[2,3], Yu Kumagai[4], Isao Tanaka[2,3], Fumiyasu Oba[2,5] （1.Center for Frontier Science, Chiba Univ., Japan, 2.Center for Materials Research by Information Integration, National Institute for Materials Science, Japan, 3.Department of Materials Science and Engineering, Kyoto Univ., Japan, 4.Materials Research Center for Element Strategy, Tokyo Institute of Technology, Japan, 5.Laboratory for Materials and Structures, Institute of Innovative Research, Tokyo Institute of Technology, Japan）

(Thu. Nov 1, 2018 11:15 AM - 12:30 PM Room8)

[SY-D2] Using Machine-Learning to Create Predictive Material Property Models

Invited

○Chris Wolverton （Northwestern University, United States of America）

Rational, data-driven materials discovery has the potential to make research and development efforts far faster and cheaper. In such a paradigm, computer models trained to find patterns in massive chemical datasets would rapidly scan compositions and systematically identify attractive candidates. Here, we present several examples of our work on developing machine learning (ML) methods capable of creating predictive models using a diverse range of materials data. As input training data, we demonstrate ML on both large computational datasets of DFT calculations, as implemented in the Open Quantum Materials Database (oqmd.org), and also experimental databases of materials properties. We construct ML models using a large and chemically diverse list of attributes, which we demonstrate can be used as an effective tool to automatically learn intuitive design rules, predict diverse properties of crystalline and amorphous materials, such as formation energy, specific volume, band gap energy, and glass-forming ability, and accelerate combinatorial searches.

(Thu. Nov 1, 2018 11:15 AM - 12:30 PM Room8)

[SY-D2] Designing mesoscale structures of Li-ion battery electrode using FIB-SEM image via machine learning

○Yoichi Takagishi, Tatsuya Yamaue （Kobelco Research Institute Inc., Japan）

Optimizations of the mesoscale structure of Li-ion battery electrode have been demonstrated by using the advanced simulation method by single 2D slice image (Quasi-3D modeling) and machine learning. The mathematical model is based on the electrochemistry and physics model[1)], and developed in order to calculate Li/Li+ concentration on the 2D plane, in consideration of virtual 3D structure. In this study, we firstly confirm the validity of the Quasi-3D model, and secondly optimize the electrode structure in mesoscale using Bayesian optimization, a method of machine learning.

In order to confirm the validity of our proposed model, full 3D discharge simulations with random packed active material particles have been performed and compared. By use of an appropriate value of “ connection factor”, quasi-3D model reproduce well a sliced Li/Li+ concentration calculated by the full 3D model in charge/discharge process, in addition that this model makes it possible to reduce computation time dramatically. Next, we have carried out optimizations of the mesoscale structure of the positive electrode $Li(Ni_{1/3}Mn_{1/3}Co_{1/3})O_2$ based on the actual FIB-SEM image via Bayesian optimization. As a result, statistical parameters of the optimized meso-scale structures, including the dispersion of active material size and location, remarkably differ depending on the objective functions for high rate charge/discharge performance or for long cycle performance.

1) M.Doyle et al. J. Electrochem.Soc. 1996, Vol.143, No.6, p.1890

(Thu. Nov 1, 2018 11:15 AM - 12:30 PM Room8)

[SY-D2] Stability Engineering of Halide Perovskite via Machine Learning

○Wan-Jian YIN, Wanjian YIN （Soochow University, China）

Perovskite stability is of the core importance and difficulty in current research and application of perovskite solar cells. Nevertheless, over the past century, the formability and stability of perovskite still relied on simplified factor based on human knowledge, such as the commonly used tolerance factor *t*. Combining machine learning with first-principles density functional calculations, we proposed a strategy to firstly calculate the decomposition energies, considered to be closely related to thermodynamic stability, of 354 kinds halide perovskites, establish the machine learning relationship between decomposition energy and compositional ionic radius and investigate the stability of 14190 halide double perovskites. The ML-predicted results lead us to rediscover a series of stable rare earth metal halide perovskites (up to ~10^3 kinds), indicating the generalization of this model and further provide elemental and concentration suggestion for improving the stability of mixed perovskite.

(Thu. Nov 1, 2018 11:15 AM - 12:30 PM Room8)

[SY-D2] Systematic evaluation of ionization potentials of divalent cation binary oxides

○Yoyo Hinuma[1,2,3], Hiroyuki Hayashi[2,3], Yu Kumagai[4], Isao Tanaka[2,3], Fumiyasu Oba[2,5] （1.Center for Frontier Science, Chiba Univ., Japan, 2.Center for Materials Research by Information Integration, National Institute for Materials Science, Japan, 3.Department of Materials Science and Engineering, Kyoto Univ., Japan, 4.Materials Research Center for Element Strategy, Tokyo Institute of Technology, Japan, 5.Laboratory for Materials and Structures, Institute of Innovative Research, Tokyo Institute of Technology, Japan）

Finding materials with suitable surface properties is unarguably important for applications including (photo)catalysis and crystal growth. Modeling of surface properties requires identification of surfaces that a given material will preferentially adopt. In a data-driven materials discovery and design approach, reasonable models of surfaces with various orientations and terminations must be obtained with minimum human intervention. Moreover, the surface energy as well as any relevant surface property, such as the ionization potential (IP), needs to be calculated systematically and results have to be stored in a database. Ultimately, reducing the number of costly first-principles calculations is desirable by using regression or some other means to estimate a certain surface property and eliminate sampling of the search space that is highly likely to have an unfavorable surface probability.

In this presentation we use first-principles calculations to systematically investigate the IPs of divalent cation binary oxides. The algorithm to make nonpolar and stoichiometric slab-and-vacuum models by Hinuma *et al.* [1] is used to construct such models. Identification of the drivers that affect the IP, which is a fundamental surface property, will be discussed. The insight obtained from this study would assist the search of descriptors that determine surface properties.

[1] Y. Hinuma, Y. Kumagai, F. Oba, I. Tanaka. Comp. Mater. Sci. **113**, 221 (2016).

Symposium | D. Data-Driven and Physics-Informed Materials Discovery and Design

[SY-D3] Symposium D-3

Chair: Daryl Chrzan(UC Berkeley, USA)

Thu. Nov 1, 2018 2:00 PM - 3:30 PM Room8

[SY-D3] Finding the needle in the haystack: Materials discovery through high-throughput ab initio computing and data mining

○Geoffroy Hautier （Universite catholique de Louvain, Belgium）

[SY-D3] High-entropy alloys investigation using machine-learned potentials

○Tatiana Kostiuchenko, Alexander Shapeev （Dept. of Material Science and Engeneering , Skolkovo Institute of Science and Technology, Moscow, Russia）

[SY-D3] Stability evaluation of high-entropy alloys via accurate on-lattice model

○Evgenii Meshkov[1], Ivan Novoselov[1], Alexander Shapeev[2], Alexey Yanilkin[1] （1.All-Russian Research Institute of Automatics (VNIIA), Russia, 2.Skolkovo Institute of Science and Technology, Russia）

[SY-D3] Atomistically informed atomic mobility databases for continuum diffusion simulations

○Katrin Abrahams[1], Daniel Gaertner[2], Maximilian Grabowski[3], Irina Roslyakova[1], Oleg Shchyglo[1], Sergiy V. Divinski[2], Ingo Steinbach[1] （1.Scalebridging Thermodynamic and Kinetic Simulation (ICAMS), Ruhr-University Bochum, Germany, 2.Institute of Materials Physics, University of Münster, Germany, 3.Atomistic Modelling and Simulation (ICAMS), Ruhr-University Bochum, Germany）

[SY-D3] The European Materials Modelling Council: standardization, interoperability and data management tools for materials modelling

○Luca Bergamasco[1], Emanuele Ghedini[2], Gerhard Goldbeck[3], Eliodoro Chiavazzo[1], Pietro Asinari[1] （1.Politecnico di Torino, Italy, 2.Università di Bologna, Italy, 3.Goldbeck Consulting Ltd, UK）

(Thu. Nov 1, 2018 2:00 PM - 3:30 PM Room8)

[SY-D3] Finding the needle in the haystack: Materials discovery through high-throughput ab initio computing and data mining

Invited

○Geoffroy Hautier （Universite catholique de Louvain, Belgium）

Essential materials properties can now be assessed through ab initio methods. When coupled with the exponential rise in computational power, this predictive power provides an opportunity for large-scale computational searches for new materials. We can now screen thousands of materials by their computed properties even before the experiments. This computational paradigm allows experimentalists to focus on the most promising candidates, and enable researchers to efficiently and rapidly explores new chemical spaces.

In this talk, I will present the challenges as well as opportunities in materials discovery in high-throughput ab initio computing using examples from transparent conducting materials. I will especially highlight computational predictions which have been followed by experimental synthesis and characterization. In addition to allowing the ability to navigate through a large volume of materials data to identify promising compounds, high-throughput computing also offers unprecedented data mining opportunities to detect new relationships between chemistry, structures, and properties. I will illustrate examples of these relationships through our recent work in crystal structure descriptors and automatic local environment identification, which merge traditional solid-state chemistry and materials science concepts through modern informatics.

The impact of high-throughput computing is multiplied when the generated data is shared with free and easy access. I will finish my talk by presenting the Materials Project (http://www.materialproject.org), a collaborative project which precisely targets such a data dissemination.

(Thu. Nov 1, 2018 2:00 PM - 3:30 PM Room8)

[SY-D3] High-entropy alloys investigation using machine-learned potentials

○Tatiana Kostiuchenko, Alexander Shapeev （Dept. of Material Science and Engeneering , Skolkovo Institute of Science and Technology, Moscow, Russia）

High-entropy alloys (HEAs) are a class of materials promising for their potential durability and high heat-resistance. HEAs are defined as alloys consisting of at least four different components that form single-phase solid solutions due to high entropy of mixing.

It is rather difficult to find which components would form a HEA since solid solutions alloys tend to split into binary or mono-atomic alloys at low temperatures and can form metallic glasses at high temperatures. This makes it difficult to experimentally investigate HEAs. Hence there is a need in computational approaches to the design of HEAs.

In this work we propose a computational framework for predicting the temperature of the order-disorder (i.e., intermetallic-solid solution) transition for HEAs. We first construct a very computationally efficient machine-learning on-lattice model of interatomic interaction (an alternative to the cluster expansion model) [Shapeev A., 2017]. The model parameters are fitted to quantum-mechanical (DFT) data with accuracy of about

1meV/atom. Then we perform canonical Monte-Carlo simulations for b.c.c. (body-centered cubic), h.c.p. (hexagonal close-packed) and f.c.c. (face-centered cubic) lattices. We validate our results against the published works [Körmann F. et al, 2017][Huhn W.P. et al, 2013][Fernández-Caballero A. et al, 2017]. Particular approach in atomistic simulations significantly reduces calculation time, enables to increase explored atomic configurations range and preserves the accuracy level in comparison with *ab initio* calculations. In the case of successful development of the method of constructing phase diagrams using machine learning, human labor can be excluded from the routine process of studying phase diagrams. This will also reduce the computational costs consumed by conventional calculations from the first principles.

(Thu. Nov 1, 2018 2:00 PM - 3:30 PM Room8)

[SY-D3] Stability evaluation of high-entropy alloys via accurate on-lattice model

○Evgenii Meshkov[1], Ivan Novoselov[1], Alexander Shapeev[2], Alexey Yanilkin[1] （1.All-Russian Research Institute of Automatics (VNIIA), Russia, 2.Skolkovo Institute of Science and Technology, Russia）

High-entropy alloys (HEA) are a new promising class of metallic materials. Some of them demonstrate excellent mechanical properties at elevated temperatures, outstanding corrosion resistance, and high radiation tolerance. However, atomistic modeling of HEAs is hindered by their high chemical diversity. A novel approach is required to perform accurate and computationally feasible atomic-scale description of HEA.

In our approach, energy of the system is represented as a sum of contributions of local atomic environments. These contributions are parameterized by low-rank multidimensional tensors in order to reproduce DFT results [1]. This model is then embedded into kinetic Monte-Carlo to perform large-scale simulations. This approach gives an accurate description of alloys with a large number of elements.

We employ the proposed approach to evaluate thermodynamic stability of several multicomponent alloys, and to search for new single-phase compositions.
[1] Shapeev, A. (2017) Computational Materials Science, 139, 26-30

(Thu. Nov 1, 2018 2:00 PM - 3:30 PM Room8)

[SY-D3] Atomistically informed atomic mobility databases for continuum diffusion simulations

○Katrin Abrahams[1], Daniel Gaertner[2], Maximilian Grabowski[3], Irina Roslyakova[1], Oleg Shchyglo[1], Sergiy V. Divinski[2], Ingo Steinbach[1] （1.Scalebridging Thermodynamic and Kinetic Simulation (ICAMS), Ruhr-University Bochum, Germany, 2.Institute of Materials Physics, University of Münster, Germany, 3.Atomistic Modelling and Simulation (ICAMS), Ruhr-University Bochum, Germany）

Diffusion is a key aspect for microstructural evolution and has to be solved in full-field models like the phase-field model. Many phase transformations are diffusion controlled that their kinetics depend crucially on mobilities of the diffusing elements as well as their thermodynamic factor. Both parameters, the Gibbs energies and the atomic mobilities are temperature, composition and pressure dependent. Parameters

representing these dependencies are stored in CALPHAD (CALculated PHAse Diagrams) type databases.

In this talk a new approach for the assessment of the temperature and composition dependence of the atomic mobility data using atomistic and experimental data is presented. The new model takes into account the physical meaning of three parameters on the basis of a mono-vacancy diffusion mechanism: the frequency factor, the vacancy formation energy and the migration energy. The temperature dependence is given by an Arrhenius equation, where the activation energy consists of the migration energy and the vacancy formation energy. The temperature dependence of both parameters is investigated using Kinetic Monte Carlo simulations. This information is used to deduce a general description of the temperature dependence of the activation energy based on these parameters. Additionally, the composition dependence of the pre-exponential factor and the activation energy is investigated separately using experimentally determined self-diffusion coefficients obtained from the tracer method and calculated self-diffusion coefficients based on kinetic Monte-Carlo simulations.

(Thu. Nov 1, 2018 2:00 PM - 3:30 PM Room8)

[SY-D3] The European Materials Modelling Council: standardization, interoperability and data management tools for materials modelling

○Luca Bergamasco[1], Emanuele Ghedini[2], Gerhard Goldbeck[3], Eliodoro Chiavazzo[1], Pietro Asinari[1]
（1.Politecnico di Torino, Italy, 2.Università di Bologna, Italy, 3.Goldbeck Consulting Ltd, UK）

The European Materials Modelling Council (EMMC) was established in 2014 as a new European network to coordinate and support the industrial uptake of materials modelling in Europe. The EMMC community consists of different types of stakeholders, namely: manufacturers (industrial end-users); software owners (academic and commercial software providers); Translators (skilled professionals able to translate industrial problems into modeling activities) and academic model developers (of electronic, atomistic, mesoscopic and continuum models). The main EMMC objectives are: to enhance the interaction and collaboration between all stakeholders; to identify materials model gaps in industry and to steer model development; to build strong foundations to ease model interoperability, integration and data management; to promote modelling in industry based on beneficial economic arguments. These activities rely on wide stakeholder consultation, with the ultimate goal to integrate materials modelling into the product life-cycle management, enhancing innovation and global competitiveness.

The aim of this talk is to present the EMMC activities, with particular regards to those related to standardization, interoperability and data management strategies for materials modelling. First, the Review of Materials Modelling (RoMM), edited by the European Commission, will be presented as the reference document for standardization. Based on this preamble, the CEN Workshop Agreement (CWA) for materials modelling terminology, the Modelling Data (MODA) sheets to document modelling in standard form, and the European Materials Modelling Ontology (EMMO) will be presented. Particular emphasis will be given to the discussion of physics-based vs data-based modelling approaches, showing how they fit into the abovementioned tools. Available results on the data-management regulation will be also shown and discussed. Finally, an outlook on how this framework will help materials discovery and design will be given.

This project has received funding from the EU H2020 project EMMC-CSA H2020-NMPB-2016-2017 GA n.

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Symposium | D. Data-Driven and Physics-Informed Materials Discovery and Design

[SY-D4] Symposium D-4

Chair: Minoru Otani(AIST, Japan)

Thu. Nov 1, 2018 4:00 PM - 5:30 PM Room8

[SY-D4] Exploration of large ab initio data spaces to design structural materials with superior mechanical properties

○Joerg Neugebauer, Jan Janssen, Tilmann Hickel, Blazej Gabowski （Max-Planck-Institut fuer Eisenforschung, Germany）

[SY-D4] Toward a machine learning aided interatomic potential for multi-element alloys: Application to binary compounds

○Doyl Dickel, David Francis, Christopher Barrett （Mississippi State University, United States of America）

[SY-D4] **Machine Learning potentials for modeling iradiation defects in iron and tungsten**

○Alexandra Goryaeva[1], Jean-Bernard Maillet[2], Mihai-Cosmin Marinica[1] （1.DEN-Service de Recherches de Métallurgie Physique, CEA, Université Paris-Saclay, 91191 Gif-sur-Yvette, France, 2.CEA-DAM DIF, 91297 Arpajon Cedex, France）

[SY-D4] Effect of friction and ductility on relaxation dynamics and mechanical memory of crumpled materials

○Mehdi Habibi, Eric van Bruggen （Wageningen University, Netherlands）

[SY-D4] Big-data insights into solute-GB segregation

○Liam Huber, Blazej Grabowski, Joerg Neugebauer （MPIE, Germany）

(Thu. Nov 1, 2018 4:00 PM - 5:30 PM Room8)

[SY-D4] Exploration of large ab initio data spaces to design structural materials with superior mechanical properties

Invited

○Joerg Neugebauer, Jan Janssen, Tilmann Hickel, Blazej Gabowski （Max-Planck-Institut fuer Eisenforschung, Germany）

Modern engineering materials have evolved from simple single phase materials to nano-composites that employ dynamic mechanisms down to the atomistic scale. The structural and thermodynamic complexity of this new generation of structural materials presents a challenge to their design since experimental trial-and-error approaches as successfully used in the past are often no longer feasible. Ab initio approaches provide perfect tools to new design routes but face serious challenges: Finite temperature free energies of the various phases are almost degenerate, requiring advanced theoretical formalisms that accurately capture all relevant entropic contributions. In addition, their hierarchical nature with respect to length and time makes it challenging to explore the large range of chemical compositions. We have therefore developed a python based framework *pyiron* that allows in a highly automated way to combine accurate finite temperature first principles calculations with big data analytics. The flexibility and the predictive power of these automated approaches will be discussed for examples ranging from the design of ductile Mg alloys to the discovery of general rules for interstitials in metals.

(Thu. Nov 1, 2018 4:00 PM - 5:30 PM Room8)

[SY-D4] Toward a machine learning aided interatomic potential for multi-element alloys: Application to binary compounds

○Doyl Dickel, David Francis, Christopher Barrett （Mississippi State University, United States of America）

As the chemical complexity of novel material systems continues to increase, the need for the rapid development of predictive, scalable interatomic potentials has grown as well. Machine learning, neural networks, and other data-driven techniques has shown promise in condensing large amounts of data from first principles and density functional theory calculation into classical dynamical equations with linear scaling, making them ideal for molecular dynamics simulation. A formalism for the development of a multi-species interatomic potential is presented and applied to binary metals. The resulting potential is then analyzed in terms of predictive power, validity, performance, and development time.

(Thu. Nov 1, 2018 4:00 PM - 5:30 PM Room8)

[SY-D4] Machine Learning potentials for modeling iradiation defects in iron and tungsten

○Alexandra Goryaeva[1], Jean-Bernard Maillet[2], Mihai-Cosmin Marinica[1] （1.DEN-Service de Recherches de Métallurgie Physique, CEA, Université Paris-Saclay, 91191 Gif-sur-Yvette, France, 2.CEA-DAM DIF, 91297 Arpajon Cedex, France）

Prediction of condensed matter properties requires an accurate description of a material at the atomic scale. Ground state properties of a material are often described well within the Density Functional Theory (DFT) while studying irradiation-induced damage requires a length scale that is pushed beyond *ab initio* level of theory. Unachievable CPU cost of such calculations have fueled the search for alternatives, accounting for reasonable approximations, which has led to development of various empirical potentials, ranging from pairwise potentials to embedded atom model and tight binding. Although these potentials have been successful in making radiation damage feasible, inconsistency of the results from different potentials is a major shortcoming that hinders conclusive theoretical predictions for such important functional materials as Fe and W.

Here we present a new strategy to achieve machine learning interatomic potentials for metals that approach accuracy of DFT calculations and at the same time preserve a reasonable balance between precision and CPU cost. Targeting to model irradiation-induced defects and plasticity, the potentials are trained on the extensive DFT database that includes EOS, elastic deformation, planar defects (GSF), self-interstitial atoms (SIA), vacancies, and liquid state.
The new potentials for Fe and W are applied to investigate the complex energy landscape of defects under irradiation such as clusters of SIA. We aim to predict the relative stability of large SIA clusters up to nanometric-size, with a particular focus on to the relative stability of the conventional dislocation loops as well as the C15 clusters [1]. The present approach enables us to account for the effect of temperature [2]. Moreover, as a perspective development, the potential will be tested to reproduce high-pressure bcc-hcp transition in Fe.

[1] M.C. Marinica *et al.* (2012) *Phys Rev Lett* **108**, 025501

[2] T.D. Swinburne, M.C. Marinica (2018) *Phys Rev Lett* **120**, 135503

(Thu. Nov 1, 2018 4:00 PM - 5:30 PM Room8)

[SY-D4] Effect of friction and ductility on relaxation dynamics and mechanical memory of crumpled materials

○Mehdi Habibi, Eric van Bruggen （Wageningen University, Netherlands）

Crumpled structures are ubiquitous in nature and technology. They combine low-density structures with surprising mechanical strength and the
ability to absorb mechanical energy. This combination of properties opens doors
to use them as mechanical metamaterials for a variety of applications.
However, in order to rationally design metamaterials, a thorough physical understanding of their unique features is needed. One remarkable physical property observed in crumpled structures is their slow mechanical relaxation
and their ability to carry a long lasting memory of previous mechanical states.
We experimentally investigate the role of material properties (ductility and friction) on relaxation dynamics of crumpled sheets by
comparing relaxation curves of different materials. We show that relaxation rates are not only dependent on material’s elastoplastic properties, but also rely on friction and adhesion between surfaces.This is further explored by using a two-step compaction protocol, that allowed us to probe deeper into the material’s relaxation behavior. We study the material dependency of the non-monotonic aging in a crumpled ball.

We show the normalized height of the non-monotonic aging peak depends linearly on the time at which it arose with a slope that revealed a material property that seemed to be correlated with the material dependent relaxation constant.

(Thu. Nov 1, 2018 4:00 PM - 5:30 PM Room8)

[SY-D4] Big-data insights into solute-GB segregation

○Liam Huber, Blazej Grabowski, Joerg Neugebauer （MPIE, Germany）

Solute-grain boundary (GB) interaction plays a critical role in the evolution and stabilization of grain structure and thus strongly impacts final material properties. Due to the large number of possible grain boundary configurations, there are a many inequivalent sites solutes can be incorporated at. Combined with the fact that there are many possible segregating chemical species in modern alloys, concepts to derive general trends in segregation are still missing. Using classical molecular statics, we perform high-throughput calculations of 1.4 million segregation energies for six solutes to 38 different boundaries in Al. The size of this data set is sufficient to apply machine learning techniques for building predictive models capable of predicting segregation energy to new GBs. It also provides useful insights into trends in the atomistic mechanisms controlling segregation behaviour. We show that the resulting segregation energy distributions can be interpreted analogously to electronic density of states and provides a useful perspective to consider solute concentration enrichment at the GB and GB embrittlement.

Symposium | H. Multiscale Mechanics of Polymers, Soft Matter and Network Materials

[SY-H7] Symposium H-7

Chair: Patrick R. Onck(Univ. of Groningen, Netherlands)

Thu. Nov 1, 2018 9:45 AM - 11:00 AM Room9

[SY-H7] Computational modeling approach for the rational design of DNA nanostructures

○Do-Nyun Kim, Jae Young Lee, Jae Gyung Lee, Young-Joo Kim, Kyung Soo Kim, Chanseok Lee (Department of Mechanical and Aerospace Engineering, Seoul National University, Korea)

[SY-H7] Quantitative Multiscale Modelling of Bionano Interface

○Vladimir Lobaskin[1], Stefano Poggio[1], David Power[1], Hender Lopez[2] (1.School of Physics, University College Dublin, Ireland, 2.Institute Laue-Langevin, Grenoble, France)

[SY-H7] Multiscale modelling of intrinsically-disordered proteins

Ankur Mishra, Henry De Vries, Hamid Jafarinia, Erik Van der Giessen, ○Patrick R. Onck (University of Groningen, Netherlands)

[SY-H7] Tracing the interplay of polymer topology and hydrodynamics

○Lisa B. Weiss[1], Arash Nikoubashman[2], Christos N. Likos[1] (1.University of Vienna, Austria, 2.Johannes Gutenberg University Mainz, Germany)

(Thu. Nov 1, 2018 9:45 AM - 11:00 AM Room9)

[SY-H7] Computational modeling approach for the rational design of DNA nanostructures

Invited

○Do-Nyun Kim, Jae Young Lee, Jae Gyung Lee, Young-Joo Kim, Kyung Soo Kim, Chanseok Lee （Department of Mechanical and Aerospace Engineering, Seoul National University, Korea）

Structural DNA nanotechnology has recently been advanced significantly enabling the construction of nanometer-scale structures with controllable three-dimensional shapes and properties. While overall mechanical properties of single and double DNA helices have been relatively well characterized both experimentally and computationally, those of various DNA motifs essential to build a DNA bundle structure are still hardly known due to experimental limits despite their importance for the rational design of DNA nanostructures. In this presentation, we introduce our computational modeling approach to establishing an efficient design process in order to achieve fine control over the geometrical shape and mechanical properties of self-assembling DNA nanostructures. Molecular dynamics simulations are highly utilized to extract the unknown mechanical properties of local DNA motifs that are fed into a more coarse-grained DNA model built on the finite element method. Then, this finite-element-based model of DNA nanostructure is used to predict its three-dimensional shape and mechanical properties, which provides designers structural feedback as quick as possible offering a chance to revise the design before actual synthesis. We expect our multiscale analysis framework facilitates the rational design of DNA nanostructures with a target shape and mechanical (or other derived) properties with precision.

This work was supported by the National Research Foundation of Korea (NRF) grants funded by the Korea government (Ministry of Science and ICT) (NRF-2016R1C1B2011098, NRF-2017M3D1A1039422, and NRF-2014M3A6B3063711).

(Thu. Nov 1, 2018 9:45 AM - 11:00 AM Room9)

[SY-H7] Quantitative Multiscale Modelling of Bionano Interface

○Vladimir Lobaskin[1], Stefano Poggio[1], David Power[1], Hender Lopez[2] （1.School of Physics, University College Dublin, Ireland, 2.Institute Laue-Langevin, Grenoble, France）

In biomedical and food technologies, the functionality of the engineered materials and potential hazards are triggered and controlled by molecular-level interactions at the biointerface, a nanoscale layer where biological fluids meet the foreign substances. The main concerns are related but not limited to the emerging risks for human health. The questions of biocompatibility of materials arise naturally in respect to medical appliances such as stents, dental and cardiac implants, or prosthetic joints as they can cause immediate hazard upon introduction into the human body. These interactions are often non-specific and unintended. Quantitative understanding of biointerface structure is therefore crucial for achieving a better control over the surface activity biomaterials and reducing the associated health risks.

In this work, we propose a systematic multiscale bottom-up method to coarse-grain the interactions of foreign materials with biological fluids of arbitrary composition. Biomolecules (lipids, proteins and carbohydrates) are coarse-grained by mapping their main chemical fragments onto single beads, and their interaction with the substrate surface is characterised by potentials of mean force (PMF) from atomistic

simulations [1]. The substrate is represented by a two-layer model where the surface interacts with the molecule beads via those PMFs, while the core interacts with via van der Waals forces calculated using Lifshitz theory. The united-atom model for biomaterial-biomolecule segment interaction is used to evaluate the adsorption free energy of arbitrary biomolecules on a specified foreign surface. This mesoscale representation is used to build a united-block model, which can address competitive adsorption of entire proteins and lipids onto the adsorbent and predict the content of biomolecular corona.

The main outcome of our work is a framework for comparative characterisation of nano- and biomaterials in terms of descriptors of bionano interface such as protein binding affinity and content of the corona, which forms a basis for construction of nanoinformatic data-driven models for predicting material functionality.

Funding: EU H2020 grant SmartNanotox, contract 686098, EU H2020 project NanoCommons, contract 731032.

[1] H. Lopez, V. Lobaskin, J. Chem. Phys. 143, 243138 (2015)

(Thu. Nov 1, 2018 9:45 AM - 11:00 AM Room9)

[SY-H7] Multiscale modelling of intrinsically-disordered proteins

Ankur Mishra, Henry De Vries, Hamid Jafarinia, Erik Van der Giessen, ○Patrick R. Onck （University of Groningen, Netherlands）

Proteins are often called the work-horse molecules of life because they are involved in almost any structure and activity in living systems. It has long been thought that proteins inherit their function from the secondary and tertiary structure in which they are folded. However, more and more evidence is appearing that show that also unfolded, intrinsically-disordered proteins (IDPs) play an important biological role, in both health and disease. In this work we focus on two of these biological roles, i.e., (i) in mediating transport through the nuclear pore complex (NPC) and (ii) in the formation of pathological protein aggregates in neurodegenerative diseases. IDPs are long chains of amino acids with conformations that are primarily dictated by the non-covalent interactions between the individual amino acids. Due to the large size of the protein complexes of interest, high-resolution (all-atom) molecular-dynamics simulations are restricted to study only a few IDPs. Here, we use a coarse-grained, one-bead-per-amino-acid model that is fine enough to capture the exact amino-acid sequence, but coarse enough to account for the collective interaction of hundreds of IDPs. In this presentation, recent results are presented on the collective behavior of IDPs in forming the selective permeability barrier of the NPC and on the phase-separation of pathological IDPs in the neurodegenerative disease ALS. For both studies the relation between amino-acid sequence and collective/aggregation behavior will be emphasized and discussed.

(Thu. Nov 1, 2018 9:45 AM - 11:00 AM Room9)

[SY-H7] Tracing the interplay of polymer topology and hydrodynamics

○Lisa B. Weiss[1], Arash Nikoubashman[2], Christos N. Likos[1] （1.University of Vienna, Austria, 2.Johannes Gutenberg University Mainz, Germany）

Polymers exhibit a variety of topologies ranging from linear to cyclic and various knot types, which are of importance in biology, rheology and material science. Macromolecules of distinct topology consist of the same type and number of monomers making it challenging to separate them using chemical approaches. Nevertheless, topology influences strongly their response to flow fields in concentrated [1] and dilute solutions [2]. Exploiting these differences for future separation strategies requires a detailed understanding of the interplay of hydrodynamic interactions and topology. Due to the inherent separation of time scales of macromolecules and solvent, here the Multi-Particle Collision Dynamics algorithm is employed to couple an explicit coarse-grained solvent to polymers treated with Molecular Dynamics.
We investigated the transport of topologically-distinct polymers in microfluidic slit channels. We find that in bare channels and in dilute solutions there is only minor difference in the migration behavior, which is not sufficient for separation. In contrast, decorating the channel walls with attractive spots arranged on a track parallel to the flow results in a reliable and novel strategy for separation of linear and ring polymers that takes full advantage of the different topologies [3]. Those spots effectively capture and immobilize linear chains, while forcing ring polymers to change their preferred orientation close to the walls. In doing so, ring polymers are enabled to roll along the spots with a finite velocity. Furthermore, investigation of the migration in semi-dilute linear and ring polymer mixtures exhibits an astonishing difference. Finally, we extend our studies to knotted polymers to construct knot-sensitive filters.

References

[1] Kapnistos, M.; Lang, M.; Vlassopoulos, D.; Pyckhout-Hintzen, W.; Richter, D.; Cho, D.; Chang, T.; Rubinstein, M. Nat. Mater. 2008, 7, 997-1002.
[2] Hsiao, K.-W. W.; Schroeder, C. M.; Sing, C. E. Macromolecules 2016, 49, 1961-1971.
[3] Weiss, L. B.; Nikoubashman, A.; Likos, C. N. ACS Macro Letters 2017, 6, 1426-1431.

Symposium | H. Multiscale Mechanics of Polymers, Soft Matter and Network Materials

[SY-H8] Symposium H-8

Chair: Patrick R. Onck(Univ. of Groningen, Netherlands)

Thu. Nov 1, 2018 11:15 AM - 12:30 PM Room9

[SY-H8] Modeling and Simulation of DNA Foldback Intercoil Structure

○Moon Ki Kim, Byung Ho Lee, Soojin Jo （School of Mechanical Engineering, Sungkyunkwan University, Korea）

[SY-H8] DNA-particle vitrimer systems

○francesco sciortino （Sapienza Universita' di Roma, Italy）

[SY-H8] Relation between Macroscopic Flows in a Contraction-Expansion Channel and Dynamics of Well-Entangled Polymer Chains

○Takeshi Sato, Takashi Taniguchi （Dept. of Chemical Engineering, Kyoto Univ., Japan）

[SY-H8] Origin of large scale spatial organization of DNA-polymer in bacterial chromosomes.

○Apratim Chatterji[1], Tejal Agarwal[2], Manjunath G.P.[3], Farhat Habib[4] （1.IISER-Pune, India 411008, India, 2.IISER-Pune, India, 411008, India, 3.NYU, USA, United States of America, 4.Inmobi, Bangalore, India 560103., India）

(Thu. Nov 1, 2018 11:15 AM - 12:30 PM Room9)

[SY-H8] Modeling and Simulation of DNA Foldback Intercoil Structure

Invited

○Moon Ki Kim, Byung Ho Lee, Soojin Jo （School of Mechanical Engineering, Sungkyunkwan University, Korea）

The stem-loop foldback intercoil (FBI) DNA is one of unique four-stranded DNA structures. Its intercoil stem region is constructed by interwinding DNA duplexes in their major groove. Although the FBI DNA is closely related with DNA homologous recombination, inversion, and deletion process, its structural and dynamic characteristics have not been yet revealed. In this study, we create a 3D FBI computer model based on homologous and palindromic DNA base sequences and its structural validity is confirmed by a variety of topological comparison with B-DNA including its diameter and helicity such as 22 angstrom and 10.5 base pairs per turn, respectively. Then, its dynamic features are investigated by normal mode analysis (NMA). NMA results show that the stem part has more rigidity compared to the other parts during the major bending and twisting motions. It is also cross-validated by the AFM experiment in which the height different of stem part is apparently measured. In addition, the DNA homologous recombination phenomenon is observed by using molecular dynamics simulation (MD) in atomic details. MD results imply that homologous recombination of the DNA FBI structure is triggered by base flipping of the stem region resulting in B-Z DNA junctions at the interface between stem and loop. Consequently, this computational modelling and simulation study enables us to better understand both structural and biological features of the FBI DNA.

(Thu. Nov 1, 2018 11:15 AM - 12:30 PM Room9)

[SY-H8] DNA-particle vitrimer systems

○francesco sciortino （Sapienza Universita' di Roma, Italy）

Vitrimers are a new class of polymeric materials in which the network nodes, despite the covalent bonding, can change their bonded partners via reversible exchange reactions with unreacted sites. The ability to dynamically rearrange the network structure and the external control (for example, via temperature) of the rate of exchange opens up the possibility to spontaneously heal internal fractures, recycle the material shape, and release applied stresses.

Along the lines of using DNA as a material, we have proposed an innovative design of a vitrimer system entirely made of DNA sequences [1]. In this DNA gel, bonds can switch without breaking, providing a mechanism for changing the network structure under an external driving force, retaining at all times the same number of bonds. To implement the bond switching mechanism, we use toehold-mediated displacement, one of the basic processes underlying dynamic DNA nanotechnology.

Beside discussing how a DNA vitrimer can be designed in silico and in the lab, I will discuss some other examples of particle vitrimer systems[2] in which the bond-swithching dynamics is modeled numerically with a three-body potential[3]. Preliminay application of this method show how the self and collective dynamics of these particles sensitively depend on microscopic swaps. Finally, I will discuss the origin of the observed non-dispersive (in wavevector) collective relaxation mode[4].

[1]Flavio Romano and Francesco Sciortino
Switching Bonds in a DNA Gel: An All-DNA Vitrimer

Phys. Rev. Letts. 114, 078104 (2015)

[2] Lorenzo Rovigatti, Giovanni Nava, Tommaso Bellini and Francesco Sciortino
Self-Dynamics and Collective Swap-Driven Dynamics in a Particle Model for Vitrimers
Macromolecules, 51 ,1232-1241 (2018).

[3] Francesco Sciortino, *Three-body potential for simulating bond swaps in molecular dynamics*
Eur. Phys. J. E (2017) 40: 3 DOI 10.1140/epje/i2017-11496-5

[4] Giovanni Nava, Marina Rossi, Silvia Biffi, Francesco Sciortino, and Tommaso Bellini
Fluctuating Elasticity Mode in Transient Molecular Networks
Phys. Rev. Lett. 119, 078002 (2017).

(Thu. Nov 1, 2018 11:15 AM - 12:30 PM Room9)

[SY-H8] Relation between Macroscopic Flows in a Contraction-Expansion Channel and Dynamics of Well-Entangled Polymer Chains

○Takeshi Sato, Takashi Taniguchi （Dept. of Chemical Engineering, Kyoto Univ., Japan）

We have successfully applied a multiscale simulation (MSS) method [T. Murashima and T. Taniguchi, *Europhys. Lett.*, **96**, 18002 (2011)] to flows of a monodispersed linear entangled polymer melt in a contraction-expansion channel. In our MSS method, a macroscopic model based on the Lagrangian picture is coupled with a microscopic polymer model through the velocity gradient tensor and the stress tensor. The smoothed particle hydrodynamics (SPH) method is employed as the macroscopic model, and the slip-link model [M. Doi and J. Takimoto, *Phil. Trans. R. Soc. Lond A*, **361**, 641 (2003)] is employed as the microscopic model. Two-dimensional flows of a well-entangled polymer melt in a 4:1:4 contraction-expansion channel are examined using our MSS method. From our MSSs, we have investigated both macroscopic and microscopic information. As for the macroscopic information, we have focused on the spatial-dependent Weissenberg number (Wi). As for the microscopic information, we have evaluated the local orientation of polymer chains, the spatial distribution of the average number of entanglements and the number density of entanglements along a polymer chain. The states of the polymer chains are altered mainly in the region corresponding to Wi >1. In this region, we have confirmed that the polymer chains are strongly oriented, the average number of entanglements decreases and the number density of entanglements decreases in the center part on the polymer chain and has peaks near the tails. Furthermore, we have examined the number density of entanglements along a polymer chain in detail. From an analysis of the number density of entanglements, we have found that an effective advection and a hooking event play an important role in forming the number density of entanglements. Microscopic information obtained by our MSSs will provide us with new insights for the molecular design of a polymer chain.

(Thu. Nov 1, 2018 11:15 AM - 12:30 PM Room9)

[SY-H8] Origin of large scale spatial organization of DNA-polymer in

bacterial chromosomes.

○Apratim Chatterji[1], Tejal Agarwal[2], Manjunath G.P.[3], Farhat Habib[4] （1.IISER-Pune, India 411008, India, 2.IISER-Pune, India, 411008, India, 3.NYU, USA, United States of America, 4.Inmobi, Bangalore, India 560103., India）

Using data from contact maps of the DNA-polymer of bacteria E. Coli (at kilo base pair resolution) as an input to our model, we introduce cross-links between monomers in a bead-spring model of a flexible ring polymer at very specific points along the chain. By suitable Monte Carlo Simulations we show that the presence of these cross-links lead to a specific architecture and organization of the chain at large (micron) length scales of the DNA. We also investigate the structure of a ring polymer with an equal number of cross-links at random positions along the chain. We find that though the polymer does get organized at the large length scales, the nature of organization is quite different from the organization observed with cross links at specific biologically determined positions. We used the contact map of E. Coli bacteria which has around 4642 kilo base pairs in a single chromosome. In our coarse grained flexible ring polymer model we used 4642 monomer beads and observe that around 82 cross links are enough to induce large scale organization of the molecule accounting for statistical fluctuations induced by thermal energy. The length of a DNA chain of a even simple bacterial cell such as E. Coli is much longer than typical proteins, hence we avoided methods used to tackle protein folding problems. We define new suitable quantities to identify large scale structure of a polymer chain with a few cross-links. We have carried out similar studies with the DNA-bacteria of C.Crecentus with cross-links at specific points relevant to the DNA of C.Crecentus, and obtain identical conclusions. This assures us about the robustness of our results.

Published in :
1. Tejal Agarwal *et al J. Phys.: Condens. Matter* **30** 034003 (2018).
2. Tejal Agarwal, Tejal Agarwal *et al EPL* **121** 18004 (2018).

Symposium | H. Multiscale Mechanics of Polymers, Soft Matter and Network Materials

[SY-H9] Symposium H-9

Chair: Kees Storm(Eindhoven University of Technology, Netherlands)

Thu. Nov 1, 2018 2:00 PM - 3:30 PM Room9

[SY-H9] **Micromechanics and instabilities in soft composite materials**

○Stephan Rudykh （University of Wisconsin - Madison, United States of America）

[SY-H9] Deformation analysis of UV curing 3d printed materials by combined molecular dynamics-finite element method

Jiwon Jung, Chanwook Park, ○Gunjin Yun （Seoul National University, Korea）

[SY-H9] Modelling and 3D Printing Kelvin Cell Acoustic Metamaterial

○Huina MAO[1], Peter Göransson[1], John Kennedy[2], Henry Rice[2], Umberto Iemma[3] （1.Dept. of Aeronautical and Vehicle Engineering, KTH Royal Institute of Technology, Sweden, 2.Dept. of Mechanical and Manufacturing Engineering, Trinity College Dublin, Ireland, 3.Engineering Department, Roma Tre University, Italy）

[SY-H9] Theoretical approach for EUV resist fabrication: DFT-MD-FDM study

○Muyoung Kim[1], Junghwan Moon[1], Joonmyung Choi[3], Sungwoo Park[1], Byunghoon Lee[3], Changyoung Jeong[3], Maenghyo Cho[2,1] （1.Divison of Multiscale Mechanical Design, School of Mechanical and Aerospace Engineering, Seoul National University, Korea, 2.Institute of Advanced Machines and Design, Seoul National University, Korea, 3.SAMSUNG ELECTRONICS CO., LTD, Korea）

(Thu. Nov 1, 2018 2:00 PM - 3:30 PM Room9)

[SY-H9] Micromechanics and instabilities in soft composite materials

Invited

○Stephan Rudykh （University of Wisconsin - Madison, United States of America）

Soft microstructured materials enable modifications of material properties and functionalities through applied deformations, or other external stimuli, for example, electric, or magnetic fields [1]. The deformation induced tunability is mainly due to controllable changes of the microstructural arrangements, on par with material nonlinearities [2]. Moreover, the microstructures can be designed to be prone to elastic instabilities giving rise to dramatic microstructure transformations, and switchable functionalities such as cancelling certain frequency ranges of elastic waves (through induced band gaps). In the presentation, we will show our numerical and theoretical results for multiphase deformable composite materials including deformable layered materials, bio-inspired nacre-like structures [3], periodic 3D fibre composites, and periodically structured particulate materials. These numerical and theoretical results will be illustrated by the experimental observations on 3D printed multiphase composites subjected to finite deformations. Finally, the ways of material properties modifications via application of external magnetic and electric fields will be explored. In particular, magnetorheological elastomers (MRE) [1] and soft dielectric elastomers (DE) with periodic microstructures will be examined, and the coupled magneto- and electro-mechanical stability of these active architectured materials will be analysed.

References

[1] Goshkoderia, A., Rudykh, S. 2017. Stability of magnetoactive composites with periodic microstructures undergoing finite strains in the presence of a magnetic field. *Composites Part B* **128**: 19-29.

[2] Galich, P.I., Fang, N.X., Boyce, M.C., Rudykh, S. 2017. Elastic wave propagation in finitely deformed layered materials. *Journal of the Mechanics and Physics of Solids* **98**, 390-410.

[3] Slesarenko, V., Kazarinov, N., Rudykh, S. 2017. Distinct failure modes in bio-inspired 3D-printed staggered composites under non-aligned loading. *Smart Materials and Structures* **26**, 035053.

(Thu. Nov 1, 2018 2:00 PM - 3:30 PM Room9)

[SY-H9] Deformation analysis of UV curing 3d printed materials by combined molecular dynamics-finite element method

Jiwon Jung, Chanwook Park, ○Gunjin Yun （Seoul National University, Korea）

3d printing technology with UV cured polymer has been applied to diverse industrial areas since it has advantages of reducing time and costs for producing complex structures. Especially in aerospace industries where parts with complex geometries are needed, 3d printing is said to be a suitable manufacturing technique for such elaborate components. However, there has been little research on the polymerization-induced deformation such as microscopic porosity and cure shrinkage strain in the 3d printing technology to our knowledge.

In this work, molecular dynamics (MD) simulation is adopted for modeling UV induced polymerization process to derive cure shrinkage strain. Based on the finite element method, the strain of the polymer from MD simulation is then applied to the structure modeled by Abaqus software, to predict macroscopic deformation. This prediction methodology is verified with experiment results observed from deformation of 3d printed structures in reality.

(Thu. Nov 1, 2018 2:00 PM - 3:30 PM Room9)

[SY-H9] Modelling and 3D Printing Kelvin Cell Acoustic Metamaterial

○Huina MAO[1], Peter Göransson[1], John Kennedy[2], Henry Rice[2], Umberto Iemma[3] (1.Dept. of Aeronautical and Vehicle Engineering, KTH Royal Institute of Technology, Sweden, 2.Dept. of Mechanical and Manufacturing Engineering, Trinity College Dublin, Ireland, 3.Engineering Department, Roma Tre University, Italy)

Anisotropic metamaterial properties could be reached from design geometric structures. It can consist of functionality unit cells including microscale complex geometries to control the wave propagation. Structures based on regular Kelvin cells were selected and aims for design innovative devices to mitigate the civil aviation noise.

Inspired by the ultrahigh resolution 3D printer technology, manually controlled cell geometry would be possible. Polymer material was used in 3D printer. Samples with 0.1 mm diameter beam element kelvin cell model was printed in our lab and shows certain acoustic properties to reduce noise.

To understand the fully anisotropic metamaterial behavior, inverse estimation method was applied to get the 21 stiffness parameters in Hooke’s matrix. Optimization method was developed to design Kelvin cell structure to target noise reduction functions. It consists in numerically fitting a solid anisotropic model on a set of transfer functions extracted from Kelvin model. The estimated stiffness matrix is updated after each iteration until converge to an optimal solution. Feedbacks from modelling were used to control the geometry and material parameters in design. It would also be used to investigate modified noise scattering patterns in acoustic metamaterial. 3D printed samples would also be tested in wind tunnel to verify the numerical analysis.

Additional sub-elements, e.g., polymer microparticles could also be imbedded in the cells to increase viscous/damping loss and widen frequency bands. The frequency band could be adjusted according to the application by changing the geometry. Most of the sound could be decreased in the selected frequencies. If titanium was used in 3D printer, the cell size of the metamaterial would be much smaller that would increase acoustic properties too. The sound absorbing capacity of the titanium metamaterials, together with their strength and weather resistance, would also make them attractive candidates in noise and vibration control of aircrafts.

This work is a part of European project AERIALIST (AdvancEd aiRcraft-noIse-AILeviation devIceS using meTamaterials), which aims at the disclosure of the potential of metamaterials to envisage innovative devices for the mitigation of the civil aviation noise (https://www.aerialist-project.eu).

(Thu. Nov 1, 2018 2:00 PM - 3:30 PM Room9)

[SY-H9] Theoretical approach for EUV resist fabrication: DFT-MD-FDM study

○Muyoung Kim[1], Junghwan Moon[1], Joonmyung Choi[3], Sungwoo Park[1], Byunghoon Lee[3], Changyoung Jeong[3], Maenghyo Cho[2,1] （1.Divison of Multiscale Mechanical Design, School of Mechanical and Aerospace Engineering, Seoul National University, Korea, 2.Institute of Advanced Machines and Design, Seoul National University, Korea, 3.SAMSUNG ELECTRONICS CO., LTD, Korea）

Size of wafer has been reduced for improving performance and productivity in semiconductor manufacturing industry, and Extreme Ultraviolet (EUV) light source is state of the art strategy to achieve the goal. Fabrication of photoresist pattern is one of the main procedures in EUV lithography, and critical problems (pattern bridging or pinching) deteriorate as downsizing its size. Even though experimental- and theoretical approaches have been reported to provide physical mechanism and solution of performance degradation, technical huddles originating from complex photochemistry (chemical reaction by electron attachment or diffusion of reactant) hinder the rigorous investigation. From this point of view, we constructed multiscale model having sequential theoretical framework of density functional theory (DFT)-molecular dynamics (MD)-finite difference method (FDM). Our newly-developed model provides full description of photo-triggered chemical reaction (acid activation by electron attachment and acid diffusion-deprotection evolution) and also quantification of sub-10 nm photoresist morphology in atomistic level. This achievement will be the cornerstone of theoretical research which facilitates fundamental understanding on important factors for EUV performance and rational design of the next-generation PR.

Symposium | H. Multiscale Mechanics of Polymers, Soft Matter and Network Materials

[SY-H10] Symposium H-10

Chair: Kees Storm(Eindhoven University of Technology, Netherlands)

Thu. Nov 1, 2018 4:00 PM - 5:30 PM Room9

[SY-H10] In silico design of self-assembly nanostructured polymer systems by multiscale molecular modelling

○Maurizio Fermeglia （University of Trieste , Italy）

[SY-H10] Dynamical properties of suspensions of star block-copolymers in shear flow.

○Diego Felipe Jaramillo - Cano[1], Manuel Camargo[2], Christos N. Likos[1] （1.Faculty of Physics, University of Vienna, Austria, 2.CICBA, Universidad Antonio Nariño - Campus Farallones, Colombia）

[SY-H10] Heterogeneous flow and internal friction in amorphous carbon

○Richard Jana[1], Lars Pastewka[1], Daniele Savio[2], Volker L Dehringer[3], Gábor Csányi[3], Julian von Lautz[2], Michael Moseler[2], Peter Gumbsch[2,4] （1.Albert Ludwigs Universitaet Freiburg, Germany, 2.Fraunhofer-Institut für Werkstoffmechanik IWM, Germany, 3.University of Cambridge, UK, 4.Institue for Applied Materials, Karlsruhe Institute of Technology, Germany）

[SY-H10] Increasing the thermal conductivity of polymer nanocomposites filled with carbon nanotubes via molecular dynamics simulation

○Yangyang Gao[1], Liqun Zhang[1], Florian Müller-Plathe[2] （1.Beijing University of Chemical Technology, China, 2.Technische Universität Darmstadt, Germany）

[SY-H10] Thermal transport in polymer-based nanocomposite materials across multiple scales

Rajat Srivastava, ○Matteo Fasano, Shahin Mohammadnejad, Hernan Chavez Thielemann, Eliodoro Chiavazzo, Pietro Asinari （Energy Department, Politecnico di Torino, Italy）

(Thu. Nov 1, 2018 4:00 PM - 5:30 PM Room9)

[SY-H10] In silico design of self-assembly nanostructured polymer systems by multiscale molecular modelling

Invited

○Maurizio Fermeglia （University of Trieste , Italy）

One of the major goals of computational material science is the rapid and accurate prediction of properties of new materials. In order to develop new materials and compositions with designed new properties, it is essential that these properties can be predicted before preparation, processing, and characterization. Despite the tremendous advances made in the modeling of structural, thermal, mechanical and transport properties of materials at the macroscopic level (finite element (FE) analysis of complicated structures), there remains a tremendous uncertainty about how to predict many critical properties related to performance, which strongly depends on nanostructure. It is then essential analyze the structure at molecular level, with all the chemical and physical implication. Currently, atomistic level simulations such as molecular dynamics (MD) or Monte Carlo (MC) techniques allows to predict the structure and properties for systems of considerably large number of atoms and time scales of the order of microseconds. Although this can lead to many relevant results in material design, many critical issues in materials design still require time and length scales far too large for practical MD/MC simulations. This requires developing techniques useful to design engineers, by incorporating the methods and results of the lower scales (e.g., MD) to mesoscale simulations. In this work, we present applications of multiscale modeling procedures for predicting macroscopic properties strongly depending of interactions at nanoscale scale. Several different polymer systems of interest in the area of materials sciences and life sciences will be considered. including (i) functionalized nanoparticles in nanostructured polymer matrices (localization of gold nanoparticles in di-block copolymers and selective placement of magnetic nanoparticles in diblock copolymer films, (ii) functionalized nanoparticles in un structured polymer matrices (effect of chain length and grafting density) and (iii) self-assembly organization for biomedical applications (on nanoparticles and multivalent self-assembly building blocks in nanoparticles.

(Thu. Nov 1, 2018 4:00 PM - 5:30 PM Room9)

[SY-H10] Dynamical properties of suspensions of star block-copolymers in shear flow.

○Diego Felipe Jaramillo - Cano[1], Manuel Camargo[2], Christos N. Likos[1] （1.Faculty of Physics, University of Vienna, Austria, 2.CICBA, Universidad Antonio Nariño - Campus Farallones, Colombia）

Star block-copolymers (SBCs) are versatile building blocks with specific softness, functionalization, shape, and flexibility. They self-organize into a large variety of soft patchy nanoparticles, whose conformations and patchiness can be tuned and modified by different chemical-physical parameters. The static equilibrium properties of concentrated suspensions of SBCs have been an object of several studies because of the rich variety of assembly scenarios that can be achieved. In this work, we took a step forward in the study of non-equilibrium properties of suspensions of SBCs. By means of a particle-based, multiscale simulation approach, which combines standard molecular dynamics (MD) for the star monomers and multiparticle collision dynamics (MPCD) for the solvent particles, we investigated the behavior of dilute suspensions of SBCs under lineal shear flow for a wide range of parameters of the system; the latter include the functionality, the polymerization degree and the amphiphilicity degree of the star, the monomer packing fraction, the solvent

quality, and the shear rate. Our analysis focus on the dynamical behavior of the at-equilibrium-formed network structures as a consequence of the patches reorganization induced by the shear flow. The obtained results have interesting implications on the system’ s rheological properties and viscoelastic responses in dilute bulk phases because the SBCs are able to form a variety of different intermolecular transient bonds involving rather weak ones between individual arms and much stronger ones between multiarm patches.

(Thu. Nov 1, 2018 4:00 PM - 5:30 PM Room9)

[SY-H10] Heterogeneous flow and internal friction in amorphous carbon

○Richard Jana[1], Lars Pastewka[1], Daniele Savio[2], Volker L Dehringer[3], Gábor Csányi[3], Julian von Lautz[2], Michael Moseler[2], Peter Gumbsch[2,4] （1.Albert Ludwigs Universitaet Freiburg, Germany, 2.Fraunhofer-Institut für Werkstoffmechanik IWM, Germany, 3.University of Cambridge, UK, 4.Institue for Applied Materials, Karlsruhe Institute of Technology, Germany）

We use molecular dynamics simulations to probe the plastic response of representative bulk volumes of amorphous carbon at densities from 2.0 g cm^{-3} to 3.3 g cm^{-3} in simple and biaxial shear. We compare multiple interatomic potential expressions, in particular classical empirical bond-order potentials (screened Tersoff and REBO2), the modified embedded atom method (MEAM) and machine learning approaches, in particular the Gaussian approximation potential (GAP). After an initial elastic response, the samples yield without any strain hardening or softening. Individual plastic events are strikingly similar to those observed for bulk metallic glasses: Like in other amorphous materials, we find that plasticity is carried by fundamental rearrangements of regions of ~100 atoms, the shear transformation zone. We find that STZs coalesce to forms a shear band and that the relationship between stress and pressure during flow is well described by a Drucker-Prager law. Amorphous carbon is a prototypical single-component network material and its pair distribution function vanishes between first and second neighbor. This allows definition of an unambiguous nearest neighbor relationship and a mean coordination number. Stress correlates well with mean coordination, suggesting a simple constitutive model for this material. This relationship breaks down at low coordination numbers. We explain this with Thorpe’ s constraint counting theory, which predicts that networks become floppy below a certain value of mean coordination.

(Thu. Nov 1, 2018 4:00 PM - 5:30 PM Room9)

[SY-H10] Increasing the thermal conductivity of polymer nanocomposites filled with carbon nanotubes via molecular dynamics simulation

○Yangyang Gao[1], Liqun Zhang[1], Florian Müller-Plathe[2] （1.Beijing University of Chemical Technology, China, 2.Technische Universität Darmstadt, Germany）

It is very important to improve the thermal conductivity of polymer nanocomposites (PNCs) to widen their application. In this work, by employing reverse nonequilibrium molecular dynamics simulations in a full atomistic resolution, we systematically investigated the effect of the chemical grafting of carbon nanotube (CNT) on the thermal conductivity of PNCs. First, the interfacial thermal conductivity is proportional to the grafting density, while it first increases and then saturates with the grafting length. Meanwhile, the intrinsic in-plane thermal conductivity of CNT drops sharply as the grafting density increases. Combined with effective

medium approximation, the maximum overall thermal conductivity of PNCs appears at an intermediate grafting density because of these two competing effects. In addition, two empirical formulas are suggested, which quantitatively account for the effects of grafting length and density on the interfacial and parallel thermal conductivity. Secondly, the thermal resistance between the CNTs gradually decreases with the increase of the grafting density and grafting length, which can be well described by an empirical equation. The heat transfer process from one CNT to another can be well described by a thermal circuit model between the CNTs. Thirdly, a stronger enhancement of the thermal conductivity is realized when chains are grafted at the end atoms of CNTs. Under deformation, the orientation of both the chains and the CNTs improves the thermal conductivity parallel to the tensile direction, but reduces the thermal conductivity perpendicular to it. We have quantified the contribution of the polymer alignment and the CNT alignment to the anisotropy of thermal conductivity. In general, computer simulation is shown to have the capability to obtain some fundamental understanding of PNCs, in hopes of providing some design principles for fabricating high performance PNCs.

(Thu. Nov 1, 2018 4:00 PM - 5:30 PM Room9)

[SY-H10] Thermal transport in polymer-based nanocomposite materials across multiple scales

Rajat Srivastava, ○Matteo Fasano, Shahin Mohammadnejad, Hernan Chavez Thielemann, Eliodoro Chiavazzo, Pietro Asinari （Energy Department, Politecnico di Torino, Italy）

The improved physical properties of composite materials are revolutionizing many fields, from automotive to biomedical industries, from electronics to space applications. Composites are typically made of polymeric matrices reinforced with macroscopic fillers, e.g. carbon fibres. Nowadays, scientists are investigating the possibility of introducing nanostructured fillers as wells, to further enhance the effective properties of composites. Carbon nanostructures such as carbon nanotubes or graphene are particularly suitable for that, because of their outstanding mechanical, electrical and thermal properties. However, the resulting nanocomposites are characterised by properties at scales spanning from nano to macro and, therefore, should be simulated by sophisticated multi-scale approaches.

In this work, an original multi-scale approach to the thermal transport in polymer-based materials reinforced with carbon nanotubes or graphene sheets is presented and experimentally validated. First, molecular dynamics simulations are adopted to compute the thermal boundary resistance at the polymer-nanofiller and nanofiller-nanofiller interfaces, according to the different structural and chemical characteristics of the nanocomposite. The thermal conductivities of nanofillers and polymer matrix are computed as well, with molecular precision. Second, these nanoscale transport properties are used to estimate the effective thermal conductivity of nanocomposite, thanks to a mesoscopic simulation approach based on Dijkstra algorithm. The accuracy of the code is verified against a finite element model. After that, sensitivity analyses are carried out to investigate the impact of different fillers on the effective thermal conductivity of nanocomposite. Modelling results are then validated by experiments, and the most severe bottlenecks in the thermal conductivity enhancement of nanocomposites are finally identified.

Our work provides guidelines towards the technical-economical optimization of novel nanostructured materials with tunable thermal properties, with the aim to transfer them from lab experiments to industrial exploitation.

This work has received funding from the European Union’ s Horizon 2020 research and innovation program MODCOMP under grant agreement N. 685844.

Symposium | B. Challenges in the Multiscale Modelling of Radiation Effects in Nuclear Materials

[SY-B5] Symposium B-5

Chair: Jean-Paul Crocombette(CEA, Univ. Paris-Saclay, France)

Thu. Nov 1, 2018 9:45 AM - 11:00 AM Room10

[SY-B5] He impurities in boron carbide : structure, kinetics, and Raman signatures

○Guido Roma, Kevin Gillet, Anton Schneider, Jean-Paul Crocombette （CEA, Univ. Paris-Saclay, France）

[SY-B5] Irradiation damage in nuclear graphite at the atomic scale

○Alain Chartier[1], Laurent Van Brutzel[1], Justin Pageot[2] （1.DEN, Service de la Corrosion et du Comportement des Materiaux dans leur Environment, CEA Saclay, France, 2.DEN, Service d’ Etudes des Materiaux Irradies, CEA Saclay, France）

[SY-B5] Using computational modeling to understand radiation damage tolerance in complex oxides both from the bottom-up and the top-down

○Blas Pedro Uberuaga （Los Alamos National Laboratory, United States of America）

[SY-B5] **Development of defect mechanics-based multi-scale simulation techniques for reliability study of high performance electronic devices in radiation environments**

○Yukeun Eugene Pak[1], Youjung Seo[2], Dhaneshwar Mishra[1], Keonwook Kang[3], Jihyun Kim[4] （1.Advanced Institutes Convergence Technology, Korea, 2.Seoul National University, Korea, 3.Yonsei University, Korea, 4.Korea University , Korea）

(Thu. Nov 1, 2018 9:45 AM - 11:00 AM Room10)

[SY-B5] He impurities in boron carbide : structure, kinetics, and Raman signatures

Invited

○Guido Roma, Kevin Gillet, Anton Schneider, Jean-Paul Crocombette （CEA, Univ. Paris-Saclay, France）

Helium impurities, produced by nuclear reactions in the neutron absorber boron carbide, are a matter of concern because they form bubbles and eventually affect the mechanical properties of the absorbing elements in fast breeder sodium reactors. In order to shed light on the mechanisms of bubble formation we have investigated, using first principles methods, the insertion of He in boron carbide (with stoichiometry B_4C) and the possible migration mechanisms. Whereas in absence of preexisting damage, at equilibrium, He is expected to occupy interstitial sites and diffuse via an interstitial mechanism [1], we show that, under irradiation where a supersaturation of vacancies is expected, He atoms can be trapped at vacancies and diffusion might be slowed down.
How to probe such kind of impurities? Raman spectroscopy is increasingly used to quantify damage in irradiated materials, including boron carbide. In order to help the interpretation of such experiments we calculated from first principles the first order Raman spectrum of B_4C containing defects ; to circumvent the size effect we devised an inclusion procedure allowing us to obtain the dynamical matrix and the Raman tensor of a supercell containing a defect at a dilution lower than 0.1 atomic %. The results show that interstitial He impurities do not significantly perturb the spectrum, while substitutional ones do.

[1] A. Schneider, G. Roma, J.-P. Crocombette, V. Motte, D. Gosset, J. Nucl. Mater. **496**, 157 (2017).

(Thu. Nov 1, 2018 9:45 AM - 11:00 AM Room10)

[SY-B5] Irradiation damage in nuclear graphite at the atomic scale

○Alain Chartier[1], Laurent Van Brutzel[1], Justin Pageot[2] （1.DEN, Service de la Corrosion et du Comportement des Materiaux dans leur Environment, CEA Saclay, France, 2.DEN, Service d’ Etudes des Materiaux Irradies, CEA Saclay, France）

Radiation response and microstructure evolution of nuclear graphite are investigated by combination of both Molecular Dynamics (MD) simulations and experimental observations with mainly High Resolution Transmission Electron Microscopy images (HRTEM) and X-ray diffraction patterns (XRD). Radiation response of single crystal graphite is examined using MD with point defects accumulation method. Results reveal that graphite structure undergoes three stages before amorphisation: (i) an increase of the number of point defects; (ii) a wrinkling of graphene layers pinned by small amorphous pockets; and (iii) a full amorphisation of the structure via percolation of the small amorphous pockets [1]. Each stage can be related to the swelling along the c-axis and the shrinking in the basal plane. In particular rippling contributes significantly to the strain. One filler particle - composed of almost aligned crystallites separated by Mrozowski cracks - is also generated to provide insights on a more realistic microstructure of an-irradiated nuclear graphite.

Subsequently, simulated XRD pattern and HRTEM images have been generated from the MD simulations and are compared with experimental observations [2]. Simulated HRTEM images show many features observed in experimental images in both virgin and irradiated nuclear graphite. Some of these features can be linked unequivocally to defined atomistic configurations. Basal grain boundaries (GBs), Mrozowski cracks, graphene

sheets and their folding belong to this category. Conversely, some patterns in simulated HRTEM cannot be related to a unique atomistic configuration and might eventually give rise to misleading interpretation. This is evidenced for edge dislocations in virgin nuclear graphite as well as for residues of graphene layers in highly damaged graphite.

These findings confirm that univocal identification of atomic scales structures in graphite from HRTEM images only is uneasy.

[1] A. Chartier, L. Van Brutzel, B. Pannier, and Ph. Baranek, Carbon 91 (2015) 395.
[2] A. Chartier, L. Van Brutzel, and J. Pageot, Carbon 133 (2018) 224.

(Thu. Nov 1, 2018 9:45 AM - 11:00 AM Room10)

[SY-B5] Using computational modeling to understand radiation damage tolerance in complex oxides both from the bottom-up and the top-down

○Blas Pedro Uberuaga （Los Alamos National Laboratory, United States of America）

Meeting the ever-increasing demand for energy is a key challenge for the 21st century. Nuclear energy is a proven and green energy source that will be a key component of the world’s energy profile. However, maximizing the efficiency of nuclear energy systems requires materials that have significantly increased tolerance against radiation damage. Computational modeling has an important role in understanding and discovering new materials for next-generation nuclear energy systems.

In this talk, we will describe research efforts that apply computational modeling to understand the response of materials to radiation damage. We will focus on a class of complex oxides, pyrochlores, that have been proposed for nuclear waste encapsulation. Pyrochlores, with the chemical formula A2B2O7, are related to the simpler fluorite structure, with the added complication of having two cation species and oxygen structural vacancies. Past work by numerous groups has shown that the radiation tolerance of these materials is sensitive to the nature of the A and B cations and, in particular, their propensity to disorder. However, these observations are empirical at best and there is still a lack of understanding on the factors that govern the radiation response of these materials.

We have tackled this problem from two different perspectives. First, using accelerated molecular dynamics, we have studied how cation disorder, often created during radiation damage, impacts defect kinetics and thus the transport mechanisms that dictate damage recovery. This bottom-up approach has revealed that a percolation transition occurs as disorder is introduced that leads to higher defect mobilities, which in turn promotes self-healing of the damage. On the other hand, we have used materials informatics to analyze the role of pyrochlore chemistry on radiation tolerance. In this case, divorced from the complexities of making true predictions of performance, we instead use machine learning to take a top-down perspective and discover heuristic relationships between the material composition and the susceptibility of the material to amorphization. While neither study provides a complete understanding of radiation damage in these materials, together they provide a more complete picture of the factors that dictate their response to

irradiation.

(Thu. Nov 1, 2018 9:45 AM - 11:00 AM Room10)

[SY-B5] Development of defect mechanics-based multi-scale simulation techniques for reliability study of high performance electronic devices in radiation environments

○Yukeun Eugene Pak[1], Youjung Seo[2], Dhaneshwar Mishra[1], Keonwook Kang[3], Jihyun Kim[4] (1.Advanced Institutes Convergence Technology, Korea, 2.Seoul National University, Korea, 3.Yonsei University, Korea, 4.Korea University , Korea)

GaN-based electronic devices are very attractive for space applications since their radiation hardness characteristics are superior to the Si-based devices. For space missions requiring very conservative design margins, the presence of fabrication-induced defects as well as the radiation-induced defects limit the utilization of space-borne electronics. Therefore, prediction models to understand the defect generation mechanisms and the radiation effects on GaN devices are needed to properly engineer the reliability of these devices for the radiation environment.

To this end, we developed the quantitative linear elasticity models that can predict the stresses and piezoelectric fields induced in multilayer quantum wells in the presence of lattice defects such as dislocations. These electroelastic field calculations are coupled with the quantum mechanical formulation to predict the electronic and optical behavior of GaN-based devices such as LEDs and high-electronic-mobility transistors(HEMTs). To characterize the radiation effects, molecular dynamics (MD) simulations were performed to study the formation mechanisms of point defects caused by the energy transfer from irradiated particles. The required parameters for MD simulations were obtained by the Monte Carlo (MC) simulation code, GEANT4, and the results are compared with the irradiation test results.

Symposium | B. Challenges in the Multiscale Modelling of Radiation Effects in Nuclear Materials

[SY-B6] Symposium B-6

Chair: Jaime Marian(University of California Los Angeles, United States of America)

Thu. Nov 1, 2018 11:15 AM - 12:30 PM Room10

[SY-B6] Ion Irradiation as a Surrogate for Reactor Irradiation: The Expected and the Surprises

○Gary S Was[1], Zhijie Jiao[1], David Woodley[1], Stephen Taller[1], Gerrit Vancoevering[1], Anthony Monterrosa[1], Elizabeth Getto[4], Brian Wirth[2], Arthur Motta[3] （1.University of Michigan, United States of America, 2.University of Tennessee, United States of America, 3.Pennsylvania State University, United States of America, 4.United Stated Naval Academy, United States of America）

[SY-B6] Dose Effect on the Irradiation Induced Loop Density and Burgers Vector in Ion-Irradiated Ferritic/Martensitic Steel HT9 Through In-Situ TEM

Ce Zheng[1], Stuart Maloy[2], ○Djamel Kaoumi[1] （1.North Carolina State University, United States of America, 2.Los Alamos National Laboratory, United States of America）

[SY-B6] Novel Deformation Mechanism of Helium Irradiated Copper

○WEIZHONG HAN （Xi'an Jiaotong University, China）

[SY-B6] Isotope effect on quantum diffusion of interstitial hydrogen in face-centered cubic metals

○Hajime Kimizuka[1], Shigenobu Ogata[1,2], Motoyuki Shiga[3] （1.Osaka University, Japan, 2.Kyoto University, Japan, 3.Japan Atomic Energy Agency, Japan）

(Thu. Nov 1, 2018 11:15 AM - 12:30 PM Room10)

[SY-B6] Ion Irradiation as a Surrogate for Reactor Irradiation: The Expected and the Surprises

Invited

○Gary S Was[1], Zhijie Jiao[1], David Woodley[1], Stephen Taller[1], Gerrit Vancoevering[1], Anthony Monterrosa[1], Elizabeth Getto[4], Brian Wirth[2], Arthur Motta[3] (1.University of Michigan, United States of America, 2.University of Tennessee, United States of America, 3.Pennsylvania State University, United States of America, 4.United Stated Naval Academy, United States of America)

Reactor core materials in both fast reactors and LWRs granted life extension must withstand irradiation to high doses at high temperature. Ferritic-martensitic (F-M) alloys are attractive candidates for structural components of fast and thermal reactors, and high chromium and high nickel-containing austenitic steels are potential replacement alloys for LWR core materials. Both require high dpa, for which ion irradiation is ideally suited. To simulate the reactor radiation environment, self-ion irradiation and He injection are conducted simultaneously into both F-M and austenitic alloys. Reactor irradiations of the same alloys have been, or are being conducted in the BOR-60 fast reactor to assess the capability of ion irradiation to emulate the evolution of reactor generated microstructures and mechanical properties. Computational models for defect cluster evolution are being developed and benchmarked against experimental data to ultimately provide predictive capability for the response of both microstructure (loops, voids, precipitates, etc.), and mechanical properties (hardening, ductility, slip behavior) to irradiation. To date, agreement is quite promising with many outcomes ocurring as expected. However, there are a number of observations or results that are unexpected. Results will be presented on the microstructure and mechanical property evolution in ion and reactor irradiation integrated with computational modelling in an effort to understand the extent to which ion irradiation can be used as a surrogate for reactor irradiation, and to illuminate processes that are not well understood.

(Thu. Nov 1, 2018 11:15 AM - 12:30 PM Room10)

[SY-B6] Dose Effect on the Irradiation Induced Loop Density and Burgers Vector in Ion-Irradiated Ferritic/Martensitic Steel HT9 Through In-Situ TEM

Ce Zheng[1], Stuart Maloy[2], ○Djamel Kaoumi[1] (1.North Carolina State University, United States of America, 2.Los Alamos National Laboratory, United States of America)

TEM samples of F/M steel HT9 were irradiated to 20 dpa at 420˚C, 440˚C and 470˚C in a TEM with 1 MeV Kr ions so that the microstructure evolution could be followed in situ and characterized as a function of dose. Dynamic observations of irradiation induced defect formation and evolution were done at the different temperatures. The irradiation-induced loops were characterized in terms of their burgers vector, size and density as a function of dose and similar observations and trends were found at the three temperatures: (i) both **a**/2 <111> and **a** <100> loops are observed; (ii) in the early stage of irradiation, the density of irradiation induced loops increases with dose (0-4 dpa) and then decreases at higher doses (above 4 dpa), (iii) the dislocation line density shows an inverse trend to the loop density with increasing dose: in the early stages of irradiation the pre-existing dislocation lines are lost by climb to the surfaces while at higher doses (above 4 dpa), the build-up of new dislocation networks is observed along with the loss of the radiation-

induced dislocation loops to dislocation networks; (iv) at higher doses, the decrease of number of loops affects more the **a**/2 <111> loop population; the possible loss mechanisms of the **a**/2 <111> loops are discussed. Also, the ratio of **a** <100> to **a**/2 <111> loops is found to be similar to cases of bulk irradiation of the same alloy using 5 MeV Fe^{2+}ions to similar doses of 20 dpa at similar temperatures.

(Thu. Nov 1, 2018 11:15 AM - 12:30 PM Room10)

[SY-B6] Novel Deformation Mechanism of Helium Irradiated Copper

○WEIZHONG HAN （Xi'an Jiaotong University, China）

The workability and ductility of metals usually degrade with exposure to irradiation, hence the phrase “ radiation damage”. Here, we found that Helium (He) radiation can actually enhance the room-temperature deformability of submicron-sized copper. In particular, Cu single crystals with diameter of 100 nm to 300 nm and containing numerous pressurized sub-10 nm He bubbles, become stronger, more stable in plastic flow and ductile in tension, compared to fully dense samples of the same dimensions that tend to display plastic instability (strain bursts). The sub-10 nm He bubbles are seen to be dislocation sources as well as shearable obstacles, which promote dislocation storage and reduce dislocation mean free path, thus contributing to more homogeneous and stable plasticity. Failure happens abruptly only after significant bubble coalescence. Furthermore, we discover that the helium bubble not only can coalesce with adjacent bubbles, but also can split into several nanoscale bubbles under tension. Alignment of the splittings along a slip line can create a bubble-free-channel, which appears softer, promotes shear localization, and accelerates the failure in shearing-off mode. Detailed analyses unveil that the unexpected bubble fragmentation is mediated by the combination of dislocation cutting and internal surface diffusion, which is an alternative micro-damage mechanism of helium irradiated copper besides the bubble coalescence. These results shed light on plasticity and damage developments in metals. Ref. PRL 117 (2016) 515501, Nano Lett.16 (2016)4118 and Nano Lett. 17 (2017) 3725.

(Thu. Nov 1, 2018 11:15 AM - 12:30 PM Room10)

[SY-B6] Isotope effect on quantum diffusion of interstitial hydrogen in face-centered cubic metals

○Hajime Kimizuka[1], Shigenobu Ogata[1,2], Motoyuki Shiga[3] （1.Osaka University, Japan, 2.Kyoto University, Japan, 3.Japan Atomic Energy Agency, Japan）

Safe control of tritium is one of the technological challenges in the development of next-generation deuterium-tritium fusion reactors where tritium is used as nuclear fuel. From a scientific viewpoint, measuring the rate of diffusion of hydrogen isotopes in metals is important for understanding the isotope effect on the kinetics of hydrogen transport and hydrogen-induced deterioration of materials. However, a consensus on the physical mechanisms and numerical values of diffusivities of hydrogen isotopes in metals is still lacking. In this study, we clarified the site preference and diffusion rate of interstitial hydrogen and tritium in several face-centered cubic (fcc) metals, such as palladium, aluminum, and copper, by performing *ab initio* path-integral molecular dynamics (PIMD) modeling in the framework of density functional theory. This was necessary as the hydrogen atom has sufficiently low mass that it exhibits significant nuclear quantum delocalization and zero-point motion even at ambient temperature. The nuclear quantum effect on the

activation free energies for hydrogen migration was characterized according to the PIMD-based free energy profiles obtained from the thermodynamic integration of the centroid force along the migration path at 75-1200 K. We found that the nuclear quantum effects significantly affected the activation barrier for hydrogen migration and the difference between the energies of the hydrogen atom at the octahedral and tetrahedral interstitial sites even at ambient temperature. Consequently, we revealed the role of quantum fluctuations on the *reversed* isotope dependence for hydrogen diffusion in certain fcc metals.

Symposium | B. Challenges in the Multiscale Modelling of Radiation Effects in Nuclear Materials

[SY-B7] Symposium B-7

Chair: Marjorie Bertolus(CEA/DEN/DEC, Centre CEA de Cadarache, France)

Thu. Nov 1, 2018 2:00 PM - 3:30 PM Room10

[SY-B7] Thermal properties of fluorite-type metal dioxides: CeO_2, ThO_2, UO_2, NpO_2, PuO_2 and AmO_2

○Masato Kato （Japan Atomic Energy Agency, Japan）

[SY-B7] **SCIANTIX: A new inert gas behaviour module ready for use**

○Davide Pizzocri, Tommaso Barani, Lelio Luzzi （Politecnico di Milano, Italy）

[SY-B7] Modeling swelling in U_3Si_2 nuclear fuel using a multi-scale computational approach

○Larry Aagesen[1], Karim Ahmed[2], Benjamin Beeler[1], Daniel Schwen[1], Yongfeng Zhang[1] （1.Idaho National Laboratory, United States of America, 2.Texas A&M University, United States of America）

[SY-B7] Why Multiscale Modeling of Nuclear Fuel is Absolutely Essential and Why it is so Challenging

○Michael R Tonks[1], Yongfeng Zhang[2], David Andersson[3], Simon Phillpot[1], Christopher Stanek[3] （1.University of Florida, United States of America, 2.Idaho National Laboratory, United States of America, 3.Los Alamos National Laboratory, United States of America）

(Thu. Nov 1, 2018 2:00 PM - 3:30 PM Room10)

[SY-B7] Thermal properties of fluorite-type metal dioxides: CeO_2, ThO_2, UO_2, NpO_2, PuO_2 and AmO_2

Invited

○Masato Kato （Japan Atomic Energy Agency, Japan）

Actinide dioxide having a fluorite structure is one of prospective candidates as a fuel of advanced reactors. Thermal property of nuclear fuels is essential data to evaluate fuel performance. Therefore, great efforts to measure properties and understand their mechanism have been made so far. It is well-known that thermal properties of actinide oxides changes significantly depending on temperature, and their mechanism is complicated. Author’ s research group has studied on thermal properties of CeO_2, UO_2, PuO_2 and their solid solution. In this work, basic properties of various fluorite-type dioxides were summarized, and temperature dependence of thermal properties were evaluated.

In fluorite-type oxides of CeO_2, ThO_2, UO_2, NpO_2, PuO_2 and AmO_2, mechanical property, Debye temperature, Grunisen constant, thermal expansion, oxygen potential, heat capacity C_p and thermal conductivity were reviewed, and the data were compared. Heat capacity at volume constant C_v and thermal expansion term C_d were considered from their data in heat capacity evaluation. The calculation result of (C_v+C_d) was in good agreement with experimental data in CeO_2 and ThO_2, but the calculated data of other actinide dioxides underestimated the experimental data by 10-20 J/molK. The extra C_p from (C_v+C_d) was considered as a Schottky term C_{sch} which related to 5f electrons. In fact, 5 f electrons do not exist in CeO_2 and ThO_2. Experimental data of UO_2, NpO_2, PuO_2 and AmO_2 were described with the calculated (C_v+C_d+C_{sch}). The extra C_p was described assuming two level energy model.

Thermal conductivity of the dioxides was evaluated by phonon conduction mechanism using Slack’ s equation. Phonon conduction of pure oxide can be represented by 1/(BT). Thermal conductivity of CeO_2 and ThO_2 was represented by Slack’ s equation very well. But, other conduction mechanism is needed to evaluate thermal conductivity of UO_2, NpO_2, PuO_2 and AmO_2.

It is reported that excited term at high temperatures which is contributed with Frenckel defect, electron and so on exists in heat capacity and thermal conductivity. The experimental data at high temperatures are lacked to evaluate the excited terms. In addition of experimental data in high temperature region, computational approach is expected to understand deeply mechanism in property change.

(Thu. Nov 1, 2018 2:00 PM - 3:30 PM Room10)

[SY-B7] SCIANTIX: A new inert gas behaviour module ready for use

○Davide Pizzocri, Tommaso Barani, Lelio Luzzi （Politecnico di Milano, Italy）

Being able to bridge lower length-scale calculations with the engineering-scale simulations of fuel performance codes requires the development of dedicated intermediate-scale codes. In this work, we present SCIANTIX, a recently developed code which aims to fill this gap. SCIANTIX is a 0D stand-alone computer code under development at Politecnico di Milano since 2016. It is designed to be included as a module in existing fuel performance codes (e.g., TRANSURANUS). It contains models describing inert gas behaviour at the scale of a fuel grain, represented as a point (i.e., 0D). Since it is 0D, no spatial discretization

is required, and all variables are treated as average in space. Nevertheless, the models available in SCIANTIX (covering intra- and inter-granular inert gas behaviour, and high burnup structure formation and evolution as well) are physics-based and not correlation-based. The main characteristic of SCIANTIX is thus the simplicity of the models (i.e., low computational burden, in line with the requirements of fuel performance codes), paired with the possibility to inform them with parameters from lower length-scale calculations. SCIANTIX is validated against hundreds of experimental data describing inert gas behaviour at the scale of fuel grains. The validation is supported by uncertainty analyses on the main model parameters. Moreover, sensitivity analyses are performed to prioritize further research activities. Showcases of validation, uncertainty and sensitivity analyses are presented in this work (e.g., concerning gas concentrations, evolution of intra- and inter-granular bubble populations, swelling, high burnup structure formation). As for the numerical treatment of the model equations, SCIANTIX is developed with full numerical consistency and entirely verified with the method of manufactured solutions (verification of different numerical solvers is also showcased in this work). The open source release of the code is planned soon.

(Thu. Nov 1, 2018 2:00 PM - 3:30 PM Room10)

[SY-B7] Modeling swelling in U_3Si_2 nuclear fuel using a multi-scale computational approach

○Larry Aagesen[1], Karim Ahmed[2], Benjamin Beeler[1], Daniel Schwen[1], Yongfeng Zhang[1] （1.Idaho National Laboratory, United States of America, 2.Texas A&M University, United States of America）

U_3Si_2 is a leading candidate for application as an accident-tolerant fuel for commercial nuclear power generation. Due to U_3Si_2' s high thermal conductivity relative to conventional UO_2 fuel, it is believed to have a wider margin to melting/relocation in accident scenarios. However, based on limited experimental data, it is believed that U_3Si_2 undergoes much more significant swelling. To predict the swelling of U3Si2, a multi-scale computational approach has been developed. A phase-field model of fission gas bubble was developed, which tracks vacancies on the U lattice sites and Xe atoms as defect species. The proportional swelling of the fuel was assumed to be equal to the volume fraction of the bubble phase. The phase-field model was parameterized using density functional theory and molecular dynamics calculations. The incorporation of the swelling predictions to engineering-scale fuel performance models will be discussed.

(Thu. Nov 1, 2018 2:00 PM - 3:30 PM Room10)

[SY-B7] Why Multiscale Modeling of Nuclear Fuel is Absolutely Essential and Why it is so Challenging

Invited

○Michael R Tonks[1], Yongfeng Zhang[2], David Andersson[3], Simon Phillpot[1], Christopher Stanek[3] （1.University of Florida, United States of America, 2.Idaho National Laboratory, United States of America, 3.Los Alamos National Laboratory, United States of America）

The performance of reactor fuel is historically determined using codes that rely on empirical fits to experimental data. However, as reactor operation becomes more variable and as we consider changes to the fuel and cladding system to increase accident tolerance, these empirical models become insufficient to meet our needs. The US Nuclear Engineering Advanced Modeling and Simulation (NEAMS) program is beginning to

implement an alternative approach to fuel performance materials models that relies on representing the evolving state of the fuel microstructure using state variables that impact the material properties. However, developing the required models for this approach using only experimental data would be extremely difficult, time consuming, and expensive. Hierarchical multiscale modeling and simulation, ranging from density functional theory to mesoscale simulation approaches, provides a powerful means to obtain additional data to inform the development of these new materials models. However, applying this multiscale approach to reactor fuel has a number of challenges. In this presentation I will summarize this multiscale approach being taken in the US and discuss a number of the issues that make it difficult.

Symposium | B. Challenges in the Multiscale Modelling of Radiation Effects in Nuclear Materials

[SY-B8] Symposium B-8

Chair: Guang-Hong Lu(Beihang University, China)

Thu. Nov 1, 2018 4:00 PM - 5:30 PM Room10

[SY-B8] Kinetic Monte Carlo study of tungsten fuzz formation under low energy helium irradiation

○Zhangcan Yang, Yingzhao He, Quansong Peng （School of Energy and Power Engineering, Huazhong University of Science and Technology, China）

[SY-B8] Constrained thermodynamic model for multi-component alloys under irradiation: A matrix formulation from first-principles Hamiltonian

○Duc Nguyen-Manh[1], J.S Wrobel[2], A. Fernandez_Caballero[3], S.L. Dudarev[1] （1.Materials Science and Scientific Computing Department, Culham Centre for Fusion Energy, UKAEA, UK, 2.Faculty of Materials Science and Engineering, Warsaw University of Technology, Poland, 3.School of Mechanical Aerospace and Civil Engineering, University of Manchester , UK）

[SY-B8] Kinetic Monte-Carlo Simulations of Radiation Damage in W(Re,Os) Alloys

○Matthew James Lloyd[1,2], David Armstrong[1], Enrique Martinez Saez[3], Duc Nguyen-Manh[2] （1.Department of Materials, University of Oxford, UK, 2.Culham Centre for Fusion Energy, UK, 3.Los Alamos National Laboratory, United States of America）

[SY-B8] Modeling Re-precipitate hardening in neutron irradiated W and W-Re alloys: from point defects to macroscopic hardening

Chen-Hsi Huang[1], Leili Gharaee[2], Paul Erhart[2], ○Jaime Marian[1] （1.University of California Los Angeles, United States of America, 2.Chalmers University, Sweden）

[SY-B8] In-situ TEM of Formation Processes of Defects in Tungsten under Irradiation: Comparison between Electron and Self-ion Irradiations

○Kazuto Arakawa （Shimane University, Japan）

(Thu. Nov 1, 2018 4:00 PM - 5:30 PM Room10)

[SY-B8] Kinetic Monte Carlo study of tungsten fuzz formation under low energy helium irradiation

○Zhangcan Yang, Yingzhao He, Quansong Peng （School of Energy and Power Engineering, Huazhong University of Science and Technology, China）

Tungsten has been considered as the primary candidate for the plasma-facing materials of fusion reactors. However, the formation of fuzz-like nanostructures on tungsten surfaces under low-energy helium plasma irradiation has raised big concerns since these fuzzy structures have been shown to be detrimental to the performance of the materials and the stability of plasma. Unfortunately, the mechanism of fuzz formation is still under debate. Here we present an Object Kinetic Monte Carlo study that links the nucleation and growth of helium bubbles with the evolution of surface morphology. The key difference of our model compared with a previous model by Lasa’ s[1] is that the motion of the punched dislocation loops and the diffusion of surface ad-atoms are modeled in detailed in our model. As a result, our model is able to produce real fuzz-like structures rather than the glassy structures in Ref [1]. We first study the sub-surface helium clustering behavior in tungsten as a function of temperature, helium implantation rate, and concentration of pre-existing defects [2]. The key parameters that affect helium clustering behavior have been identified. We then investigate the possible processes that may contribute to the surface evolution and quantitatively analyze their relative contribution. We find that the motion of dislocation loops and the surface diffusion are the two key processes to the surface evolution. Bubble rupture only affects the initial surface roughness, but plays a negligible role in the growth of fuzz structures.

Reference:
[1] A. Lasa et al 2014, EPL, 105(2), 25002.
[2] Z. Yang et al 2017, Fusion Science and Technology, 71(1), 60.

(Thu. Nov 1, 2018 4:00 PM - 5:30 PM Room10)

[SY-B8] Constrained thermodynamic model for multi-component alloys under irradiation: A matrix formulation from first-principles Hamiltonian

○Duc Nguyen-Manh[1], J.S Wrobel[2], A. Fernandez_Caballero[3], S.L. Dudarev[1] （1.Materials Science and Scientific Computing Department, Culham Centre for Fusion Energy, UKAEA, UK, 2.Faculty of Materials Science and Engineering, Warsaw University of Technology, Poland, 3.School of Mechanical Aerospace and Civil Engineering, University of Manchester , UK）

Understanding the behaviour of multi-component alloys under irradiation is one of the great challenges for the development of materials for nuclear applications. Recent experimental investigations revealed that micro-structural evolution of multi-component metallic alloys formed by transmulation under neutron irradiation can be very complicated since they may undergo spinodal decomposition and radiation-induced precipitation due to the strong coupling between defects and local chemical environment. Very recently, it was shown that concentrated solute solution alloys including high-entropy alloys (HEAs) may exhibit significantly improved performance under irradiation that depends strongly on the number of alloying elements and local alloy composition.

In this work, a revisited constrained thermodynamic model, initially proposed by Georges Martin, has been developed to model multi-component alloys under irradiation. The model is based on ab initio calculations in combination with a cluster-expansion Hamiltonian generalized for systems containing vacancy (V) and interstitial (I) defects. It is found that this formalism can be mathematically represented in terms of a matrix formulation for any N-component system via cluster correlation functions, which in turn can be deduced consistently from Monte-Carlo simulations. Analytical expressions for local short-range order parameters for alloy components and configurational entropies as functions of temperature and composition have been derived explicitly from this matrix representation. In the first nearest-neighbour approximation, the new approach reproduces the ABVI Ising model for a binary system as well as the thermodynamic limit of the Cluster Variation Method. We apply this formalism to anomalous precipitation in W(Re,Os,Ta) alloys under neutron irradiation as well as in low activation bcc and high-radiation resistance fcc HEAs and their derivatives.

(Thu. Nov 1, 2018 4:00 PM - 5:30 PM Room10)

[SY-B8] Kinetic Monte-Carlo Simulations of Radiation Damage in W(Re,Os) Alloys

○Matthew James Lloyd[1,2], David Armstrong[1], Enrique Martinez Saez[3], Duc Nguyen-Manh[2] （1.Department of Materials, University of Oxford, UK, 2.Culham Centre for Fusion Energy, UK, 3.Los Alamos National Laboratory, United States of America）

The realisation of fusion energy is dependant on the development of high performance materials that can withstand the extreme conditions that they will be subjected to. The plasma facing components of a fusion reactor will experience a combination of high thermal loading (~10MWm^{-2}) and an intense flux of both 14MeV neutrons and high energy He/H ions (~5-20dpa/yr), meaning they will have to operate at very high temperatures (~1300 K). Tungsten is currently the leading candidate material due to its high melting temperature (~3695K); good thermal conductivity (~150Wm^{-1}K^{-1}) and resistance to sputtering (Eth=200eV). But at such a high neutron flux, transmutation of W in a fusion reactor is significant, resulting in several at.% Re, Os and Ta over the lifetime of the reactor. Precipitation of Re and Os has been observed well below their solubility limit in W, resulting in embrittlement, hardening, and a reduction in thermal conductivity.

The research presented examines irradiated W-(Re,Os,Ta) alloy systems, using a combination of DFT parametrised, multicomponent atomistic kinetic Monte-Carlo (AKMC) modelling, and high resolution nanoscale characterisation techniques such as atom probe tomography (APT). The role of interstitial defects in W-Re and W-Os is thought to play an important role in precipitation, because of the low rotation energy of the W-Re/W-Os mixed dumbbell. This enables the 3D transport of solute atoms, that would otherwise be confined to the <111> direction. We present a multicomponent kinetic Monte Carlo model, incorporating both vacancy and interstitial defects, and solute concentration dependant interactions. The predictions made by our model are supported by APT data of W-Re and W-Os alloys irradiated at high temperature, using W ions.

(Thu. Nov 1, 2018 4:00 PM - 5:30 PM Room10)

[SY-B8] Modeling Re-precipitate hardening in neutron irradiated W and W-Re alloys: from point defects to macroscopic hardening

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High-temperature, high-dose, neutron irradiation of W results in the formation of Re-rich clusters at concentrations one order of magnitude lower than the thermodynamic solubility limit. These clusters may eventually transform into brittle W-Re intermetallic phases, leading to severe embrittlement and loss of thermal conductivity. Standard theories of radiation-enhanced diffusion and precipitation cannot explain the formation of these precipitates and so understanding the mechanism by which nonequilibrium clusters form under irradiation is crucial to predict material degradation and devise mitigation strategies. In this work, we integrate neutronics, primary damage calculations, molecular dynamics results, Re transmutation calculations, and stochastic cluster dynamics simulations to study neutron damage in single-crystal tungsten to mimic divertor materials. We study the material response under experimental conditions at the JOYO fast reactor and the High Flux Isotope Reactor, for which measurements of cluster densities and hardening levels exist. We then provide calculations under expected DEMO fusion conditions. Several key mechanisms involving Re atoms and defect clusters are found to govern the accumulation of irradiation damage in each case. We use established correlations to translate damage accumulation into hardening increases and compare our results to the experimental measurements. We find hardening increases in excess of 5000 MPa in all cases, which calls into question the performance of these materials under service conditions in fusion reactors.

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[SY-B8] In-situ TEM of Formation Processes of Defects in Tungsten under Irradiation: Comparison between Electron and Self-ion Irradiations

Invited

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Nuclear-fission and fusion materials are degraded primarily due to the accumulation of radiation-produced lattice defects, such as point defects (self-interstitial-atoms (SIAs) and vacancies) and point-defect clusters (dislocation loops and cavities). In order to precisely predict the lifetimes of nuclear materials, accurate understanding of the origins of the defect accumulation—generation of defects and their subsequent dynamics—is crucial.

In-situ transmission electron microscopy (TEM) is a powerful technique for probing defect dynamics, in response to external stimuli such as irradiation under heating or cooling. As the irradiation sources for the in-situ TEM, electrons and ions are available. In the electron irradiation, only point defects are generated as the primary damage via knock-on displacement. In contrast, in the ion irradiation, point-defect clusters are also generated as the primary damage, which is called “collision cascade”, like neutron irradiation.

In this presentation, we focus on the formation process of dislocation loops in tungsten under irradiation. Firstly we show our results on dynamic properties of SIAs [1] and SIA dislocation loops, which have been

mainly obtained with high-voltage electron microscopes in Osaka University and Nagoya University in Japan. And, we provide our results on the formation processes of dislocation loops under self-ion irradiation, which have been obtained with an ion-accelerators combined microscope in the JANNuS-Orsay facility in France. Through the comparison between these results, we try to extract the effects of collision cascade on the formation processes of dislocation loops.

References

[1] T. Amino, K. Arakawa, and H. Mori, *Scientific Reports* 6 (2016) 26099.