Mon. Oct 29, 2018

Poster Hall

Poster Session | A. Advances in Materials Theory for Multiscale Modeling

[PO-A1] Poster Session 1

5:45 PM - 8:00 PM Poster Hall

[P1-01] The Coadsorption Effect of Cl- and H_2O on the Various Defect Al_2O_3 Film Surface

○Chuan-Hui Zhang, Bao Chen, Peng Shi （University of Science and Technology Beijing, China）

[P1-02] Incorporation of double cross-slip in continuum dislocation dynamics

○Xingjian Zhou, Yichao Zhu （Faculty of vehicle Engineering and Mechanics, Dalian University of Technology, China）

[P1-03] **Effect of Defect on Structural and Optical Properties in Methyl-Ammonium Lead Iodide(MAPI) Perovskite via First Principles Calculations**

○Abdullah Al ASAD, Keiichi MITANI, Atsushi ISHIKAWA, Kenji TSURUTA （Dept. of Electrical and Electronic Engineering, Okayama University, Japan）

[P1-04] Isogeometric modeling and large-scale computation for stress field around lattice defects

○Shunsuke Kobayashi[1], Ryuichi Tarumi[2], Atsushi Suzuki[3], Masao Ogino[4], Yoji Shibutani[1] （1.Graduate School of Engineering, Osaka Univ., Japan, 2.Graduate School of Engineering Science, Osaka Univ., Japan, 3.Cybermedia Center, Osaka Univ., Japan, 4.Information Technology Center, Nagoya Univ., Japan）

[P1-05] **A local/nonlocal plasticity model for upscaling microstructural effects**

○John Mitchell （Sandia National Laboratories, United States of America）

[P1-06] **First-principles investigation of atomic hydrogen adsorption and diffusion on/into Mo-doped Nb (100) surface**

○Zhong-min Wang, Yang Wu, Qingrong Yao, Yan Zhong, Chaohao Hu, Huaiying Zhou （Guilin University of Electronic Technology, China）

[P1-07] **First-principles Study on Electronic Properties of Hybrid MA*BX*$_3$ perovskites (MA= $CH_3NH_3^+$; *B*= Pb, Sn, Ge; *X*= I, Br, Cl)**

○Narasak Pandech[1,2], Thanundon Kongnok[1], Sirichok Jungthawan[1], Sukit Limpijumnong[1], Walter R.L Lambrecht[2] （1.School of Physics and NANOTEC-SUT Center of Excellence on Advanced Functional Nanomaterials, Suranaree University of Technology, NakhonRatchasima 30000, Thailand, Thailand, 2.Department of Physics, Case Western Reserve University, Cleveland, Ohio 44106-7079, USA., United States of America）

Poster Session | C. Crystal Plasticity: From Electrons to Dislocation Microstructure

[PO-C1] Poster Session 1

5:45 PM - 8:00 PM Poster Hall

[P1-08] Pressure effects on dislocation core structures in Mg_2SiO_4 olivine: insights from atomic-scale modeling

○Philippe Carrez, Srinivasan Mahendran, Patrick Cordier （Lille University, Lab. UMET UMR-CNRS 8207, France）

[P1-09] Structural and magnetic properties of long-period stacking ordered (LPSO) structure of iron; A first-principles study

○Takao Tsumuraya[1], Ikumu Watanabe[2], Takahiro Sawaguchi[2] （1.Magnesium Research Center/POIE, Kumamoto Univ., Japan, 2.Research Center for Structural Materials, National Institute for Materials Science, Japan）

[P1-11] Dislocation transmission behaviors of bi-crystal BCC Tantalum with high and low angle symmetric tilt grain boundaries: Multiscale simulation study

○Moon Sunil, Kang Keonwook （Dept. of Mechanical Engineering, Yonsei Univ., Korea）

[P1-12] Ab Initio Dislocation Core Calculations using a Cluster Model

○Jonas Frafjord[1,3], Bjørn Holmedal[4], Jesper Friisj[2,3], Randi Holmestad[1,3], Ingeborg-Helene Svenum[2], Inga Gudem Ringdalen[2] （1.Dept. of Physics, Norwegian University of Science and Technology, Norway, 2.SINTEF Industry, Trondheim, Norway, 3.Centre for Advanced Structural Analysis, SIMLab, Norway, 4.Dept. of Materials Science and Engineering, Norwegian University of Science and Technology, Norway）

[P1-13] Anelastic recovery of a steel wire under pure shear strain with various magnetic treatments

○Shigeo Kotake, Takuro Murata （Dept. of Mechanical Engineering, Mie Univ., Japan）

[P1-14] Possible explanation of sudden stress drop at upper yield point in iron by magnetostriction and

unpinning dislocations with law of approach in residual magnetization

○Shigeo Kotake （Dept. of Mechanical Engineering, Mie Univ., Japan）

[P1-15] Investigation of dislocation core structure in Aluminum by using a generalized Peierls-Nabarro model

○Hideki MORI （College of Industrial Technology, Japan）

[P1-16] Crystal orientation evolution analysis during deformation using molecular dynamics

○Keisuke Kinoshita （Nippon Steel &Sumitomo Metal Corporation, Japan）

[P1-17] Nanoindentation of Nanoparticles -A Molecular Dynamics and Discrete Dislocation Dynamics Simulations Study

Roy Shyamal[1], Riccardo Gatti[2], Benoit Devincre[2], ○Dan Mordehai[1] （1.Mechanical Engineering, Technion - Israel Institute of Technology, Haifa, Israel, Israel, 2.LEM, UMR 104, CNRS-ONERA, 29 Av. de la Division Leclerc, 4 Chatillon, France, France）

[P1-18] Machine learning interatomic potentials for molecular dynamics simulations of dislocations

○Eyal Oren, Guy Makov （Dept. of Materials Engineering, Ben-Gurion University of the Negev, Israel）

Poster Session | E. Deformation and Fracture Mechanism of Materials

[PO-E1] Poster Session 1

5:45 PM - 8:00 PM Poster Hall

[P1-21] Large-scale molecular dynamics simulations: coupling with dislocation dynamics

○Pavel A. Pokatashkin, Denis K. Ilnitsky, Alexei V. Yanilkin （Dukhov Research Institute of Automatics (VNIIA), Russia）

[P1-22] **Hydrogen embrittlement controlled by reaction of dislocation with grain boundary in alpha-iron polycrystals**

○Liang Wan[1,2], Wen Tong Geng[2,3], Akio Ishii[2], Jun-Ping Du[2,4], Nobuyuki Ishikawa[5], Hajime Kimizuka[2], Shigenobu Ogata[2,4] （1.Wuhan University, China, 2.Osaka University, Japan, 3.University of Science and Technology Beijing, China, 4.Kyoto University, Japan, 5.JFE Steel Corporation, Japan）

[P1-23] Study of solute effect on the yield strength of Fe-based dilute alloy using atomistically informed kinetic Monte Carlo method

○Shuhei Shinzato[1], Masato Wakeda[2], Shigenobu Ogata[1] （1.Dept. of Mechanical Science and Bioengineering, Osaka Univ., Japan, 2.National Institute for Materials Science, Japan）

[P1-24] **Molecular Dynamics Simulations of Low-cycle Fatigue Behavior in Single Layer Molybdenum Disulfide**

Yu-Chieh Lo[1], ○Yu-Cheng Su[1], Ming-Chen Chung[2], Alice Hu[3] （1.National Chiao Tung University, Taiwan, 2.National Cheng Kung University, Taiwan, 3.City University of Hong Kong, Hong Kong）

[P1-25] Fracture behavior of multi-walled carbon nanotube under biaxial loading condition

○Masaomi Nishimura[1], Naoki Kazami[2], Daiki Kato[2] （1.Dept. of Mechanical Systems Engineering, Shinshu Univ., Japan, 2.Graduate School of Science and Technology, Shinshu Univ., Japan）

[P1-26] **On the role of amorphous shells on mechanical properties of fcc Ni nanoparticles under compression**

○Alexandra Goryaeva[1,2], Claudio Fusco[2], Matthieu Bugnet[2], Jonathan Amodeo[2] （1.DEN-Service de Recherches de Métallurgie Physique, CEA, Université Paris-Saclay, 91191 Gif-sur-Yvette, France, 2.INSA-Lyon, Université de Lyon, MATEIS, 69621 Villeurbanne, France）

[P1-27] Molecular dynamics analysis of hydrogen diffusion behavior in alpha-Fe bi-crystal under stress gradient

○Ken-ichi Saitoh[1], Haruka Koga[2], Tomohiro Sato[1], Masanori Takuma[1], Yoshimasa Takahashi[1] （1.Kansai Univ., Japan, 2.Kobe Steel, Ltd., Japan）

[P1-28] Understanding Interactions of Dislocations with Interfaces in Nickle-based Superalloys: Insights from Molecular Dynamics Simulations

○Jian Huang[1], Yunjiang Wang[2] （1.Shanghai Institute of Ceramics Chinese Academy of Sciences, China, 2.Institute of Mechanics, Chinese Academy of Sciences, China）

[P1-29] The influence of nano-sized Ti_3Al particles on the mechanical properties of α-titanium alloys

○Yan He[1,2,3], Wang Hao[1], Dongsheng Xu[1], Yang Rui[1] （1.IMR, CAS, China, 2.Coll. of Physics Science and Technology, SYNU, China, 3.Univ. of chinese Academy of Sciences, China）

[P1-30] **The atomic study of tensile property for nickel nanowires with helium bubble**

○Hengfeng Gong, Rui Li, Tong Liu （CGN, China）

[P1-31] **Componets of fracture response of alkali-activated slag mortars with steel fibers**

○Hana Simonova, Petr Frantik, Zbynek Kersner, Pavel Schmid, Pavel Rovnanik （Brno University of Technology, Faculty of Civil Engineering, Czech Republic）

[P1-32] Molecular Dynamics Simulation of Crack Growth Behavior of Single Crystal γ-TiAl Alloy Under Different Nb Substitution Mode

○Yuxi Feng[1,2], Zhiyuan Rui[1,2], Hui Cao[1,2], Ruicheng Feng[1,2], Xiaocui Fan[1,2], Xing Yang[1,2] （1.Mechanical and Electronical Engineering College, Lanzhou University of Technology, China, 2.Key Laboratory of Digital Manufacturing Technology and Application, the Ministry of Education, Lanzhou University of Technology, China）

Poster Session | F. From Microstructure to Properties: Mechanisms, Microstructure, Manufacturing

[PO-F1] Poster Session 1

5:45 PM - 8:00 PM Poster Hall

[P1-33] UNDERSTANDING OF DELAYED HYDRIDE CRACKING FAILURE MECHANISM IN E110 ZIRCONIUM BASED FUEL CLADDINGS BY EBSD AND IN-SITU MECHANICAL TESTING

○Hygreeva Kiran NAMBURI[1], Zbynek Spirit[1], Patricie Halodova[1], Ondrej Libera[1], Jakub krejci[2] （1.Research Centre REZ, Czech Republic, 2.UJP Praha, Czech Republic）

[P1-34] Transition-metal alloying of γ ‘-Ni_3Al: Effects on the ideal uniaxial compressive strength from first-principles calculations

○Minru Wen[2,1], Chongyu Wang[2] （1.Guangdong University of Technology, China, 2.Tsinghua University , China）

[P1-35] **The Influence of Deposition Pattern on Stress and Mechanical Properties in Wire Arc Additive Manufacturing**

○Changmeng Liu, Qianru Wu, Jiping Lu, Shuyuan Ma （Beijing Institute of Technology, China）

[P1-36] On the Significance of the Higher-Order Neighbors for Abnormal Grain Growth and Recrystallization Nucleation

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

[P1-37] **Hydrogen trapping in carbon supersaturated a-iron and its decohesion effect in martensitic steel**

○Wen-Tong Geng[1,2], Vei Wang[1,3], Jin-Xu Li[2], Nobuyuki Ishikawa[4], Hajime Kimizuka[1], Kaneaki Tsuzaki[5,6], Shigenobu Ogata[1,6] （1.Department of Mechanical Science and Bioengineering, Osaka University, Japan, 2.University of Science and Technology Beijing, China, 3.Department of Applied Physics, Xi’ an University of Technology, China, 4.Steel Research Laboratory, JFE Steel Corporation, Japan, 5.Department of Mechanical Engineering, Kyushu University, Japan）

[P1-38] **Size Scale Effect on Energy Absorption Property of Aluminum Foam**

○zengyou liang, fudi liang, dezhi deng, chunzhuang miao, mingguang wang （North University of China, China）

[P1-39] Development of charge-transfer type interatomic potential for SiC oxidation

○So Takamoto[1], Takahiro Yamasaki[2], Takahisa Ohno[2], Chioko Kaneta[3], Asuka Hatano[1], Satoshi Izumi[1] （1.The Univ. of Tokyo, Japan, 2.NIMS, Japan, 3.Fujitsu Lab., Japan）

[P1-40] Alpha-phase in engineering aluminum alloys: a multiscale modeling approach to its mechanical behavior

○Duancheng Ma （Leichtmetallkompetenzzentrum Ranshofen GmbH, Austria）

[P1-41] Multi-phase-field lattice Boltzmann modeling and simulation of equiaxed structure

○Ryotaro Sato[1], Tomohiro Takaki[1], Shinji Sakane[1], Munekazu Ohno[2], Yasushi Shibuta[3] （1.Kyoto Institute of Technology, Japan, 2.Hokkaido University, Japan, 3.Tokyo University, Japan）

[P1-42] Simulation of Extrusion Process of TiAl alloy prepared by Triple VAR

○Fan Gao, Zhenxi Li （AECC BEIJING INSTITUTE OF AERONAUTICAL MATERIALS, China）

[P1-43] Experimental-Computational Analysis of Primary Static Recrystallizazion in DC04 Steel

○Martin Diehl, Markus Kühbach, Dierk Raabe （Max-Planck-Institut fuer Eisenforschung GmbH, Germany）

[P1-44] Combining 4D experiments and phase-field modeling to determine reduced grain boundary mobilities

○Jin Zhang[1,2], Peter W Voorhees[1], Henning F Poulsen[2] (1.Northwestern University, United States of America, 2.Technical University of Denmark, Denmark)

[P1-45] Fiber-intersectant microstructure of fish scale and biomimetic research

○Bin Chen[1], Jinghong Fan[2], Miao Li[1], Wei Ye[1] (1.College of Aerospace Engineering, Chongqing University, China, 2.Division of Mechanical Engineering, Alfred University, United States of America)

[P1-46] Microstructures of turtle shell and biomimetic fabrication

○Bin Chen[1], Jinghong Fan[2], Wei Ye[1], Miao Li[1] (1.College of Aerospace Engineering, Chongqing University, China, 2.Division of Mechanical Engineering, Alfred University, United States of America)

[P1-47] **Phase-field Simulation of Solidification Process in Welding Pool of Fe-C Binary Alloy**

○Ian zhan, Xiangge Qin (Jiamusi Univ., China)

[P1-48] **Phase field simulation of the phase separation in the TiC-ZrC-WC system**

○Zelin Luo[1], Hong Ma[1], Sai Tang[1], Yingbiao Peng[2], Yong Du[1], Zikui Liu[3], Qianhui Min[1], Yafei Pan[4] (1.State Key Lab of Powder Metallurgy, Central South University, China, 2.College of Metallurgy and Materials Engineering, Hunan University of Technology, China, 3.Department of Materials Science and Engineering, Pennsylvania State University, United States of America, 4.School of materials science and engineering, Hefei University of Technology, China)

[P1-49] Switching of coordinate transformations of a repetitive bar-and-joint framework under uniaxial compression

○Hiro Tanaka[1], Kazutoshi Hamada[1], Yoji Shibutani[1,2] (1.Dept. of Mechanical Engineering, Osaka Univ., Japan, 2.Nanotechnology Program, Vietnam Japan Univ., Viet Nam)

[P1-50] Understanding the effect of Residual Stresses in 3D Printed Metals

○Alankar Alankar, BVSS Bharadwaja, Ritam Chatterjee (IIT Bombay, India)

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

[PO-H1] Poster Session 1
5:45 PM - 8:00 PM Poster Hall

[P1-51] Multi-scale modeling of DNA-dendrimers in electrolyte solutions

○Natasa Adzic[1], Clemens Jochum[2], Gerhard Kahl[2], Christos Likos[1] (1.Faculty of Physics, University of Vienna, Austria, 2.Institute for Theoretical Physics, Vienna University of Technology, Austria)

[P1-52] Structural and dynamical properties 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)

[P1-53] Multiscale simulation of polymeric solids for fracture processes

○Takahiro Murashima[1], Shingo Urata[2] (1.Dept. of Physics, Tohoku Univ., Japan, 2.AGC, Japan)

[P1-54] Quantification and validation of the mechanical properties of DNA nicks

○Jae Young Lee, Jae Gyung Lee, Do-Nyun Kim (Dept. of Mechanical and Aerospace Engineering, Seoul National Univ., Korea)

[P1-55] Investigating the mechanical properties of azobenzene-tethered DNA for controlling self-assembling DNA nanostructures

○Jae Gyung Lee, Chanseok Lee, Do-Nyun Kim (Dept. of Mechanical and Aerospace Engineering, Seoul National Univ., Korea)

[P1-56] FTMP-based Modeling and Simulations of Glassy Polymers.

○Soushi Miyamoto, Tadashi Hasebe (Dept. of Mechanical Engineering, Kobe Univ., Japan)

[P1-57] Shock Wave Induced Damage in Tumor Cells: Experiments and Simulations

○Martin Steinhauser (Fraunhofer Ernst-Mach-Institute, EMI, Germany)

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

[PO-I1] Poster Session 1
5:45 PM - 8:00 PM Poster Hall

[P1-58] Phase-field modeling of anisotropic grain growth with incorporation of Sigma 3 CSL grain boundaries.

○Kunok Chang (Kyung Hee Univ., Korea)

[P1-59] Direct mapping from molecular dynamics to phase-field simulations for accurate prediction of grain growth

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

[P1-60] Density functional theory plus Hubbard U study of the segregation of Pt to the CeO_{2-x} grain boundary

Guoli Zhou, Pan Li, Qingmin Ma, ○Zhixue Tian, Ying Liu (Hebei Normal Univ., China)

[P1-61] **Interfacial charge transfer and enhanced photocatalytic mechanism for Bi_2WO_6/BiOCl heterostructure: A first-principles theoretical study**

○Pan Li (Hebei Normal Univ., China)

[P1-62] Investigation of abnormal grain growth conditions by phase-field method

○Nobuko Mori, Eisuke Miyoshi, Tomohiro Takaki (Kyoto Institute of Technology, Japan)

[P1-63] **Phase Field Crystal Modeling of Mechanism of Strain-Driven for Nucleation and Grain of Deformed-Grain**

○Ying-Jun Gao (Guangxi University, China)

[P1-64] **Diffusion and trapping of hydrogen at grain boundaries scale in fcc polycrystalline nickel: some implications of the atomic volume and the interstitial self-stress**

○xavier Feaugas, jiaqi Li, abdel malek Hallil, abdelali oudriss, arnaud metsue, jamaa bouhattate (university of La Rochelle, France)

Poster Session | J. Multiscale Modeling of Heterogeneous Layered Media

[PO-J1] Poster Session 1

5:45 PM - 8:00 PM Poster Hall

[P1-65] Multiscale Model for Interlayer Defects in Heterogeneous Bilayer Material

○Shuyang Dai[1], David Joseph Srolovitz[2], Yang Xiang[3] (1.Wuhan University, China, 2.University of Pennsylvania, United States of America, 3.Hong Kong University of Science and Technology, Hong Kong)

Poster Session | L. Structure, Statistics and Mechanics in Crystal Dislocation Plasticity

[PO-L1] Poster Session 1

5:45 PM - 8:00 PM Poster Hall

[P1-66] Molecular dynamics study on temperature and loading rate dependence of nano-indentation pop-in load

○Yuji Sato[1], Shuhei Shinzato[1], Takahito Ohmura[2], Shigenobu Ogata[1,3] (1.Department of Mechanical Science and Bioengineering, Osaka University, Japan, 2.Research Center for Structural Materials, National Institute for Materials Science, Japan, 3.Center for Elements Strategy Initiative for Structural Materials (ESISM), Kyoto University, Japan)

[P1-67] Geometry of curved surface and energetics of in graphene with defects

○Ako Kihara[1], Xiao-Wen Lei[1], Akihiro Nakatani[2] (1.Dept. of Mechanical Engineering, Univ.of Fukui, Japan, 2.Dept. of Adaptive Machine Systems, Osaka Univ., Japan)

[P1-68] Collective motion of dislocation associated with local plasticity initiation and subsequent behavior in bcc metals

○Takahito Ohmura (National Institute for Materials Science, Japan)

Poster Session | M. Time- and History-Dependent Material Properties

[PO-M1] Poster Session 1

5:45 PM - 8:00 PM Poster Hall

[P1-69] FORMATION OF PHYSICAL GELS BY ARRESTED SPINODAL DECOMPOSITION IN CHARGED COLLOIDS

○Jose Manuel Olais-Govea[1], Alonso Gomez-Canales[1], Leticia Lopez-Flores[2], Martin Chavez-Paez[2], Magdaleno Medina-Noyola[2] (1.Instituto Tecnologico y de Estudios Superiores de Monterrey, Mexico, 2.Universidad Autonoma de San Luis Potosi, Mexico)

[P1-70] How to improve the ductility of CuZr BMGs based on cyclic pre-straining: MD simulations and mechanical testing

○Jonathan Amodeo[1], Oriane Baulin[1], Damien Fabregue[1], David Rodney[2] (1.MATEIS, Univ. Lyon 1, France, 2.ILM, Univ. Lyon 1, France)

[P1-71] **Modeling plastic deformation of amorphous solids from atomic scale mechanisms**

○Francesca Boioli[1], Tristan Albaret[2], David Rodney[2] (1.LEM, CNRS-ONERA, Chatillon, France, France, 2.ILM, University of Lyon 1, France, France)

[P1-72] Thermally Activated Creep and Constant Shear Rate Deformation in Amorphous Materials

○Samy MERABIA[1], Julien LAM[2], François DETCHEVERRY[1] (1.CNRS and Universite Lyon 1, France, 2.Université de Bruxelles, Belgium)

[P1-73] Numerical analysis of shrinkage process based on the experimental data

○Barbara Kucharczykova[1], Hana Simonova[2], Petr Frantik[2] （1.Brno University of Technology, Faculty of Civil Engineering, Institute of Building Testing, Czech Republic, 2.Brno University of Technology, Faculty of Civil Engineering, Institute of Structural Mechanics, Czech Republic）

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

[PO-O1] Poster Session 1

5:45 PM - 8:00 PM Poster Hall

[P1-74] Designing Lubricant Additives for Titanium Carbide Surface: First-principles and Molecular Dynamics Investigations

○Tasuku Onodera, Jun Nunoshige, Hiroshi Kanemoto （Research &Development Group, Hitachi, Ltd., Japan）

[P1-75] Crystal Growth Molecular Dynamics Simulation of alpha-Al_2O_3 Cutting Tools for Realizing Their Best Tribological Properties

○Shandan BAI[1], Hiroya Nakata[1], Jingxiang Xu[2], Nobuki Ozawa[2], Momoji Kubo[2] （1.KYOCERA Cop., Japan, 2.Tohoku Univ., Japan）

[P1-76] Atomistic modeling of polymer friction

○Robin Sam Vacher （SINTEF-NTNU, Norway）

[P1-77] A two degree-of-freedom extension to the Prandtl Tomlinson-model for friction strengthening in layered materials

○David Andersson[1,2], Astrid de Wijn[2] （1.Department of Physics, Stockholm University, Sweden, 2.Department of Mechanical and Industrial Engineering, Norwegian University of Science and Technology, Norway）

[P1-78] Analysis of Friction Characteristics of Steel Powders using Parallelized Discrete Element Method

○Naoki Yashiro[1,2], Kouya Oohira[2], Natsuko Sugimura[1], Hitoshi Washizu[1] （1.Graduate School of Simulation Studies, University of Hyogo, Japan, 2.Advanced Technology R&D Center, NTN Corporation, Japan）

[P1-80] Dynamics of Polymer Under Shear in Confinement Geometry

○Taiki Kawate[1], Soma Usui[1], Hiroaki Yoshida[2], Hitoshi Washizu[1] （1.Univ. of Hyogo, Japan, 2.Toyota Central R&D Labs, Japan）

[P1-81] Dynamics of a Polymer in Bulk Solution under Shear Flow

○Soma Usui[1], Taiki Kawate[1], Hiroaki Yoshida[2], Hitoshi Washizu[1] （1.Univ. of Hyogo, Japan, 2.Toyota Central R&D Labs., Japan）

[P1-82] Mechanochemistry induced atomic wear in chemical mechanical polishing processes

○Jialin Wen, Tianbao Ma, Xinchun Lu （Dept. of Mechanical Engineering, Tsinghua Univ., China）

[P1-83] Adsorption property of a fatty acid on iron surface with grain boundary

○Yuki Uchiyama, Yoshinori Shiihara, Ivan Lobzenko （Toyota Technological Institute, Japan）

Wed. Oct 31, 2018

Poster Hall

Poster Session | A. Advances in Materials Theory for Multiscale Modeling

[PO-A2] Poster Session 2

5:45 PM - 8:00 PM Poster Hall

[P2-01] Multiscale model of solid state amorphization during processing of pharmaceutical materials

Chunyu Li[1], Yifei Zeng[1], Lorena Alzate-Vargas[1], Pilsun Yoo[1], Rachel Frocino[2], Jeff Brum[2], Peilin Liao[1], Marisol Koslowski[1], ○Alejandro Strachan[1] （1.Purdue University, United States of America, 2.GlaxoSmithKline, Analytical Sciences and Development, United States of America）

[P2-02] FTMP-based Modeling and Simulations of HCP Mg Single Crystal

○Takahiro Kitano, Tadashi Hasebe （Dept. of Mechanical Engineering, Kobe Univ., Japan）

[P2-03] Nonlinear elasticity on Riemannian manifold and its application to general surface development

○Yuto Horikawa[1], Ryuichi Tarumi[2], Yoji Shibutani[1] （1.Dept. of Mechanical Engineering, Osaka Univ., Japan, 2.Grad. Sch. of Engineering Science, Osaka Univ., Japan）

[P2-04] The challenge of achieving quantitative phase field models for microstructure evolution in irradiated solids - the case of voids

○Anter El-Azab （Purdue University, United States of America）

[P2-05] A Molecular-Dynamics Study of Surface Tension: From Alloy Droplets to Bubbles in Molten Alloy

○Xiangming Ma, Hongtao Liang, Yang Yang （East China Normal Univercity, China）

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

[PO-B2] Poster Session 2

5:45 PM - 8:00 PM Poster Hall

[P2-06] Effects of rhenium on the mechanical behavior of irradiated tungsten: a molecular dynamics study using neural-network potential

○Ryo KOBAYASHI （Nagoya Institute of Technology (NITech), Japan）

[P2-07] Diffusion behavior and temperature dependence of hydrogen in tungsten and molybdenum under isotropic strain state

○QuanFu Han[1], Yue-Lin Liu[2], Ying Zhang[1], Guang-Hong Lu[1] （1.Beihang University, China, 2.Yantai University, China）

[P2-08] **Diffusion of Point Defects on Tungsten Surface**

Jiannan Hao[1], ○Shuo Jin[1], Haixuan Xu[2], Xiaolin Shu[1], Guanghong Lu[1] （1.School of Physics and Nuclear Energy Engineering, Beihang University, China, 2.Department of Material Science and Engineering, The University of Tennessee, Knoxville, United States of America）

[P2-09] Influence of anisotropic strain and temperature on hydrogen dissolution in tungsten

○Ying zhang[1], Quan Fu Han[1], Yue lin Liu[2], Guang Hong Lu[1] （1.Beihang University, China, 2.Yantai University, China）

[P2-10] Screw dislocation-interstitial solute coevolution in W-O alloys using atomistically-informed kinetic Monte Carlo simulations

○Yue Zhao[1], Lucile Dezerald[3], Jaime Marian[1,2] （1.Dept. of Materials Science and Engineering, University of California, Los Angeles, United States of America, 2.Dept. of Mechanical Engineering, University of California, Los Angeles, United States of America, 3.Institut Jean Lamour, University of Lorraine, France）

[P2-11] 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）

[P2-13] **Dynamics of Magnetism in Neutron Irradiated Iron-Chromium Steels**

○Jacob B. J. Chapman, Pui-Wai Ma, Sergei L. Dudarev （Culham Centre for Fusion Energy (CCFE), UK）

[P2-14] **Atomistic insights into the grain boundaries interaction with radiation-induced point defects in bcc Fe-Cr alloys**

○Marcin Roland Zemla, Jan Stanislaw Wrobel, Tomasz Wejrzanowski （Faculty of Materials Science and Engineering, Warsaw University of Technology, Woloska 141, 02-507 Warsaw, Poland）

[P2-15] Production and Process of Cascade Development in Irradiated Pure α-Zr from Molecular Dynamics Simulations

○Rongjian Pan[1], Lu Wu[1], Xiaoyong Wu[1], Aitao Tang[2], Bang Wen[1], Wen He[1], Y.R. Ovcharenko[3], D.O.

Kharchenko[3] (1.The First Sub-Institute, Nuclear Power Institute of China, China, 2.College of Materials Science and Engineering, Chongqing University, China, 3.Institute of Applied Physics, National Academy of Science of Ukraine, Ukraine)

[P2-16] Microstructure evolution of cascade annealing in irradiated pure α-Zr from molecular dynamics simulations

○Bang Wen[1], Rongjian Pan[1], Wei Zhang[1], Lu Wu[1], Xiaoyong Wu[1], Aitao Tang[2], Wen He[1], Y.R. Ovcharenko[3], D.O. Kharchenko[3] (1.The First Sub-Institute, Nuclear Power Institute of China, China, 2.College of Materials Science and Engineering, Chongqing University, China, 3.Institute of Applied Physics, National Academy of Science of Ukraine, Ukraine)

Poster Session | C. Crystal Plasticity: From Electrons to Dislocation Microstructure

[PO-C2] Poster Session 2

5:45 PM - 8:00 PM Poster Hall

[P2-18] **Prediction of Biaxial Tensile Deformation Behavior of Aluminum Alloy Sheets using Crystal Plasticity Finite Element Method and Machine Learning**

○Kota Koenuma[1], Akinori Yamanaka[1], Ikumu Watanabe[2], Toshihiko Kuwabara[1] (1.Tokyo University of Agriculture and Technology, Japan, 2.National Institute of Materials Science, Japan)

[P2-19] MobiDiC: A 3-D Dislocation Dynamics Simulation

○Ronan MADEC[1], Laurent COLOMBET[1], Ladislas KUBIN[2] (1.CEA, DAM, DIF, France, 2.LEM, UMR 104 CNRS-ONERA, Université Paris Saclay, France)

[P2-20] Temperature dependence of fatigue crack growth in Ti-6Al-4V

○Bhargavi Rani Anne, Masaki Tanka, Tatsuya Morikawa (Dept. of Materials Science and Engineering, Kyushu University, Japan)

[P2-21] Parametric model of discrete dislocation dynamics based on mathematical theory of moving curves

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

[P2-22] On Visualization of Multiscale Information Transfer/Exchange Processes via FTMP-based Duality Diagram Representation Scheme

○Takuya Takagi, Tadashi Hasebe (Dept. of Mechanical Engineering, Kobe Univ., Japan)

[P2-23] **Rotational Field Evolutions based on Field Theory of Multiscale Plasticity (FTMP)**

○Tadashi Hasebe[1], Yasutaka Matsubara[2] (1.Kobe Univ., Japan, 2.Graduate School of Kobe Univ., Japan)

[P2-24] **A 2D MESOSCALE STUDY OF DISLOCATIONS, CRACKS AND MARTENSITIC PHASE TRANSFORMATIONS**

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

[P2-25] Effects of Stress Distribution on the Plastic Deformation of Metallic Glasses under Different Geometries

○Chih-Jen Yeh[1], Hsuan-Teh Hu[1], Chang-Wei Huang[2], Yu-Chieh Lo[3] (1.National Cheng Kung University, Taiwan, 2.Chung Yuan Christian University, Taiwan, 3.National Chiao Tung University, Taiwan)

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

[PO-D2] Poster Session 2

5:45 PM - 8:00 PM Poster Hall

[P2-26] Generalized nano-thermodynamic model for predicting size-dependent surface segregation in multi-metal alloy nanoparticles from smaller particles

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

[P2-27] Development of thermodynamic database of Nd-Fe-B-based permanent magnet alloys

○Jiang Wang, Lei Xu, Kaicheng Yang, Qingrong Yao, Guanghui Rao, Huaiying Zhou (School of Material Science and Engineering, Guilin University of Electronic Technology, China)

[P2-28] Design of proteins and biopolymers: role of directional interactions and of water.

○Valentino Bianco[1], Ivan Coluzza[2] (1.University of Vienna, Austria, 2.CIC biomaGUNE, center for cooperative research in biomaterials, Spain)

[P2-29] Aquatic pollutant removal by adsorption in zeolite structures: An experimental and molecular simulation study

○Mate Erdos[1], Nan Jiang[2], Sebastian G. J. Heijman[2], Othonas A. Moultos[1] (1.Process &Energy Department, Faculty of Mechanical, Maritime and Materials Engineering, Delft University of Technology,

Netherlands, 2.Department of Water Management, Faculty of Civil Engineering and Geosciences, Delft University of Technology, Netherlands）

[P2-30] Optimizing elastic moduli of the silicate glasses through high-throughput atomistic modeling and machine learning techniques

Yong-Jie Hu[1], Ge Zhao[2], Tyler Del Rose[1], ○Liang Qi[1] （1.Dept. of Materials Science and Engineering, University of Michigan, United States of America, 2.Department of Statistics, Pennsylvania State University, United States of America）

[P2-31] High pressure phase transition and structural stability of transition metal compounds

○Fanyan Meng[1], Wandong Xing[1,2], Rong Yu[2] （1.Dept. of Physics, University of Science and Technology Beijing, China, 2.School of Materials Science and Engineering, Tsinghua University , China）

[P2-32] Development of artificial neural network model for prediction of electronic density of states in atomistic systems

○Atsushi Kubo, Yoshitaka Umeno （Institute of Industrial Science, the University of Tokyo, Japan）

[P2-33] Development of First-principles Platform Technology for Energy Research

○Kanghoon Yim[1], Chan-Woo Lee[1], Jehyun Lee[1], Incheol Jeong[2], Yong Youn[3], Seungwu Han[3] （1.R&D Platform Center, Korea Institute of Energy Research, Korea, 2.Dept. of Energy Science and Engineering, Daegu Gyeongbuk Institute of Science &Technology, Korea, 3.Seoul National University, Korea）

Poster Session | E. Deformation and Fracture Mechanism of Materials

[PO-E2] Poster Session 2

5:45 PM - 8:00 PM Poster Hall

[P2-34] Dynamics of a solidification front made by invasion of fluid with a different temperature

○So Kitsunezaki, Chika Yamanaka （Nara Women's Univ., Japan）

[P2-35] Strengthening through solid solution in $W_{1-x}Ta_xB$ system

○lijuan liu[1], Wandong Xing[2], Fanyan Meng[1], Rong Yu[2] （1.Dept. of Applied Physics, University of Science and Technology Beijing, China, 2.School of Materials Science and Engineering, Tsinghua University , China）

[P2-36] Desiccation crack patterns based on phase-field modeling and their statistical properties

○Shin-ichi Ito[1], Satoshi Yukawa[2] （1.The Univ. of Tokyo, Japan, 2.Osaka Univ., Japan）

[P2-37] Ce-terminated (111) surface of CeO_2

○YaNan Zhao[1], Wandong Xing[2], Fanyan Meng[1], Rong Yu[2] （1.Dept. of Applied Physics, University of Science and Technology Beijing, China, 2.School of Materials Science and Engineering, Tsinghua University , China）

[P2-39] **Numerical analysis of elasto-plastic behavior of metallic architectured materials**

○Filip Siska[1], Ivo Dlouhy[1], Jan Cizek[2], Hanus Seiner[3] （1.Institute of Physics of Materials, Czech Academy of Sciences, Czech Republic, 2.Institute of Materials Science and Engineering, Brno University of Technology, Czech Republic, 3.Institute of Thermomechanics, Czech Academy of Sciences, Czech Republic）

[P2-40] Automatic analysis and numerical prediction of flow stress curves for aluminium alloys

○Evgeniya Kabliman, Johannes Kronsteiner, Ana-Helena Kolody （Light Metals Technologies Ranshofen, Center fo Low-Emission Transport, Austrian Institute of Technology, Austria）

[P2-41] Comparison of different alkali activated mortars with hemp fibres response during fracture test by acoustic emission method

Libor Topolar[1], ○Hana Simonova[1], Barbara Kucharczykova[1], Zbynek Kersner[1], Jelena Dragas[2], Ivan Ignjatovic[2], Miroslav Komljenovic[3], Violeta Nikolic[3] （1.Brno University of Technology, Faculty of Civil Engineering, Czech Republic, 2.University of Belgrade, Faculty of Civil Engineering, Serbia, 3.University of Belgrade, Institute for Multidisciplinary Research, Serbia）

Poster Session | F. From Microstructure to Properties: Mechanisms, Microstructure, Manufacturing

[PO-F2] Poster Session 2

5:45 PM - 8:00 PM Poster Hall

[P2-43] Design of spontaneous formation-based 3D plasmonic optical structure, using multyphysics modeling

○Jihwan Song[1], Inhee Choi[2], Yonghee Shin[3], SoonGweon Hong[5], Younggeun Park[5], Dongchoul Kim[4], Taewook Kang[3], Luke Lee[5] （1.Dept. of Mechanical Engineering, Hanbat National University, Korea, 2.Dept. of Life Science, University of Seoul, Korea, 3.Dept. of Chemical and Biomolecular Engineering, Sogang

University, Korea, 4.Dept. of Mechanical Engineering, Sogang University, Korea, 5.Dept. of Bioengineering and Berkeley Sensor and Actuator Center, University of California, Berkeley, United States of America）

[P2-44] **Characterization of $K_xNa_{1-x}NbO_3$ powders and ceramics prepared by hydrothermal synthesis**

○Jing Yang, Aifen Tian, Xuan Xi, Huiling Du （Dept. of Materials Science and Engineering, Xi An Univ. of Science and Technology, China）

[P2-45] Numerical and experimental investigation of liquid metal dealloying of Cu-Ni alloy in liquid silver.

○Pierre-Antoine Geslin[1,2,3], Takumi Suga[2], Takeshi Wada[2], Hidemi Kato[2] （1.INSA Lyon/CNRS, France, 2.Institute for Materials Research, Tohoku University, Japan, 3.Frontier Research Institute for Interdisciplinary Sciences, Tohoku University, Japan）

[P2-46] **Application of DLVO theory to predict dispersion stability of ZrO_2 submicron particles in electrolyte solutions**

○Ming-Hong Chiueh, Tien-Jung Huang （Industrial Technology Research Institute, Taiwan）

[P2-47] Multi-GPU large-scale phase-field lattice Boltzmann simulation of dendrite growth with thermal-solutal convection

○Shinji Sakane[1], Tomohiro Takaki[1], Munekazu Ohno[2], Yasushi Shibuta[3], Takayuki Aoki[4] （1.Kyoto Institute of Technology, Japan, 2.Hokkaido University, Japan, 3.The University of Tokyo, Japan, 4.Tokyo Institute of Technology, Japan）

[P2-48] Stress analysis of 4H-SiC power devices via FEM and Raman spectroscopy

○Hiroki Sakakima[1], Asuka Hatano[1], Akihiro Goryu[2], Kenji Hirohata[2], Satoshi Izumi[1] （1.The Univ. of Tokyo, Japan, 2.Toshiba, Japan）

[P2-49] A Functionally Graded Multi-Phase Micromechanical Model for Carbon Nanotube - Polymer Composites

○Vahidullah Tac[1,2], Ercan Gurses[1] （1.Middle East Technical University, Turkey, 2.Turkish Aerospace Industries, Turkey）

[P2-50] **Atomic surface treatment of copper nanowires by electron beam irradiation simulated by first principle calculation**

○Shih Kuang Lee （National Chiao Tung University, Taiwan）

[P2-51] Molecular-Dynamic Simulation of Rapid Solidification of Dipolar Molecular Crystal from Its Melt

○Xianqi Xu, Yang Yang （East China Normal University, China）

[P2-52] Intrinsic Analysis of Structural Order Parameter at Equilibrium Crystal-Melt Interfaces

○Wenliang Lu, Hongtao Liang, Yang Yang （EAST CHINA NORMAL UNIVERSITY, China）

[P2-53] Multiscale Modelling of Indirect-to-Direct Band Gap Transition in Silicon Nanosheets

○Byung-Hyun Kim[1], Chan-Woo Lee[1], Mina Park[2], Gyubong Kim[2], Kersti Hermansson[3], Peter Broqvist[3], Heon-Jin Choi[4], Kwang-Ryeol Lee[2] （1.R&D Platform Center, Korea Institute of Energy Research, Korea, 2.Computational Science Research Center, Korea Institute of Science and Technology, Korea, 3.Dept. of Chemistry-Ångström Laboratory, Uppsala University, Sweden, 4.Dept. of Materials Science and Engineering, Yonsei University, Korea）

Poster Session | G. Modeling Mechanical Behavior of Materials under Harsh Environments

[PO-G2] Poster Session 2

5:45 PM - 8:00 PM Poster Hall

[P2-54] **Component-wise Effect of Incompatibility Tensor on Misorientation Development in Lath Block Structure Model based on FTMP**

○Yuta Amano, Tadashi Hasebe, Yasutaka Matsubara （Dept. of Mechanical Engineering, Kobe Univ., Japan）

[P2-55] Construction of virtual ITZ specimens using extended stochastic optimization and evaluation of their permeability

○Se-Yun Kim, Tong-Seok Han （Dept. of Civil and Environmental Engineering, Yonsei Univ., Korea）

[P2-56] Estimation for probabilistic distribution of material response according to microstructural characteristics

○JI-SU KIM, Tong-Seok Han （Yonsei Univ., Korea）

[P2-57] **Hypervelocity impact and shock behavior of pillared graphene foams**

○Stefano Signetti, Seunghwa Ryu （Department of Mechanical Engineering, Korea Advanced Institute of Science and Technology (KAIST), Korea）

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

[PO-H2] Poster Session 2

5:45 PM - 8:00 PM Poster Hall

[P2-58] Studying the kinetics of a self-propelled cruiser in 2D granular media under gravity

○Guo-jie Jason Gao （Dept. of Mathematical and Systems Engineering, Shizuoka Univ., Japan）

[P2-59] A Discrete Tetris model showing two flow regimes for hard particles exiting a hopper with an adjustable obstacle

○Tomoya Yasuno[1,2], Guo-jie Jason Gao[1] （1.Dept. of Mathematical and Systems Engineering, Shizuoka Univ., Japan, 2.Dept. of Complex Systems Science, Nagoya Univ., Japan）

[P2-60] Effect of water molecules on polymer chain motion in dense chain ensembles of nafion membrane

○Isamu Riku, Ryoma Oka, Koji Mimura （Osaka Prefecture Univ., Japan）

[P2-61] A Coarse-Grained Model for Competitive Adsorption on the Surface of Inorganic Nanomaterials

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

[P2-62] Molecular Dynamics of Inorganic and Organic Interfaces with Force-Field Parameters Based on DFT Simulations

○Kosuke Ohata, Hiroya Nitta, Kenta Chaki, Taku Ozawa （JSOL Corporation, Japan）

[P2-63] **Molecular dynamics screening for developing compounds of electrolytes with high performance in lithium ion batteries**

○Yoshihiro Takai[1], Ken-ichi Saitoh[2], Masanori Takuma[2], Yoshimasa Takahashi[2], Tomohiro Sato[2] （1.Graduate school of Science and Engineering, Kansai Univ., Japan, 2.Faculty of Engineering Science, Kansai Univ., Japan）

[P2-64] Molecular dynamics study on transmission mechanism of torsional deformation in cellulose nanofibers with hierarchical structure

○Kentaro Takada[1], Ken-ichi Saitoh[2], Masanori Takuma[2], Yoshimasa Takahashi[2], Tomohiro Sato[2] （1.Graduate School of Science and Engineering, Kansai Univ., Japan, 2.Faculty of Engineering Science, Kansai Univ., Japan）

[P2-65] Bubble dynamics of foam flow around an obstacle

○Antti Puisto, Juha Koivisto, Leevi Viitanen, Mikko J Alava （Aalto University, Department of Applied Physics, Finland）

[P2-66] Shape Deformation and Mechanical Relationship of Ionic Droplet Under An Electric Field

Bo-Yu Shih[1], ○Wei-Chun Lin[1], Alice Hu[2], Hsuan-Teh Hu[1], Yu-Chieh Lo[3] （1.Department of Civil Engineering,National Cheng Kung University, Taiwan, 2.Department of Mechanical and Biomedical Engineering, City University of Hong Kong, Hong Kong, 3.Department of Materials Science and Engineering, National Chiao Tung University, Taiwan）

[P2-67] Multiscale modeling of surface functionalized graphene/polymer nanocomposites: insight into the effect of covalent grafting

○Jeong-ha Lee[1], Seunghwa Yang[2] （1.Dept. of Energy Engineering, Chung-Ang Univ., Korea, 2.Dept. of Energy Systems Engineering, Chung-Ang Univ., Korea）

[P2-68] Durability analysis on the environmental aging of epoxybased nanocomposite

○Sunyong Kwon[1], Man Young Lee[2], Seunghwa Yang[3] （1.Dept. of Energy Engineering, Chung-Ang Univ., Korea, 2.Agency for Defense Development, Korea, 3.Dept. of Energy Systems Engineering, Chung-Ang Univ., Korea）

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

[PO-I2] Poster Session 2

5:45 PM - 8:00 PM Poster Hall

[P2-69] **Topological evolution of the microstructures of thin films during grain growth**

○Ahu Oencue[1], Thorsten Halle[2], Dana Zoellner[3] （1.Institute of Experimental Physics, Otto-von-Guericke University Magdeburg, Germany, 2.Institute of Materials and Joining Technology, Otto-von-Guericke University Magdeburg, Germany, 3.B CUBE Center for Molecular Bioengineering, TU Dresden, Germany）

[P2-70] Molecular dynamics simulations of phase transformations in nanocrystalline NiTi shape-memory alloys

○Won-Seok Ko （University of Ulsan, 93 Daehak-ro, Nam-gu, Ulsan, 44610, Korea）

[P2-71] An attempt to connect migration of grain boundaries to their atomic structures with help of Molecular Dynamics

Zakaria El Omari, ○Sylvain Queyreau, Charlie Kahloun,

Brigitte Bacroix （Universite Paris XIII, Sorbonne Paris Cite, Laboratoire des Sciences des Procedes et des Materiaux, LSPM UPR 3407, France）

[P2-72] Disconnection interaction in Cu grain boundaries

○Christian Brandl （Karlsruhe Institute of Technology, Germany）

[P2-73] Phase-field Approach to Thermo-mechanical Behavior of Through-silicon Vias

Wooju Lee, ○jaekeun yoon, Dongchoul Kim （Sogang Univ., Korea）

[P2-74] **Grain-Growth in Nanocrystalline Metals under Ion Irradiation: A Thermal Spike Model**

○Djamel Kaoumi[1], Robert Birtcher[2], Arthur Motta[3]（1.North Carolina State University, United States of America, 2.Argonne National Laboratory, United States of America, 3.Penn State University, United States of America）

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

[PO-N2] Poster Session 2

5:45 PM - 8:00 PM Poster Hall

[P2-75] **Why the structure-property relationship in metallic glasses should be established beyond short-range order: Insight from potential energy landscape**

○Dan Wei[1,2], Yunjiang Wang[1,2], Lanhong Dai[1,2]（1.University of Chinese Academy of Sciences, China, 2.Institute of Mechanics, Chinese Academy of Sciences, China）

[P2-76] Vacancy segregation analysis near grain boundaries in metallic systems by long-time atomistic simulations

○Shotaro Hara （Dept. of Mechanical Engineering, Chiba Institute of Technology, Japan）

[P2-77] **EXPERIMENTAL AND DENSITY FUNCTIONAL THEORY STUDIES OF PRECIPITATE INTERFACES IN ALUMINIUM ALLOYS, WITH FOCUS ON β" & β**

○Haris Rudianto, Deni Hariadi, Andriansyah Andriansyah（Gunadarma University, Indonesia）

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

[PO-O2] Poster Session 2

5:45 PM - 8:00 PM Poster Hall

[P2-78] Adsorption of Volatile Organic Compounds (VOCs) on Silicene by Density Functional Theory Calculations

○Thi Viet Bac Phung[1], Trong Lam Pham[1], Van An Dinh[1,2]（1.Nanotechnology Program, Vietnam Japan University - Vietnam National University, Viet Nam, 2.Center for Atomic and Molecular Technologies, Graduate School of Engineering, Osaka University, Japan）

[P2-79] Atomistic insights into defect formation mechanism in single crystal SiC based on molecular dynamics simulation

○Kenji Nishimura[1], Koji Miyake[1], Ken-ichi Saitoh[2]（1.AIST, Japan, 2.Kansai Univ., Japan）

[P2-80] **Potential cathode material Na_xVOPO_4 for rechargeable Sodium - ion batteries: DFT investigation**

○Duc Huu Luong[1], An Van Dinh[1,2], Yoshitada Morikawa[3], Yoji Shibutani[2,1] （1.Nano Technology Program, Vietnam Japan University, Viet Nam, 2.Center for Atomic and Molecular Technology, Graduate School of Engineering, Osaka University, Japan, 3.Department of Precision Science and Technology, Graduate School of Engineering, Osaka University, Japan）

[P2-81] **Two-dimensional Na_xSiS as a promising anode material for rechargeable Sodium-based batteries: Ab initio material design.**

Thi Dung Pham[1], ○Van An Dinh[1,2], Kazunori Sato[3], Yoji Shibutani[1,2] （1.Nanotechnology Program, Vietnam Japan University, Viet Nam, 2.Center for Atomic and Molecular Technology, Graduate School of Engineering, Osaka University, Japan, 3.Division of Materials and Manufacturing Science, Graduate School of Engineering, Osaka University, Japan）

[P2-82] Modelling and analysis of SiO2 interfaces of non-firing solids

○Tomohiro Sato[1], Ken-ichi Saitoh[1], Masayoshi Fuji[2], Chika Yamashita Takai[2], Hadi Razavi[2], Masanori Takuma[1], Yoshimasa Takahashi[1] （1.Dept. of Mechanical Engineering, Kansai Univ., Japan, 2.Advanced Ceramics Reserch Center, Nagoya Institute of Technology, Japan）

Poster Session | A. Advances in Materials Theory for Multiscale Modeling

[PO-A1] Poster Session 1

Symposium A

Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall

[P1-01] The Coadsorption Effect of Cl- and H_2O on the Various Defect Al_2O_3 Film Surface

○Chuan-Hui Zhang, Bao Chen, Peng Shi （University of Science and Technology Beijing, China）

[P1-02] Incorporation of double cross-slip in continuum dislocation dynamics

○Xingjian Zhou, Yichao Zhu （Faculty of vehicle Engineering and Mechanics, Dalian University of Technology, China）

[P1-03] **Effect of Defect on Structural and Optical Properties in Methyl-Ammonium Lead Iodide(MAPI) Perovskite via First Principles Calculations**

○Abdullah Al ASAD, Keiichi MITANI, Atsushi ISHIKAWA, Kenji TSURUTA （Dept. of Electrical and Electronic Engineering, Okayama University, Japan）

[P1-04] Isogeometric modeling and large-scale computation for stress field around lattice defects

○Shunsuke Kobayashi[1], Ryuichi Tarumi[2], Atsushi Suzuki[3], Masao Ogino[4], Yoji Shibutani[1] （1.Graduate School of Engineering, Osaka Univ., Japan, 2.Graduate School of Engineering Science, Osaka Univ., Japan, 3.Cybermedia Center, Osaka Univ., Japan, 4.Information Technology Center, Nagoya Univ., Japan）

[P1-05] **A local/nonlocal plasticity model for upscaling microstructural effects**

○John Mitchell （Sandia National Laboratories, United States of America）

[P1-06] **First-principles investigation of atomic hydrogen adsorption and diffusion on/into Mo-doped Nb (100) surface**

○Zhong-min Wang, Yang Wu, Qingrong Yao, Yan Zhong, Chaohao Hu, Huaiying Zhou （Guilin University of Electronic Technology, China）

[P1-07] **First-principles Study on Electronic Properties of Hybrid MABX_3 perovskites (MA= $CH_3NH_3^+$; *B*= Pb, Sn, Ge; *X*= I, Br, Cl)**

○Narasak Pandech[1,2], Thanundon Kongnok[1], Sirichok Jungthawan[1], Sukit Limpijumnong[1], Walter R.L Lambrecht[2] （1.School of Physics and NANOTEC-SUT Center of Excellence on Advanced Functional Nanomaterials, Suranaree University of Technology, NakhonRatchasima 30000, Thailand, Thailand, 2.Department of Physics, Case Western Reserve University, Cleveland, Ohio 44106-7079, USA., United States of America）

(Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall)

[P1-01] The Coadsorption Effect of Cl- and H_2O on the Various Defect Al$_2O_3$ Film Surface

○Chuan-Hui Zhang, Bao Chen, Peng Shi （University of Science and Technology Beijing, China）

First-principles calculations have been performed on the perfect surface, point-defect surface, step-defect surface, layer-defect surface of Al_2O_3 film with water molecules and chloride ions. The coadsorption mechanism has effect on the reaction and erosion of the surface. The adsorption energies (E_{ads}), stable adsorbed sites, binding of film, charge transfer, reactants and products, activation energies and transition states are calculated and discussed. The results evidence that for the perfect Al_2O_3 surface, the critical monolayer of Cl- is 3/7, the E_{ads} decrease in three steps, each E_{ads} step only relate to the adsorbed site and the morphology. For point-defect surface, substitution point defects are more sensitive than vacancy point defects for reaction and erosion. The species of products depend on the energy barrier and orientation of water. For step-defect surface, Al1 step-defect and Al3 step-defect surfaces prefer to obtain Al-H_2O compounds, while O2 step-defect surface prefers to form Al-Cl products. There is no obvious linear relationship between the number of products and the number of steps. For layer-defect surface, when low concentrations of Cl ions reach the surface, they prefer to erode the Al layer-defect surface with producing Al-Cl compounds, while they prefer to interact with H_2O upon the O layer-defect surface.

(Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall)

[P1-02] Incorporation of double cross-slip in continuum dislocation dynamics

○Xingjian Zhou, Yichao Zhu （Faculty of vehicle Engineering and Mechanics, Dalian University of Technology, China）

It is widely agreed that the cross-slip mechanism of screw dislocations plays a key role as crystalline materials deform plastically. In discrete dislocation dynamics (DDD) models, the onset of cross-slip is widely formulated as a random event. However, a proper formulation of cross-slip in models of continuum dislocation dynamics (CDD), where dislocation microstructures are described as a density distribution, is still missing. In this presentation, we present a CDD framework incorporating cross-slip mechanism. The discrete-to-continuum (D2C) transition is carried out by translating the probability of a discrete event into a collective frequency. This work is conducted under the framework of dislocation density potential function (DDPFs), where the mean-field stress can be evaluated with related ease. Numerical examples will be shown to demonstrate the role of cross-slip in the determination of material’ s stress-strain relation.

(Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall)

[P1-03] Effect of Defect on Structural and Optical Properties in Methyl-Ammonium Lead Iodide(MAPI) Perovskite via First Principles Calculations

○Abdullah Al ASAD, Keiichi MITANI, Atsushi ISHIKAWA, Kenji TSURUTA （Dept. of Electrical and Electronic Engineering, Okayama University, Japan）

Hybrid organic/inorganic perovskites(HOIPs) have drawn significant research interests due to the incomparable rapid rise in energy conversion efficiency seen in photovoltaic devices based on $CH_3NH_3PbI_3$. Current research attempts in this field have concentrated on searching for similar perovskites with better properties, especially stability under a humid condition and/or irradiation [1]. In this work, employing first-principles calculations based on the density functional theory, we have investigated effects of vacancy on the optimized structures, bandgap, total and partial density of state, effective on-site and bond charge, by comparing with relevant experimental and/or theoretical data [2]. These analyses reveal that a Pb vacancy induces an asymmetric distortion of the lattice, which leads to a local volume expansion at low temperature [3]. The degenerate states at the conduction band minimum(CMB) are split each other due to the defect and it promotes broadening of the light absorption spectra. Possible effects of interstitial impurity, such as a water molecule, will also discussed in the presentation.

[1] A. K. Chauhan and P. Kumar, J. Phys. D: Appl. Phys. 50 (2017) 325105.
[2] Y. Wang et al., Phys. Chem. Chem. Phys. 16 (2014)1424.
[3] A. Walsh et al., Angewandte Chemie 2 (2015) 1791.

(Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall)

[P1-04] Isogeometric modeling and large-scale computation for stress field around lattice defects

○Shunsuke Kobayashi[1], Ryuichi Tarumi[2], Atsushi Suzuki[3], Masao Ogino[4], Yoji Shibutani[1] （1.Graduate School of Engineering, Osaka Univ., Japan, 2.Graduate School of Engineering Science, Osaka Univ., Japan, 3.Cybermedia Center, Osaka Univ., Japan, 4.Information Technology Center, Nagoya Univ., Japan）

It is well known that classical elasticity yields singular stress field around the core of lattice defects such as point defects and dislocations. Regularization of the stress singularity is therefore primarily important to understand mechanical behavior of defects from a continuum viewpoint. First strain gradient elasticity (FSGE) generalizes the classical elasticity by introducing the characteristic length l in the constitutive equation. Recent theoretical investigations revealed that FSGE removes the stress singularity at the core of dislocations and disclinations. Hence, the *non-local* elasticity theory is suitable for multiscale modeling of defects in solid. In the present study, we aim to develop (i) isogeometric models for lattice defects and (ii) their numerical implementation for large-scale computation within the framework of FSGE. At first, we derive the weak form stress equilibrium equation for Cauchy-type FSGE. The integrodifferential Euler-Lagrange equation is then solved numerically using isogeometric analysis (IGA), *i.e.*, Galerkin method with the non-uniform rational B-spline (NURBS) basis functions. Consequently, the boundary value problem is cast into a system of linear algebraic equations whose degree of freedom exceeds 20 million. The large-scale computation was conducted on a supercomputer OCTOPUS which is installed in the cyber media center of Osaka Univ. Point defects were modeled using the first-order approximation for the force dipole and implemented into the weak form equation through the body force. The resulting stress fields showed singularity free distribution and they converged to classical solution with increasing in distance from the core. Dislocation model was constructed referring to the extended finite element method (XFEM). This model successfully reproduces the kink deformation from the pairs of equally arrayed edge dislocations.

(Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall)

[P1-05] A local/nonlocal plasticity model for upscaling microstructural effects

○John Mitchell （Sandia National Laboratories, United States of America）

Despite its importance, why is mesoscale plasticity advancing so slowly? The fundamental equations of equilibrium used for mesoscale modeling have not changed in centuries. In this talk, I will present an innovative idea for combining nonlocal/local models to upscale effects of microstructures on plastic deformations. A local von Mises plasticity model is evolved using a nonlocal and peridynamics [1] inspired yield condition [2]. The application area is the analysis ofadditively manufactured metal parts.

Additive manufacturing produces heterogeneous and poorly understood material microstructures. Practical macroscale models that reflect the nature of AM microstructures do not currently exist: length scale effects, grain shape morphologies, grain orientations, intragrain defects, grain boundary heterogeneities, aggregrate textures. For the purpose of engineering design and qualification, it is essential that we develop and advance models for AM built parts.

[1] S.A. Silling, Reformulation of elasticity theory for discontinuities and long-range forces, Journal of the Mechanics and Physics of Solids, 48(1), (2000), 175-209.

[2] J.A. Mitchell, A nonlocal, ordinary, state-based plasticity model for peridynamics, Sandia National Laboratories, tech report SAND2011-3166, May, 2011.

(Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall)

[P1-06] First-principles investigation of atomic hydrogen adsorption and diffusion on/into Mo-doped Nb (100) surface

○Zhong-min Wang, Yang Wu, Qingrong Yao, Yan Zhong, Chaohao Hu, Huaiying Zhou （Guilin University of Electronic Technology, China）

Based on sequential study of the surface model, surface-model slab, H-adsorption sites, and H-diffusion coefficient (D), we investigate the most likely process of atomic hydrogen adsorption and diffusion on/into Mo-doped Nb (100) surface/subsurface (in the $Nb_{12}Mo_4$ case) via first-principles. Our results reveal that the (100) surface is the most stable Mo-doped Nb surface with the smallest surface energy (2.75 J/m^2). Hole sites (HSs) in the Mo-doped Nb (100) surface are H-adsorption-favorable mainly due to their large adsorption energy (4.27 eV), and the H-diffusion path should preferentially be HS→TIS (tetrahedral interstitial site) over HS→OIS (octahedral interstitial site) because of the correspondingly lower H-diffusion energy barrier. With respect to a pure Nb (100) surface, the Mo-doped Nb (100) surface has a smaller energy barrier along the HS→TIS pathway (0.31 eV) and larger H-diffusion coefficient (5.65×10^{-10} m^2s^{-1}).

(Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall)

[P1-07] First-principles Study on Electronic Properties of Hybrid MABX_3 perovskites (MA= $CH_3NH_3^+$; B= Pb, Sn, Ge; X= I, Br, Cl)

○Narasak Pandech[1,2], Thanundon Kongnok[1], Sirichok Jungthawan[1], Sukit Limpijumnong[1], Walter R.L Lambrecht[2] （1.School of Physics and NANOTEC-SUT Center of Excellence on Advanced Functional Nanomaterials, Suranaree University of Technology, NakhonRatchasima 30000, Thailand, Thailand, 2.Department of Physics, Case Western Reserve University, Cleveland, Ohio 44106-7079, USA., United States of America）

Recently, hybrid MABX_3perovskites (MA= $CH_3NH_3^+$; B= Pb, Sn, Ge; X= I, Br, Cl) have revolutionized emerging photovoltaic technologies with the development of highly efficient solar cells, and have attracted significant fundamental research interest. Despite the extremely fast progress in device fabrication, the materials electronic properties, which determine the photovoltaic performance, are not yet fully understood. Here, we performed calculations of these materials, using a van der Waals-corrected density functional theory (DFT) method using the Perdew-Burke-Ernzerhof (PBE) and Heyd-Scuseria-Ernzerhof (HSE) hybrid functionals. Subsequently, we use the GW-approximation to calculate the bands as quasiparticle excitations including also the spin-orbit coupling. The orientation and position of the MA-cation is found to significantly affect the electronic properties around the band edges of the Pb and Sn based compounds. Because Ge based halides already prefer a rhombohedrally distorted perovskite structure with off-centered Ge even for a simple inorganic cation (e.g. Cs), the three-fold symmetry of the MA ion is compatible with a preferred orientation of the molecules along the rhombohedral axis. The interplay between its dipole and the Ge off-centering leads to interesting ferro-electric behavior.

Poster Session | C. Crystal Plasticity: From Electrons to Dislocation Microstructure

[PO-C1] Poster Session 1

Symposium C

Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall

[P1-08] Pressure effects on dislocation core structures in Mg_2SiO_4 olivine: insights from atomic-scale modeling

○Philippe Carrez, Srinivasan Mahendran, Patrick Cordier （Lille University, Lab. UMET UMR-CNRS 8207, France）

[P1-09] Structural and magnetic properties of long-period stacking ordered (LPSO) structure of iron; A first-principles study

○Takao Tsumuraya[1], Ikumu Watanabe[2], Takahiro Sawaguchi[2] （1.Magnesium Research Center/POIE, Kumamoto Univ., Japan, 2.Research Center for Structural Materials, National Institute for Materials Science, Japan）

[P1-11] Dislocation transmission behaviors of bi-crystal BCC Tantalum with high and low angle symmetric tilt grain boundaries: Multiscale simulation study

○Moon Sunil, Kang Keonwook （Dept. of Mechanical Engineering, Yonsei Univ., Korea）

[P1-12] Ab Initio Dislocation Core Calculations using a Cluster Model

○Jonas Frafjord[1,3], Bjørn Holmedal[4], Jesper Friisj[2,3], Randi Holmestad[1,3], Ingeborg-Helene Svenum[2], Inga Gudem Ringdalen[2] （1.Dept. of Physics, Norwegian University of Science and Technology, Norway, 2.SINTEF Industry, Trondheim, Norway, 3.Centre for Advanced Structural Analysis, SIMLab, Norway, 4.Dept. of Materials Science and Engineering, Norwegian University of Science and Technology, Norway）

[P1-13] Anelastic recovery of a steel wire under pure shear strain with various magnetic treatments

○Shigeo Kotake, Takuro Murata （Dept. of Mechanical Engineering, Mie Univ., Japan）

[P1-14] Possible explanation of sudden stress drop at upper yield point in iron by magnetostriction and unpinning dislocations with law of approach in residual magnetization

○Shigeo Kotake （Dept. of Mechanical Engineering, Mie Univ., Japan）

[P1-15] Investigation of dislocation core structure in Aluminum by using a generalized Peierls-Nabarro model

○Hideki MORI （College of Industrial Technology, Japan）

[P1-16] Crystal orientation evolution analysis during deformation using molecular dynamics

○Keisuke Kinoshita （Nippon Steel &Sumitomo Metal Corporation, Japan）

[P1-17] Nanoindentation of Nanoparticles -A Molecular Dynamics and Discrete Dislocation Dynamics Simulations Study

Roy Shyamal[1], Riccardo Gatti[2], Benoit Devincre[2], ○Dan Mordehai[1] （1.Mechanical Engineering, Technion - Israel Institute of Technology, Haifa, Israel, Israel, 2.LEM, UMR 104, CNRS-ONERA, 29 Av. de la Division Leclerc, 4 Chatillon, France, France）

[P1-18] Machine learning interatomic potentials for molecular dynamics simulations of dislocations

○Eyal Oren, Guy Makov （Dept. of Materials Engineering, Ben-Gurion University of the Negev, Israel）

(Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall)

[P1-08] Pressure effects on dislocation core structures in Mg_2SiO_4 olivine: insights from atomic-scale modeling

○Philippe Carrez, Srinivasan Mahendran, Patrick Cordier （Lille University, Lab. UMET UMR-CNRS 8207, France）

Olivine $(Mg,Fe)_2SiO_4$, a silicate with orthorhombic structure, is one of the most common minerals. As an abundant phase of the upper Earth mantle, its plastic properties strongly constrained the thermal convection of Earth mantle in its upper part. Plastic deformation of olivine involves two types of dislocation corresponding to the shortest Burgers vector [001] and [100]. At low temperature and high stress, [001] slip is supposed to be the most predominant slip system whereas at high temperature and low stress, [100] dislocations dominate. Over the last decades, a number of different slip systems have been thus identified in various domain of temperature, strain rate or pressure.
In this study, we revisit plasticity of this silicate by computing at the atomic scale the intrinsic properties of dislocation in Mg_2SiO_4 single crystal. All the calculations rely on a parametrized potential combining coulombic interactions and a core-shell interaction model for oxygen atoms. We performed a systematic investigation of [100] dislocations metastable configurations and possible dissociations.
Our calculations show that at low pressure, the atomic arrangement within the dislocation core is compatible with the [100](010) slip system observed experimentally. Also we show that the occurrence of several metastable core configurations allows to various cross slip events for which the cross slip energy barrier have been computed. Finally, we will show that the various core configurations are strongly sensitive to pressure leading to some change in the relative metastable states of the dislocation core and ultimately inhibiting some known slip plane at higher pressure.

(Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall)

[P1-09] Structural and magnetic properties of long-period stacking ordered (LPSO) structure of iron; A first-principles study

○Takao Tsumuraya[1], Ikumu Watanabe[2], Takahiro Sawaguchi[2] （1.Magnesium Research Center/POIE, Kumamoto Univ., Japan, 2.Research Center for Structural Materials, National Institute for Materials Science, Japan）

Fe-Mn-Si based alloys is known to exhibit a shape-memory effect associated with deformation-induced martensitic transformation from face-centered cubic (fcc) γ-austenite to hexagonal closed packed (hcp) ε-martensitic phase. The Fe-Mn-Si-based alloys with modified chemical compositions appeared to have outstanding properties of low-cycle fatigue lives, and a Fe-15Mn-10Cr-8Ni-4Si (mass%) alloy developed is practically used in a seismic damping component of architectural constructions. Recently, under cyclic push-pull loading of Fe-Mn-Si-based alloys, a new phase different from ε-phase was found by transmission electron microscopy. The new phase shows electron diffraction spots at the 1/3 position of the {10-11} spots of the ε-phase, which suggests the existence of a long-period stacking ordered (LPSO) structure. In 1960s, a similar phase was reported after several times of thermal cycles of γ-ε phase phase transitions in Fe-Mn-C alloys. However, actual stacking sequence of the LPSO phase and relative stability with γ and ε-phases still remain unclear. To understand these issues, we proposed several structural models of LPSO structure of pure Fe, such as 4H, $6H_1$ and $6H_2$, and discuss structural and magnetic stabilities among the candidate of LPSO structures with first-principles calculation methods. [1] L. I. Lysak, and B. I. Nikolin, Fiz Met. Mettaloved **20**,

547 (1965), *ibid*. **23**, 93 (1967).

(Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall)

[P1-11] Dislocation transmission behaviors of bi-crystal BCC Tantalum with high and low angle symmetric tilt grain boundaries: Multiscale simulation study

○Moon Sunil, Kang Keonwook （Dept. of Mechanical Engineering, Yonsei Univ., Korea）

In this research, we conducted multiscale (molecular dynamics and dislocation dynamics) simulations to study dislocation transmission behaviors of bi-crystal BCC Tantalum (Ta) with high and low angle symmetric tilt grain boundaries. To investigate dislocation transmission behaviors, we introduced a dislocation loop to describe the Frank-Read source, one of the dislocation multiplications in molecular dynamics simulation. We put dislocation loop on the slip plane where maximum resolved shear stress occurs. In molecular dynamics simulation, we observed interactions between dislocation and grain boundary such as dislocation transmission and absorption. Furthermore, we performed dislocation dynamics simulation to observed similar dislocation transmission behaviors. Finally, we analyzed mechanical property changes (e.g. stress-strain response) as dislocation interacts with grain boundary.

Acknowledgement

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(Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall)

[P1-12] Ab Initio Dislocation Core Calculations using a Cluster Model

○Jonas Frafjord[1,3], Bjørn Holmedal[4], Jesper Friisj[2,3], Randi Holmestad[1,3], Ingeborg-Helene Svenum[2], Inga Gudem Ringdalen[2] （1.Dept. of Physics, Norwegian University of Science and Technology, Norway, 2.SINTEF Industry, Trondheim, Norway, 3.Centre for Advanced Structural Analysis, SIMLab, Norway, 4.Dept. of Materials Science and Engineering, Norwegian University of Science and Technology, Norway）

Solute strengthening is an important mechanism contributing to the strength of metallic alloys. In order to create an accurate framework for strength calculations, this mechanism must be fully understood. In that regard, studies have shown that it is crucial to include the core region of a dislocation in models [1-3], as the core interacts strongly with solute atoms through short-range interactions, and affects the dislocation mobility. The core region can be treated from first principles to include electronic effects. One challenge has been to correctly describe the dissociation of a dislocation at atomic level [4,5]. Dissociation of a perfect dislocation results in a more favourable configuration by reduction of the elastic energy. The equilibrium separation of the partial dislocations generated is due to the cost of the intrinsic stacking fault. This separation width is important for the strengthening mechanism of solutes since it affects the solute-dislocation interaction-energy map.

In this work, a cluster model for dislocation core structures is applied. The model takes the shape of a cylinder, where the dislocation line is elongated through the centre [6]. It consists of an outer region surrounded by vacuum, where the atoms are fixed by an elastic displacement field, and a core region that is relaxed. This model is strongly dependent on the assumption that the elastic theory is respected within the fixed region. The advantage of this model is the simplicity, and its transparency towards the assumptions that are taken. The aim is to improve the capability to set up an atomistic model for dislocations in fcc metals using a cluster model with sufficient accuracy. The setup has been tested for Aluminium with a pure edge dislocation. It will be extended further to screw dislocations.

Using this simple model, the static configuration of a dislocation core structure can be compared to experimental observations and results using the flexible boundary condition applied by other groups [1,4].

[1] doi.org/10.1016/j.actamat.2016.09.046
[2] doi.org/10.1016/j.scriptamat.2014.04.018
[3] doi.org/10.1016/j.actamat.2010.06.045
[4] doi.org/10.1016/j.msea.2005.03.039
[5] 10.1103/PhysRevLett.100.045507
[6] doi.org/10.1016/j.actamat.2016.09.049

(Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall)

[P1-13] Anelastic recovery of a steel wire under pure shear strain with various magnetic treatments

○Shigeo Kotake, Takuro Murata （Dept. of Mechanical Engineering, Mie Univ., Japan）

Elastic property of a metal under pure shear strain is quite different from that under other strain, since the former doesn’ t have the volume change of the specimen. Without the volume change, elasticity under the pure shear strain is mainly caused from bowing-out deformation of dislocations in slip planes. After external force is removed, the solid will immediately return to its original size. It indicates deformed dislocation lines are straitened instantly in this condition. On the other hand, people has observed slow recovery of the size of the specimen after unloading, which is called anelasticity. When anelastic phenomenon occurs under pure shear strain, it indicates some dislocations slowly recover its bowing-out shape because of the existence of weak pinning sites. Since dislocations are known to interact with magnetic domain walls in ferrous materials, the domain walls can partially act for weak pinning sites for anelasticity.

To prove this mechanism, we will observe anelastic recovering of steel compression coil spring, whose strain is mainly pure shear state, under various magnetic treatments. The residual elongation cannot be explained from simple relaxation phenomenon of macroscopic spring dynamics. Since the amount of anelastic recover is influenced with magnetic treatment during compression condition, magnetic domain walls can work as weak pinning sites for some dislocations. As temporal change of elongation is logarithmically changed, resultant number of bowing-out dislocations is inversely proportionally decreased with time during recovering.

At last, we will discuss the mechanism of interaction between dislocation and magnetic domain wall. In iron, easy-magnetization axes are <100> and 180-degree magnetic domain walls are located along {011} plane. Slip planes of bcc iron are {110} plane, and dislocation lines are perpendicular to {110}. Since [01-1]

dislocation line, which is perpendicular to a magnetic domain wall, has no interactions to the wall, most dislocation lines across the 180-degree wall in this manner. We will discuss the origin of weak pinning sites of dislocation from the distribution of Bloch wall and Bloch line in the domain wall. And we will show the possibility to understand the interaction from magnetic force caused by swirling flow of electron along dislocation line.

(Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall)

[P1-14] Possible explanation of sudden stress drop at upper yield point in iron by magnetostriction and unpinning dislocations with law of approach in residual magnetization

○Shigeo Kotake （Dept. of Mechanical Engineering, Mie Univ., Japan）

Unique mechanical properties of iron is one of important resources of engineering in modern technology. Since elastic deformation is dominant below the yield stress in iron, people can design a machine under strength of materials. Although sudden drop of stress at the upper yield point is one of prominent phenomena in iron, its mechanism has been a point of controversy in the study of mechanical properties.

On the other hand, Pitman (1990) reported sudden changes in residual magnetization of iron, which shifts towards an anhysteresis curve after applying mechanical stress. Jiles (1995) and Jiles and Li (2004) studied the magnetomechanical effect and discovered the existence of the “law of approach” in residual magnetization, in which the hysteresis converts to an anhysteresis curve under applied stress.

In this study we will try to explain the sudden drop of stress at the upper yield point from magnetostriction and unpinning dislocation with the sudden change of residual magnetization under the law of approach. Because of the positive magnetostriction coefficient of iron, specimen will show sudden drop of stress from the sudden decrease of residual magnetization, in case the initial magnetization is perpendicular to the direction of the applied force. Since the decreased magnetization has been kept, the sudden drop of stress has not been observed just after the first tensile test. Recovery of the phenomenon can be explained from remagnetization of the specimen during the heat treatment of annealing. It will be remaining study to explain the effect from temperature or strain rate to the upper yield stress.

Moreover, it has been noticed there are pinning effects between dislocation lines and magnetic domain walls. The law of approach has been explained from unpinning effect of the dislocations from the magnetic domain walls. Therefore, at the upper yield point, unpinned dislocations can move freely until contact another pinning site to enhance the decrease of stress. And we will show the possibility to understand the pinning interaction from magnetic potential between magnetic domain wall and dislocation line, where swirling electron flows.

(Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall)

[P1-15] Investigation of dislocation core structure in Aluminum by using a generalized Peierls-Nabarro model

○Hideki MORI （College of Industrial Technology, Japan）

We investigate the dislocation core structure in Aluminum (Al) by using generalized Peierls-Nabarro (PN) model.
Same as classical PN model, a generalized PN model expresses the total energy of dislocation core as a sum of local misfit energy and non-local elastic energy.
To integrate micromechanics in classical PN model, the generalized PN model can flexibly and efficiently evaluate the non-local elastic energy [1].
Especially, in isotropic case, the generalized PN model can evaluate the non-local elastic energy with high accuracy [1,2].
In this work, we calculate the generalized stacking fault energy surface by density functional theory (DFT) calculation and empirical atomic potential and evaluate dislocation core structure in Al.
Then we discuss the accuracy of generalized PN model by comparing to result of empirical atomic potential.
We also demonstrate that the generalized PN model is a useful tool to investigate the mesoscopic dislocation behavior.

[1] H.Wei,Y.Xiang and P.Ming: Commun. Comput. Phys. 4 (2008) 275-293
[2] V.V.Bulatov and W.Cai: Computer simulations of dislocations (Oxford,2006)

(Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall)

[P1-16] Crystal orientation evolution analysis during deformation using molecular dynamics

○Keisuke Kinoshita （Nippon Steel &Sumitomo Metal Corporation, Japan）

Usually, metallic materials are anisotropic material, for example, in a tensile testing of single crystal, stress and strain relationship depends on tensile direction. Although, when grains in polycrystalline metals have fully random crystal orientation, respectively, anisotropy of the metals is reduced. However, in the actual metallic materials, the grains don’ t have fully random crystal orientation and the grains have been limited to specific crystal orientations that depends on crystal structures and/or plastic deformation processes, etc. In other words, the polycrystalline metals have the texture. Mechanical properties of the polycrystalline metals that have texture is depended on the texture. Therefore, controlling the texture is one of important problems for improving the mechanical properties of metals. The mechanism of the texture formation during deformation is rotation of each grain, macroscopically. An elementary step of the rotation of the grains is dislocation movement, microscopically. The dislocation movements depend on the crystal structures and the stress state, etc. In result, the texture depends on the crystal structures, etc. Although, the dislocation movement is the elementary step of the texture formation, the texture formation should be reproducible by molecular dynamics. But the simulation result reports are not many.
In this study, we will show molecular dynamics simulation results for the crystal rotation of body-centered cubic iron during deformation at 300 K. We will show two results. First, an algorithm that is determined equivalent crystal orientation from atomic configures is described and inspected. Second, crystal rotation evolution during tensile deformation on molecular dynamics simulation using the algorithm will be shown. As a result, we will show two results, 1) the crystal rotation of the simulation is corresponded to the theoretical result, and 2) when multi slip systems are activated, crystal orientation is stable, but when single slip system is activated, crystal orientation is changed.

(Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall)

[P1-17] Nanoindentation of Nanoparticles -A Molecular Dynamics and Discrete Dislocation Dynamics Simulations Study

Roy Shyamal[1], Riccardo Gatti[2], Benoit Devincre[2], ○Dan Mordehai[1] （1.Mechanical Engineering, Technion - Israel Institute of Technology, Haifa, Israel, Israel, 2.LEM, UMR 104, CNRS-ONERA, 29 Av. de la Division Leclerc, 4 Chatillon, France, France）

When decreasing the size of metallic specimens into the sub-micrometer scale, they can drastically change their mechanical properties. While plasticity at this scale is commonly studied using compression tests, nanoindentation can reveal the importance of free surfaces on the depletion of dislocations during the deformation. In this talk, we present a computational study on how the size and shape of defect-free nanoparticles affect the mechanical response to nanoindentation. Using Molecular Dynamics (MD) simulations and Discrete Dislocation Dynamic (DDD) simulations, we simulate nanoindentation of Au faceted nanoparticles in a height range of 9-150 nm. The DDD simulations are coupled with a finite element analysis, in order to reproduce the stress field generated during nanoindentation. Since the nanoparticles are initially pristine (dislocation free), a nucleation criterion for dislocations is introduced in the DDD simulations. When indenting along a <111> direction, the simulations show that shear dislocation loops are nucleated beneath the indent on all {111} slip planes. Those shear dislocation loops interact and form v- and u-shaped dislocations or prismatic loops that glide towards the lower part of the nanoparticles, facilitating their escape from beneath the indent. Two other mechanisms are shown to control the escape of dislocations laterally from the upper part of the nanoparticle. In one, segments of shear dislocation loops, that are nucleated on the {111} slip plane parallel to the upper surface of the nanoparticle, cross-slip and escape from the upper surface, forming two half prismatic loops that glides parallel to the upper facet. In another mechanism, dislocations on two different slip planes interact and form a glissile dislocation segment that glides lateraly and escapes the nanoparticles. The effect of size on the various dislocation mechanisms is discussed.

(Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall)

[P1-18] Machine learning interatomic potentials for molecular dynamics simulations of dislocations

○Eyal Oren, Guy Makov （Dept. of Materials Engineering, Ben-Gurion University of the Negev, Israel）

The mechanical response of crystalline materials is largely controlled by the mobility of dislocations. It is possible to study the mobility of individual dislocations using molecular dynamics simulations, e.g. [1], but the validity of these studies depends on the quality of the interatomic potentials employed. In the present contribution we employ machine learning techniques for the construction of interatomic potentials using ab-initio data as input, validate the interatomic potential accuracy against experimental and ab-initio observables and apply to the study of dislocations.

[1] E. Oren, E. Yahel, G. Makov, Dislocation kinematics: a molecular dynamics study in Cu, Model. Simul. Mater. Sci. Eng. 25 (2017) 25002.

Poster Session | E. Deformation and Fracture Mechanism of Materials

[PO-E1] Poster Session 1

Symposium E

Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall

[P1-21] Large-scale molecular dynamics simulations: coupling with dislocation dynamics

○Pavel A. Pokatashkin, Denis K. Ilnitsky, Alexei V. Yanilkin （Dukhov Research Institute of Automatics (VNIIA), Russia）

[P1-22] **Hydrogen embrittlement controlled by reaction of dislocation with grain boundary in alpha-iron polycrystals**

○Liang Wan[1,2], Wen Tong Geng[2,3], Akio Ishii[2], Jun-Ping Du[2,4], Nobuyuki Ishikawa[5], Hajime Kimizuka[2], Shigenobu Ogata[2,4] （1.Wuhan University, China, 2.Osaka University, Japan, 3.University of Science and Technology Beijing, China, 4.Kyoto University, Japan, 5.JFE Steel Corporation, Japan）

[P1-23] Study of solute effect on the yield strength of Fe-based dilute alloy using atomistically informed kinetic Monte Carlo method

○Shuhei Shinzato[1], Masato Wakeda[2], Shigenobu Ogata[1] （1.Dept. of Mechanical Science and Bioengineering, Osaka Univ., Japan, 2.National Institute for Materials Science, Japan）

[P1-24] **Molecular Dynamics Simulations of Low-cycle Fatigue Behavior in Single Layer Molybdenum Disulfide**

Yu-Chieh Lo[1], ○Yu-Cheng Su[1], Ming-Chen Chung[2], Alice Hu[3] （1.National Chiao Tung University, Taiwan, 2.National Cheng Kung University, Taiwan, 3.City University of Hong Kong, Hong Kong）

[P1-25] Fracture behavior of multi-walled carbon nanotube under biaxial loading condition

○Masaomi Nishimura[1], Naoki Kazami[2], Daiki Kato[2] （1.Dept. of Mechanical Systems Engineering, Shinshu Univ., Japan, 2.Graduate School of Science and Technology, Shinshu Univ., Japan）

[P1-26] **On the role of amorphous shells on mechanical properties of fcc Ni nanoparticles under compression**

○Alexandra Goryaeva[1,2], Claudio Fusco[2], Matthieu Bugnet[2], Jonathan Amodeo[2] （1.DEN-Service de Recherches de Métallurgie Physique, CEA, Université Paris-Saclay, 91191 Gif-sur-Yvette, France, 2.INSA-Lyon, Université de Lyon, MATEIS, 69621 Villeurbanne, France）

[P1-27] Molecular dynamics analysis of hydrogen diffusion behavior in alpha-Fe bi-crystal under stress gradient

○Ken-ichi Saitoh[1], Haruka Koga[2], Tomohiro Sato[1], Masanori Takuma[1], Yoshimasa Takahashi[1] （1.Kansai Univ., Japan, 2.Kobe Steel, Ltd., Japan）

[P1-28] Understanding Interactions of Dislocations with Interfaces in Nickle-based Superalloys: Insights from Molecular Dynamics Simulations

○Jian Huang[1], Yunjiang Wang[2] （1.Shanghai Institute of Ceramics Chinese Academy of Sciences, China, 2.Institute of Mechanics, Chinese Academy of Sciences, China）

[P1-29] The influence of nano-sized Ti_3Al particles on the mechanical properties of α-titanium alloys

○Yan He[1,2,3], Wang Hao[1], Dongsheng Xu[1], Yang Rui[1] （1.IMR, CAS, China, 2.Coll. of Physics Science and Technology, SYNU, China, 3.Univ. of chinese Academy of Sciences, China）

[P1-30] **The atomic study of tensile property for nickel nanowires with helium bubble**

○Hengfeng Gong, Rui Li, Tong Liu （CGN, China）

[P1-31] **Componets of fracture response of alkali-activated slag mortars with steel fibers**

○Hana Simonova, Petr Frantik, Zbynek Kersner, Pavel Schmid, Pavel Rovnanik （Brno University of Technology, Faculty of Civil Engineering, Czech Republic）

[P1-32] Molecular Dynamics Simulation of Crack Growth Behavior of Single Crystal γ-TiAl Alloy Under Different Nb Substitution Mode

○Yuxi Feng[1,2], Zhiyuan Rui[1,2], Hui Cao[1,2], Ruicheng Feng[1,2], Xiaocui Fan[1,2], Xing Yang[1,2]
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(Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall)

[P1-21] Large-scale molecular dynamics simulations: coupling with dislocation dynamics

○Pavel A. Pokatashkin, Denis K. Ilnitsky, Alexei V. Yanilkin （Dukhov Research Institute of Automatics (VNIIA), Russia）

Various dislocation-related mechanisms: phonon drag, forest-harderning, thermal activated processes (climb, cross-slip) contribute to material properties e.g. strength. Until recently, studying of deformation via molecular dynamics (MD) considered simulations of only extremely high strain-rates. However contribution of various mechanisms might change significantly while proceeding to lower strain rates. Therefore the accuracy of dislocation dynamics (DD) models used for large strain rate range is an open question due to extrapolation.

Recent advances in computational powers increased both spatial and temporal scales available for atomistic modeling. Therefore it is possible to make coulping between MD and DD for strain rates ~10^7 s^{-1} and higher. We consider such materials as: iron, molybdenum, and uranium.

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[P1-22] Hydrogen embrittlement controlled by reaction of dislocation with grain boundary in alpha-iron polycrystals

○Liang Wan[1,2], Wen Tong Geng[2,3], Akio Ishii[2], Jun-Ping Du[2,4], Nobuyuki Ishikawa[5], Hajime Kimizuka[2], Shigenobu Ogata[2,4] （1.Wuhan University, China, 2.Osaka University, Japan, 3.University of Science and Technology Beijing, China, 4.Kyoto University, Japan, 5.JFE Steel Corporation, Japan）

Hydrogen atoms absorbed by metals in the hydrogen-containing environments can lead to the premature fracture of the metal components used in load-bearing conditions. Since metals used in practice are mostly polycrystalline, grain boundaries (GBs) can play an important role in hydrogen embrittlement of metals. Here we show that the reaction of GB with lattice dislocations is a key component in hydrogen embrittlement mechanism for polycrystalline metals. We use atomistic modeling methods to investigate the mechanical response of GBs in alpha-iron with various hydrogen concentrations. Analysis indicates that dislocations impingement and emission on the GB cause the GB to locally transform into an activated state with a more disordered atomistic structure, and introduce a local stress concentration. The activation of the GB segregated with hydrogen atoms can greatly facilitate decohesion of the GB. We show that the hydrogen embrittlement model proposed here can give better explanation of many experimental observations.

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[P1-23] Study of solute effect on the yield strength of Fe-based dilute alloy using atomistically informed kinetic Monte Carlo method

○Shuhei Shinzato[1], Masato Wakeda[2], Shigenobu Ogata[1] （1.Dept. of Mechanical Science and Bioengineering, Osaka Univ., Japan, 2.National Institute for Materials Science, Japan）

Solid solution hardening/softening is one of the ways to control mechanical properties of alloys. The trend of change in mechanical properties of solid solution alloys due to solute addition is generally non-linear against a solute element, concentration, strain rate, and temperature. In order to develop the advanced alloy, prediction of mechanical strength is important to reduce the cost and development time.
It is well known that the solute atoms in crystalline metals affect mechanical strength by interacting other lattice defects such as dislocation. Although many researchers have studied the interaction between dislocation and solute atoms to understand solid solution hardening/softening, detail of solute effect on dislocation motion is not fully clarified yet.
In this work, we investigate the solute effect on the yield strength of body-centered cubic (BCC) alloy by analyzing dislocation motion using kinetic Monte Carlo (kMC) model based on atomistic understanding. We focus on dilute BCC Fe-based alloy including substitutional solute Si atom.
First, we analyze the solute effect on screw dislocation motion, which mainly dominates plastic deformation of BCC metals, based on atomistic modeling. In order to estimate the solute effect on screw dislocation motion, we performed nudged elastic band calculation to obtain activation energy of dislocation motion via kink mechanism which includes a kink-pair nucleation and kink migration processes.
Then, obtained activation enthalpy of each process and solute effect on them is introduced to kMC model to calculate activation rate of dislocation motion. By performing kMC simulation, we estimate dislocation velocity in different concentration, temperature, and stress conditions, and evaluate the solute effect on dislocation velocity.
Finally, we predict yield strength from estimated dislocation velocity and discuss the effect of solute atoms.

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[P1-24] Molecular Dynamics Simulations of Low-cycle Fatigue Behavior in Single Layer Molybdenum Disulfide

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Graphene-like two-dimensional transition metal dichalcogenides (TMDs) have attracted much interest in the last decade because of it astonishing properties. Molybdenum disulfide (MoS2) is one of TMDs. It has direct band gap of 1.8 eV in monolayer but its bandgap can change with the number of layers. Such properties make it industrial important. In order to ensure the reliability of nano-devices made by MoS2, much attention has been focused on their mechanical properties including elastic modulus, stiffness and breaking strength. However, only limited studies have been done on cyclic deformation and fracture behavior. As a result, we report on molecular dynamics simulations of low-cycle fatigue behavior in single layer molybdenum disulfide. We choose the Reactive Empirical Bond Order (REBO) potential to describe the interatomic interactions. The REBO potential is used to estimate the failure strain and the tensile strength. The simulations and subsequent analysis suggest that the tensile stress will make the vacancies penetrate the whole plane, and induce the fracture for incremental brittle crack growth to occur during near-threshold fatigue. We want to clarify whether the plastic-strain-controlled fatigue tests would show the Coffin-Manson relation in fatigue life. Such power-law form originates from plastic-strain-dependent microscopic damage accumulation. Lastly, the effect of a crack on low-cycle fatigue of monolayer MoS2 in terms of failure mode and fatigue life is also discussed.

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[P1-25] Fracture behavior of multi-walled carbon nanotube under biaxial loading condition

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One-dimensional carbon materials such as Carbon Fibers (CFs) and Carbon nanotubes (CNTs) are applied in a wide range of areas. For example, carbon fiber reinforced plastics are put to practical use for bodyworks of cars and airplanes. Though carbon materials in composites are subjected to complex deformation by multiaxial loading, the fracture mechanism of them is not clarified under multiaxial stress conditions.
In this study, we have performed deformation simulations on multi-walled CNTs under biaxial loadings in order to clarify the fracture criterion of one-dimensional carbon materials from nanometer scale viewpoints. CNTs in simulation cell are compressed in a radial direction, and extended in a longitudinal direction by molecular dynamics simulation using the adaptive intermolecular reactive empirical bond order (AIREBO) potential. Fracture of CNTs originates from a bond breaking by the tensile loading for longitudinal direction, under small compressive stresses for the radial direction. On the other hand, high compressive stresses for the radial direction trigger a collapse of six-membered ring structures before the bond breaking by the longitudinal tension. The collapse occurs in the neighborhood of the innermost layer in highly compressed CNTs.
In addition, we have also performed biaxial deformations of composite models which are made by filling amorphous polyethylene structure in the space between MWCNTs. As a result, fracture behavior varies with stress conditions, as in the case of models without polyethylene. A collapse of six-membered ring structures under high compressive stresses occurs not from the innermost layer but from the outermost layer by the interaction between polyethylene and CNTs.

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[P1-26] On the role of amorphous shells on mechanical properties of fcc Ni nanoparticles under compression

○Alexandra Goryaeva[1,2], Claudio Fusco[2], Matthieu Bugnet[2], Jonathan Amodeo[2] （1.DEN-Service de Recherches de Métallurgie Physique, CEA, Université Paris-Saclay, 91191 Gif-sur-Yvette, France, 2.INSA-Lyon, Université de Lyon, MATEIS, 69621 Villeurbanne, France）

Nano-objects, such as nanoparticles, nanowires, nanopillars *etc.*, are characterized by the large surface to volume ratio that, to a certain degree, defines their exceptional physical properties, significantly different from those in their bulk counterparts. In particular, nanocrystals are known for their promising mechanical properties: a size-dependent elastic regime, large values of yield strength and ductility, that are mainly linked to the dislocation nucleation from surface.

In this context, the various surface states of a sample are expected to lead to significant differences in terms of mechanical behavior. So far, *in situ* nano-compression experiments in the TEM occasionally report the presence of amorphous overlay at the top of nano-objects [1], while theoretical atomic scale studies are mainly focused on perfect crystalline systems [2, 3, 4].

Here we present a Molecular Dynamics (MD) study that aims to investigate the influence of amorphous shells

on mechanical response of Ni nanospheres upon compression. In order to avoid complex effects of chemistry on the onset of plasticity, we focus on pure Ni compound, without adding alloying elements to the amorphous overlay. Based on multiple EAM potentials and various sample elaboration tests, a unique methodology that provides a reasonably slow “crystallization” rate of the amorphous Ni on fcc substrate is proposed. Then, mechanical properties of the designed 20 nm nanospheres with different shell thickness are investigated under uniaxial compression. The mechanical response of the composite systems is compared with that of purely crystalline and amorphous particles, with a particular focus on dislocation-based deformation processes.

References

[1] W. Han *et al.*, Advanced Materials **27**, 3385 (2015)

[2] J.-J. Bian &G.-F. Wang, J Comput Theor Nanosci **10**, 2299 (2013)

[3] D. Mordehai *et al.*, Acta Materialia **59**, 5202 (2011)

[4] S. Bel Haj Salah *et al.*, Comput Mater Sci **129**, 273 (2017)

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[P1-27] Molecular dynamics analysis of hydrogen diffusion behavior in alpha-Fe bi-crystal under stress gradient

○Ken-ichi Saitoh[1], Haruka Koga[2], Tomohiro Sato[1], Masanori Takuma[1], Yoshimasa Takahashi[1] (1.Kansai Univ., Japan, 2.Kobe Steel, Ltd., Japan)

Delayed fracture in high-strength steel wires produced by drawing is an important issue. The major cause of the delayed fracture is supposed hydrogen embrittlement (HE), and some researches so far show that HE phenomena is very sensitive to the amount of plastic deformation in drawing process. The hydrogen(H)-atom diffusion is affected largely by ambient thermal and mechanical conditions, such as, stress, pressure and temperature. Besides, effect of stress gradient (SD) on atomic diffusion is supposed to be crucial, but is still unclear. Most of metallic materials which have been provided plastic deformation, like drawn pearlitic steel wires, have a enormous residual stresses particularly in surface and interface region, which shows strong SD. In this study, we investigate the behavior of H-atoms diffusing in pure iron (α-Fe) in the condition accompanied by SD. Since the behavior is observable just in atomic-scale, molecular dynamics (MD) simulation using EAM potentials for Fe and H atomic system is conducted. There are two types of SD condition: one is the gradient for overall specimen, which can be reproduced by bending deformation of specimen. Another is an atomic-scale gradient in the interface region, e.g. one provided by grain boundary (GB) structure. Thus, we build a bi-crystal model including GB structure, and it is applied bending deformation. For a moderate flexure, the bending stress distributes in a linear fashion along the lateral cross-section of the specimen. Diffusion coefficient of H-atoms in bulk region increases with increase of the SD value. Besides, it is clearly observed that the direction of diffusion depends on the distribution of SD. It is found that H-atom diffusion increases with the decrease of cohesive energy evaluated around the H-atom. From these MD results, we realize that the increase of H-atom diffusion shows exactly exponential relation to

SD values. So, we can successfully obtain an expression between diffusion coefficient and SD value. We also understand that, by setting temperature effects aside, the increase of SD will lead to substantial change of entropy effect for diffusion.

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[P1-28] Understanding Interactions of Dislocations with Interfaces in Nickle-based Superalloys: Insights from Molecular Dynamics Simulations

○Jian Huang[1], Yunjiang Wang[2] (1.Shanghai Institute of Ceramics Chinese Academy of Sciences, China, 2.Institute of Mechanics, Chinese Academy of Sciences, China)

Nickel-base superalloys, as the favorite material for the turbine blade of the engines, have attracted a lot of attention due to their excellent creep properties and good microstructure stability. The evolution of dislocations during creep procedure and core structures of dislocations play an important role in the strengthening mechanism of nickel-base superalloys. Especially, the dislocation reactions and their interaction with γ / γ' interfaces of nickel-base superalloys contribute to a stable stage of creep. Here, based on developed mechanistic framework, we study the interactions of dislocations with interfaces to better understand the origin of ductility of nickel-base superalloys. Using atomistic reaction pathway calculations based nudged elastic band (NEB) method, we elucidate the slip transfer reaction mediated by interfaces of nickel-base superalloys. The findings offer new idea on the possible means to optimize the ductility and strength through interfacial engineering for nickel-base superalloys.

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[P1-29] The influence of nano-sized Ti_3Al particles on the mechanical properties of α-titanium alloys

○Yan He[1,2,3], Wang Hao[1], Dongsheng Xu[1], Yang Rui[1] (1.IMR, CAS, China, 2.Coll. of Physics Science and Technology, SYNU, China, 3.Univ. of chinese Academy of Sciences, China)

In α-titanium alloys, Ti_3Al (α_2 phase) precipitates under a perceivable aluminum content. The size and distribution of α_2 particles has significant influence on the mechanical property of α-Ti alloys. Experimentally, it is found that nanometric α_2 particles drastically decrease the toughness of α-Ti alloys after certain thermal treatment. However, the strength and the ductility do not vary linearly with the size of α_2 particles and the atomic details of hardening and fracture remain unclarified. Therefore, we employed molecular dynamic simulation with the embedded-atom potential to systematically study the deformation process of α-Ti with different size and distribution of α_2 particles. The result shows that 1) the α / α_2 interface is coherent; 2) in an α grain with an α_2 particle and incoming dislocations, the existence of an α_2 particle blocks the dislocations and the strength increases with the size of the α_2 particle; and subsequently cracks nucleate at the impacting site on the gain boundary with the crack stress decreasing with the size of the α_2 particle; 3) the resulting strength and toughness vary with the size of the α_2 particle in a parabola manner. The present simulation result quantitatively agrees with experiments and helps identifying the critical α_2 particle size for the design of structural titanium alloys.

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[P1-30] The atomic study of tensile property for nickel nanowires with helium bubble

○Hengfeng Gong, Rui Li, Tong Liu （CGN, China）

Tensile deformation behavior of nickel nanowires with helium bubble has been investigated using molecular dynamics (MD) simulation. MD simulations were performed at 1K to 300K employing a strain rate of $2\times10^{9}s^{-1}$ and $2\times10^{10}s^{-1}$ for the nanowires with cross section width(***S***)ranging from $8a_0$ to $12a_0$(a_0=3.5157Å). The diameters were set from 1.2 *nm* to 1.6*nm* for helium bubbles, and the ratio of helium-to-vacancy inside bubble for 1:1, 2:1, 4:1 and 1:0. With the strain rate increasing, the elastic modulus and yield stress are also increased. However, they present the declined trend at the high temperature. As the helium bubble size increases or the cross section of nanowires decreases, the elastic modulus and yield stress increases, while the yield strain become smaller. In addition, the mechanism of yielding is discussed in details based on the snapshots of defects evolution. As the radio of helium-vacancy increases, the elastic modulus and yield stress also decrease. The helium bubble could accelerate the fracture to some extent. This study on the plastic properties of metal nanowires will be helpful to further understanding of the mechanical properties of nanomaterials.

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[P1-31] Componets of fracture response of alkali-activated slag mortars with steel fibers

○Hana Simonova, Petr Frantik, Zbynek Kersner, Pavel Schmid, Pavel Rovnanik （Brno University of Technology, Faculty of Civil Engineering, Czech Republic）

Knowledge of mechanical fracture parameters of composites based on brittle matrix is essential for the quantification of their resistance against crack initiation and propagation as well as for the definition of material models used to simulate the quasi-brittle behaviour of the structures or their parts made from this type of composites. The variability of results experimentally obtained from fracture tests of composites with different kind of fibres is much higher in comparison with composite without fibres due to the natural heterogeneity of composite containing fibres. Therefore, the main objective of this paper is to quantify the contribution of the matrix of alkali-activated slag mortars with steel fibres on their fracture response.
First alkali-activated slag material was a reference without fibres; the other composites contain steel fibres in amount 5, 10, 15 and 20 % of weight of slag, respectively. The mechanical fracture parameters were determined using evaluation of fracture tests carried out on 40 × 40 × 160 mm beam specimens with an initial central edge notch. The load vs. displacement (deflection in the middle of span length) and load vs. crack mouth opening displacement diagrams were recorded during the fracture tests. Each diagram was processed in order to obtain the component that corresponds to the structural response of the matrix of the composite consisting from alkali-activated slag and steel fibres reinforcing that matrix. The values of fracture parameters were determined using work-of-fracture method and double-*K* fracture model.
This outcome has been achieved with the financial support of the Czech Science Foundation, project No. 16-00567S and the Ministry of Education, Youth and Sports of the Czech Republic under the “ National

Sustainability Programme I” (project No. LO1408 AdMaS UP).

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[P1-32] Molecular Dynamics Simulation of Crack Growth Behavior of Single Crystal γ-TiAl Alloy Under Different Nb Substitution Mode

○Yuxi Feng[1,2], Zhiyuan Rui[1,2], Hui Cao[1,2], Ruicheng Feng[1,2], Xiaocui Fan[1,2], Xing Yang[1,2] (1.Mechanical and Electronical Engineering College, Lanzhou University of Technology, China, 2.Key Laboratory of Digital Manufacturing Technology and Application, the Ministry of Education, Lanzhou University of Technology, China)

Because of the low plasticity at room temperature, high rate of crack propagation of TiAl alloy, its application in the aerospace has been severely restricted. The addition of Nb contributes to solving this problem.The Ti-Al-Nb ternary system has become the main trend of development of TiAl alloys, and the influence of alloying elements Nb on the properties of TiAl alloys has become the focus of extensive attention and research in the field of materials engineering.In this paper,the effect of different substitution modes of Nb on the crack propagation of γ-TiAl alloy was studied from the microscopic scale by molecular dynamics method.The effect of cracks on the performance of γ-TiAl alloys without Nb, Nb substitutional Al systems, and Nb substitutional Ti systems was analyzed.The results show that the interaction between Nb and the neighboring matrix atoms is stronger than the interaction between Ti-Al atoms before the substitution, and the doped Nb is enhanced compared to the γ-TiAl alloy without Nb. The bonding and bonding strengths between the atoms in the matrix and the atoms in the TiAl alloy increase the bond strength of the unit cell, increase the bonding force and cohesion between the surrounding atoms, and make the atoms in the crack tip region bond tightly, making it difficult to break bonds and become crack propagation. An obstacle is the passivation of the crack tip, the slower rate of crack propagation, and the change in the crack propagation path, which increases the tensile and fracture toughness of the alloy.The substitutional Ti system has a higher yield strength than the substitutional Al system, Nb occupies a sublattice of Ti, and the short-range interaction between dislocations and Nb atoms results in solid solution strengthening, which enhances the strength of the alloy.The lattice distortion of the substitutional Al system is more serious than that of the substitutional Ti system, and the dislocation density is higher and the fracture toughness is higher. The difference in this phenomenon is more pronounced at a high Nb concentration of 6%.

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[PO-F1] Poster Session 1

Symposium F

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[P1-33] UNDERSTANDING OF DELAYED HYDRIDE CRACKING FAILURE MECHANISM IN E110 ZIRCONIUM BASED FUEL CLADDINGS BY EBSD AND IN-SITU MECHANICAL TESTING

○Hygreeva Kiran NAMBURI[1], Zbynek Spirit[1], Patricie Halodova[1], Ondrej Libera[1], Jakub krejci[2] （1.Research Centre REZ, Czech Republic, 2.UJP Praha, Czech Republic）

[P1-34] Transition-metal alloying of γ ‘-Ni_3Al: Effects on the ideal uniaxial compressive strength from first-principles calculations

○Minru Wen[2,1], Chongyu Wang[2] （1.Guangdong University of Technology, China, 2.Tsinghua University , China）

[P1-35] **The Influence of Deposition Pattern on Stress and Mechanical Properties in Wire Arc Additive Manufacturing**

○Changmeng Liu, Qianru Wu, Jiping Lu, Shuyuan Ma （Beijing Institute of Technology, China）

[P1-36] On the Significance of the Higher-Order Neighbors for Abnormal Grain Growth and Recrystallization Nucleation

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

[P1-37] **Hydrogen trapping in carbon supersaturated a-iron and its decohesion effect in martensitic steel**

○Wen-Tong Geng[1,2], Vei Wang[1,3], Jin-Xu Li[2], Nobuyuki Ishikawa[4], Hajime Kimizuka[1], Kaneaki Tsuzaki[5,6], Shigenobu Ogata[1,6] （1.Department of Mechanical Science and Bioengineering, Osaka University, Japan, 2.University of Science and Technology Beijing, China, 3.Department of Applied Physics, Xi’ an University of Technology, China, 4.Steel Research Laboratory, JFE Steel Corporation, Japan, 5.Department of Mechanical Engineering, Kyushu University, Japan）

[P1-38] **Size Scale Effect on Energy Absorption Property of Aluminum Foam**

○zengyou liang, fudi liang, dezhi deng, chunzhuang miao, mingguang wang （North University of China, China）

[P1-39] Development of charge-transfer type interatomic potential for SiC oxidation

○So Takamoto[1], Takahiro Yamasaki[2], Takahisa Ohno[2], Chioko Kaneta[3], Asuka Hatano[1], Satoshi Izumi[1] （1.The Univ. of Tokyo, Japan, 2.NIMS, Japan, 3.Fujitsu Lab., Japan）

[P1-40] Alpha-phase in engineering aluminum alloys: a multiscale modeling approach to its mechanical behavior

○Duancheng Ma （Leichtmetallkompetenzzentrum Ranshofen GmbH, Austria）

[P1-41] Multi-phase-field lattice Boltzmann modeling and simulation of equiaxed structure

○Ryotaro Sato[1], Tomohiro Takaki[1], Shinji Sakane[1], Munekazu Ohno[2], Yasushi Shibuta[3] （1.Kyoto Institute of Technology, Japan, 2.Hokkaido University, Japan, 3.Tokyo University, Japan）

[P1-42] Simulation of Extrusion Process of TiAl alloy prepared by Triple VAR

○Fan Gao, Zhenxi Li （AECC BEIJING INSTITUTE OF AERONAUTICAL MATERIALS, China）

[P1-43] Experimental-Computational Analysis of Primary Static Recrystallizazion in DC04 Steel

○Martin Diehl, Markus Kühbach, Dierk Raabe （Max-Planck-Institut fuer Eisenforschung GmbH,

Germany）

[P1-44] Combining 4D experiments and phase-field modeling to determine reduced grain boundary mobilities

○Jin Zhang[1,2], Peter W Voorhees[1], Henning F Poulsen[2] （1.Northwestern University, United States of America, 2.Technical University of Denmark, Denmark）

[P1-45] Fiber-intersectant microstructure of fish scale and biomimetic research

○Bin Chen[1], Jinghong Fan[2], Miao Li[1], Wei Ye[1] （1.College of Aerospace Engineering, Chongqing University, China, 2.Division of Mechanical Engineering, Alfred University, United States of America）

[P1-46] Microstructures of turtle shell and biomimetic fabrication

○Bin Chen[1], Jinghong Fan[2], Wei Ye[1], Miao Li[1] （1.College of Aerospace Engineering, Chongqing University, China, 2.Division of Mechanical Engineering, Alfred University, United States of America）

[P1-47] **Phase-field Simulation of Solidification Process in Welding Pool of Fe-C Binary Alloy**

○Ian zhan, Xiangge Qin （Jiamusi Univ., China）

[P1-48] **Phase field simulation of the phase separation in the TiC-ZrC-WC system**

○Zelin Luo[1], Hong Ma[1], Sai Tang[1], Yingbiao Peng[2], Yong Du[1], Zikui Liu[3], Qianhui Min[1], Yafei Pan[4] （1.State Key Lab of Powder Metallurgy, Central South University, China, 2.College of Metallurgy and Materials Engineering, Hunan University of Technology, China, 3.Department of Materials Science and Engineering, Pennsylvania State University, United States of America, 4.School of materials science and engineering, Hefei University of Technology, China）

[P1-49] Switching of coordinate transformations of a repetitive bar-and-joint framework under uniaxial compression

○Hiro Tanaka[1], Kazutoshi Hamada[1], Yoji Shibutani[1,2] （1.Dept. of Mechanical Engineering, Osaka Univ., Japan, 2.Nanotechnology Program, Vietnam Japan Univ., Viet Nam）

[P1-50] Understanding the effect of Residual Stresses in 3D Printed Metals

○Alankar Alankar, BVSS Bharadwaja, Ritam Chatterjee （IIT Bombay, India）

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[P1-33] UNDERSTANDING OF DELAYED HYDRIDE CRACKING FAILURE MECHANISM IN E110 ZIRCONIUM BASED FUEL CLADDINGS BY EBSD AND IN-SITU MECHANICAL TESTING

○Hygreeva Kiran NAMBURI[1], Zbynek Spirit[1], Patricie Halodova[1], Ondrej Libera[1], Jakub krejci[2] (1.Research Centre REZ, Czech Republic, 2.UJP Praha, Czech Republic)

Zirconium based alloys are commonly used as material for fuel claddings in the light water reactors. Claddings act as first metallic barriers against loss of fission products during the nuclear power plant operation, intermittent storage or final dry storage. During the reactor operation, metallic claddings are prone to water side corrosion and subsequent hydrogen pick-up (in 10’s to 100’s of ppm) due to higher operating temperatures in reactor. Under specific favorable conditions (stress, temperature and hydrogen concentration level) claddings fail by a time dependent mechanism called Delayed Hydride Cracking (DHC). This results in critical issue for the safe performance of the power plants and storage used claddings.

In this work we present results from the DHC study on zirconium based E110 metallic fuel claddings. Test specimen is oxidized in an autoclave to have desired hydrogen content. DHC experiments are performed in scanning electron microscope chamber by using in-situ tensile testing device at high temperatures.

The paper emphases on microstructural studies, evaluation of threshold stress intensity, crack propagation rate, understanding fialure mechanism and role of crack tip hydrides fracture during the DHC failure in E110 fuel claddings.

Keywords: Zirconium alloys, nuclear fuel claddings, microstructure, crack tip hydride fracture, delayed hydride cracking failure.

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[P1-34] Transition-metal alloying of γ'-Ni_3Al: Effects on the ideal uniaxial compressive strength from first-principles calculations

○Minru Wen[2,1], Chongyu Wang[2] (1.Guangdong University of Technology, China, 2.Tsinghua University , China)

The addition of transition metal (TM) elements into the γ' precipitate phase of a Ni-based single-crystal superalloy can significantly affect its mechanical properties, including the intrinsic mechanical property of compressive strength. Using first-principles density functional calculations, the effects of 3*d* (Sc-Zn), 4*d* (Y-Cd) and 5*d* (Hf-Au) TM alloying elements on the ideal uniaxial compressive strength of γ'-Ni_3Al were investigated. The stress-strain relationships of pure Ni_3Al under [100], [110] and [111] compressive loads and the site occupancy behavior of TM elements in Ni_3Al were prior studied using a total-energy method based on density functional theory. Our results showed that the capacity of TM elements for strengthening the ideal compressive strength was associated with the *d*-electron number. The alloying elements with half-filled *d*-bands (*i.e.*, Cr, Mo, W, Tc and Re) manifested the greatest efficacy for improving the ideal strength of Ni_3Al under a deformation along the weakest compressive direction. Furthermore, the charge redistribution of Ni_3Al doped with 5*d* elements were also analyzed to understand the strengthening mechanisms of TM elements

in the γ'-Ni_3Al phase.

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[P1-35] The Influence of Deposition Pattern on Stress and Mechanical Properties in Wire Arc Additive Manufacturing

○Changmeng Liu, Qianru Wu, Jiping Lu, Shuyuan Ma （Beijing Institute of Technology, China）

Wire arc additive manufacturing (WAAM) has exhibited great advantages of high deposition rate, large fly-to-buy ratio and low cost in aerospace applications. However, the deformation caused by internal stress is still a technical challenge in additive manufacturing, especially during the manufacturing process of the large-scale components. In this work, based on numerical modelling method and physical experiments, by investigating the stress and deformation distribution of Ti6Al4V components deposited by five typical patterns, the preferred deposition pattern will be selected to fabricate components with minimum deformation and uniform stress distribution. The morphology, microstructure and mechanical properties of the components with different deposition patterns were studied as well. The results illustrate that short S-shape pattern is identified as the optimal one which has uniform stress distribution and minimum deformation. The stress distribution of the components with spiral pattern and subarea pattern varies a lot and the reasons have been discussed based on the thermomechanical behavior in WAAM.

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[P1-36] On the Significance of the Higher-Order Neighbors for Abnormal Grain Growth and Recrystallization Nucleation

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

Successful nucleation of abnormal grain growth and primary static recrystallization constitutes a rare event which affects in many cases only each thousandth (sub-) grain if at all. Consequently, the making of more quantitatively substantiated number density predictions can be improved by studying million-scale initial grain populations. Thanks to representative volume element (RVE) method development and software parallelization, simulating the evolution of such large grain populations has recently become possible.

This work details how 2d and 3d resolved RVE computer simulations with such millions of (sub-) grains within each single domain allow quantifying the process of preferential grain evolution during abnormal grain growth and nucleation to primary static recrystallization to hitherto unachieved statistical significance. By assessing not only the nearest but additionally higher-order neighbors of each grain more precise and accurate predictions at which sites nucleation will likely initiate are possible. Albeit, the study proofs also that to definitely identify which grains succeed --- and as such also the number density --- requires assessing their entire topological event sequence surplus quantifying the distribution of their individual capillary- and stored elastic energy-induced grain boundary face migration speeds.

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[P1-37] Hydrogen trapping in carbon supersaturated a-iron and its decohesion effect in martensitic steel

○Wen-Tong Geng[1,2], Vei Wang[1,3], Jin-Xu Li[2], Nobuyuki Ishikawa[4], Hajime Kimizuka[1], Kaneaki Tsuzaki[5,6], Shigenobu Ogata[1,6] （1.Department of Mechanical Science and Bioengineering, Osaka University, Japan, 2.University of Science and Technology Beijing, China, 3.Department of Applied Physics, Xi’ an University of Technology, China, 4.Steel Research Laboratory, JFE Steel Corporation, Japan, 5.Department of Mechanical Engineering, Kyushu University, Japan）

It is generally accepted that the martensite in steels is more susceptible to hydrogen embrittlement than the ferrite. The atomic-scale mechanism underlying this phenomenon, nevertheless, is not fully understood yet. Our first-principles calculations demonstrate hydrogen is more stable in carbon supersaturated martensite than in a-iron, due to the carbon-induced tetragonality in martensite lattice. The trapped hydrogen leads to remarkable decohesion between (110) planes both inside the martensite and along the martensite/ferrite interface, with the former being more significant than the latter. This decohesion can explain recent precise observations that in martensite/ferrite dual-phase steels the hydrogen-promoted crack was initiated in the martensite region and that in lath martensite steel it propagated not on lath boundaries but showed quasi-cleavage feature along (110) planes at very high hydrogen concentration.

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[P1-38] Size Scale Effect on Energy Absorption Property of Aluminum Foam

○zengyou liang, fudi liang, dezhi deng, chunzhuang miao, mingguang wang （North University of China, China）

Abstract: Foam metal is extensively used in the fields of petrochemical engineering, aerospace and automobile manufacturing for its excellent properties. As a typical representative of foam metal,Aluminum foam is an excellent material in energy absorption,that it can produce larger plastic deformation under the lower flow stress.Relative to the cell dimension,the size of specimen is an important factor which affects the performance of its energy absorption. Based on the technological process of the infiltration casting method, a microscopic structure model of aluminum foam is established by Monte Carlo method and Gravity Accumulation method ,with the assistance of PFC3D software so as to study the influence of size scale effect on energy absorption property of aluminum foam. A finite element model of aluminum foam is generated according to MATLAB software. Combining with SPH algorithm, numerical simulation to the compression behavior of the different specimen size of aluminum foam is performed. From numerical simulation,we can draw the conclusion that the greater the ratio of specimen dimension to cell dimension is,the better energy absorption property it performs. The results can provide assistance on design buffer suction device with foam mental.

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[P1-39] Development of charge-transfer type interatomic potential for SiC oxidation

○So Takamoto[1], Takahiro Yamasaki[2], Takahisa Ohno[2], Chioko Kaneta[3], Asuka Hatano[1], Satoshi Izumi[1]
（1.The Univ. of Tokyo, Japan, 2.NIMS, Japan, 3.Fujitsu Lab., Japan）

Silicon carbide (SiC) is an attractive semiconductor material for applications in power electronic devices and the fabrication of a high-quality SiC/SiO_2 interface is desired. It is well known that there is a great difference in oxidation rate between the Si-face and C-face, and that the quality of oxide layer on the Si-face is better than that on the C-face. However, the atomistic mechanism of the thermal oxidation of SiC remains to be solved. In this work, we developed a new Si-C-O interatomic potential to reproduce the kinetics of the thermal oxidation of SiC. More than 1000000 properties obtained by DFT calculations were used for the fitting process. Using this interatomic potential, large-scale SiC oxidation simulations were performed. In order to focus on the reaction of O_2 molecules, the oxidation process is realized by inserting O_2 molecules into SiO_2 region. The results showed that the activation energy of the Si-face is much larger than that of the C-face. Also, the numbers of intermediate oxide states of Si atoms are in good agreement with the experimental result. In the case of the Si-face, a flat and aligned interface structure including Si^{1+} was created. We estimated activation energies of the change of intermediate oxide states and proposed that the stability of the flat interface structure is the origin of the high activation energy of the oxidation of the Si-face. In contrast, in the case of the C-face, it is found that the Si atom at the interface are pulled up by the O atoms. This process generates the disordered interface and decreases the activation energy of the oxidation.

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[P1-40] Alpha-phase in engineering aluminum alloys: a multiscale modeling approach to its mechanical behavior

○Duancheng Ma （Leichtmetallkompetenzzentrum Ranshofen GmbH, Austria）

Alpha-phase, i.e., Al(Fe,Mn)Si, is very common in engineering aluminium alloys. During ingot casting, coarse beta-phase forms. In the subsequent homogenization heat treatment, the beta-phase transforms into coarse alpha-phase. In the following forming and solution annealing processes, the coarse alpha-phase remains in the matrix and never dissolve. Since the size of the coarse alpha-phase is large (a few micrometers), they hardly contribute to the strengthening effect. There are many examples, however, showing that it is one of the potential damage nucleation sites. Despite being common in engineering aluminium alloys and being the damage nucleation sites, little is known about the mechanical properties of the alpha-phase. In this study, we use a multiscale modeling approach, i.e. from electronic to continuum scale, to investigate its mechanical behavior in aluminium.

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[P1-41] Multi-phase-field lattice Boltzmann modeling and simulation of equiaxed structure

○Ryotaro Sato[1], Tomohiro Takaki[1], Shinji Sakane[1], Munekazu Ohno[2], Yasushi Shibuta[3] （1.Kyoto Institute of Technology, Japan, 2.Hokkaido University, Japan, 3.Tokyo University, Japan）

Equiaxed structure formed during a solidification process of metals and alloys determines the mechanical property of materials. Therefore, it is crucial to accurately predict and control the formation process of the equiaxed structure. However, the formation process of equiaxed structure is a complicated multiphysics problem including a motion of multiple grains.

In this study, we construct a multi-phase-field-lattice Boltzmann model which can express the growth, motion, collision, and coalescence of multiple dendrites and following grain growth. In this model, the growth and motion of multiple dendrites are expressed by a multi-phase-field method and equations of motion, respectively, and the liquid flow is computed by lattice Boltzmann method. The collision and coalescence of multiple dendrites and/or grains are also modeled in a concept of diffuse interface. Moreover, the simulation is accelerated by employing the active parameter tracking and graphics processing unit. By using the developed method, the formation simulations of the equiaxed structure are demonstrated.

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[P1-42] Simulation of Extrusion Process of TiAl alloy prepared by Triple VAR

○Fan Gao, Zhenxi Li （AECC BEIJING INSTITUTE OF AERONAUTICAL MATERIALS, China）

TiAl alloy with low density and excellent mechanical properties at the high temperature is one of the most potential materials in aerospace industry, however the extrusion of the ingot with industrial scale is difficult due to the poor ductility. In this study, FEM was employed to describe the extrusion plastic deformation behavior of this alloy which prepared by triple VAR. Under various extrusion conditions, the strain distribution and the extrusion load were studied by numerical analysis. The influence of the die angle and the extrusion ratio were examined. The results showed that the peak extrusion force was enhanced with the increased die angle with a certain slop coefficient. The die angle with 100° was suggested to obtain the uniform deformation. With the raising of extrusion ratio, the effective strain, extrusion load in billet would be increased. Then extrusion experiment of triple VAR TiAl ingot was carried out successfully with extrusion ratio of 10.

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[P1-43] Experimental-Computational Analysis of Primary Static Recrystallizazion in DC04 Steel

○Martin Diehl, Markus Kühbach, Dierk Raabe （Max-Planck-Institut fuer Eisenforschung GmbH, Germany）

Low-alloyed steels with body-centered cubic crystal structure (bcc, ferrite) are a material class which is widely used in automotive sheet metal forming applications. When produced with an adequate crystallographic texture, the mechanical behavior of steels for forming applications is characterized by an isotropic in-plane flow behavior in combination with a low yield strength. To obtain these beneficial mechanical properties, an adequate cold rolling strategy in terms of the number of passes, deformation rates,

and total reduction needs to be followed by an annealing procedure with a time-temperature profile that facilitates primary static recrystallization. The most fundamental connection between cold rolling and heat treatment consists in the reduction of the dislocation-related free energy stored during deformation by the formation of new grains with a very small dislocation content. Hence, the local variation in crystallographic orientation and defect population lead to very inhomogeneous grain boundary migration velocities.

We present here results of a coupled experimental-computational approach for studying microstructure evolution in industrially cold rolled DC04 steel under quasi-isothermal conditions. For the experimental characterization, quasi in-situ experiments consisting of interrupted isothermal holding at 600˚C and subsequent Electron Backscatter Diffraction (EBSD) orientation imaging were conducted. The results reveal a strong correlation between local dislocation density, quantified via the Kernel Average Misorientation (KAM), and the local increase of recrystallized volume fraction. To complement the experimental findings and gain further insights into the influence of the sub-surface microstructure, a Cellular Automata (CA) model was utilized. The employed three-dimensional microstructure model was directly built from the experimentally characterized deformation microstructure. Different approaches of scaling the KAM into dislocation density values, i.e. the driving force for recrystallization, are employed. Similarities and deviations between experimental and computational results are discussed with the aim at increasing the understanding the mechanisms of static primary recrystallization.

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[P1-44] Combining 4D experiments and phase-field modeling to determine reduced grain boundary mobilities

○Jin Zhang[1,2], Peter W Voorhees[1], Henning F Poulsen[2] (1.Northwestern University, United States of America, 2.Technical University of Denmark, Denmark)

Reduced grain boundary mobilities play an essential role in accurate multi-scale modeling of grain growth in polycrystalline materials. The reduced mobility is a function of a large five-dimensional parameter space. Traditional bi-crystal experiments only determine one point in this space at a time. In this paper, we present a method to determine the reduced mobilities by comparison between 4D experiments and phase-field simulations. The growth of 1327 grains in a pure iron sample is visualized in 3D using diffraction contrast tomography (DCT) at a synchrotron source. Using the first time-step from the experimental microstructure as input, the evolution of the entire grain structure is simulated using a phase-field model. A fitting approach is applied to find the set of reduced mobilities that yield the best match between the experimental microstructure and the simulated microstructure. An efficient fitting algorithm is constructed based on a sensitivity analysis. The fitting algorithm converges fast, and more than 1000 reduced mobilities can be determined simultaneously.

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[P1-45] Fiber-intersectant microstructure of fish scale and biomimetic research

○Bin Chen[1], Jinghong Fan[2], Miao Li[1], Wei Ye[1] （1.College of Aerospace Engineering, Chongqing University, China, 2.Division of Mechanical Engineering, Alfred University, United States of America）

The microstructures of the scale of a chub fish are observed with scanning electronic microscope (SEM). It is shown that the scale is a kind of natural biocomposite consisting of parallel hydroxyapatite fiber layers and collage matrix. The hydroxyapatite fiber layers consist of long and thin hydroxyapatitefiber fiber sheets. It is also observed that the fiber sheets in adjacent fiber layers compose a fiber-intersectant microstructure. Based on the observed result, the fiber-intersectant microstructure is employed as the pattern for the design of man-made fiber-reinforced composite. A kind of fiber-reinforced composite with the fiber-intersectant structure is biomimetically fabricated. The fracture toughness of the biomimetical composite is tested and compared with that of the conventional composite with fiber-parallel structure. It is indicated that the fracture toughness of the biomimetical composite is remarkably larger than that of the composite with the fiber-parallel structure.

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[P1-46] Microstructures of turtle shell and biomimetic fabrication

○Bin Chen[1], Jinghong Fan[2], Wei Ye[1], Miao Li[1] （1.College of Aerospace Engineering, Chongqing University, China, 2.Division of Mechanical Engineering, Alfred University, United States of America）

Scanning electron microscope (SEM) observation shows that the shell of red-ear turtle is a kind of natural sandwich composite consisting of exterior cortex and interior cancellus. It is also observed that the hydroxyapatite fibers in the composite continuously surround the holes of the composite forming a particular fiber-surrounded-hole structure. Based on the result of the observation, a biomimetic composite with the fiber-surrounded-hole structure is fabricated. The ultimate strength of the biomimetic composite is tested and compared with that of the conventional composite with the non-fiber-surrounded-hole structure. It is indicated that the ultimate strength of the biomimetic composite is remarkably larger than that of the conventional composite.

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[P1-47] Phase-field Simulation of Solidification Process in Welding Pool of Fe-C Binary Alloy

○Ian zhan, Xiangge Qin （Jiamusi Univ., China）

Abstract: In this paper, the phase field method was used to study the growth process of Fe-C binary alloy welding pool dendrite. In the phase field model, the characteristics of small volume, fast cooling rate, large temperature difference and high degree of superheat of the welding pool were considered. And base on the model, the influence of undercooling on the crystal morphology of the alloy was predicted. Firstly, the growth morphology of Fe-C alloy dendrites in welding pool was successfully simulated by using the phase field model. Meanwhile, The effects of C concentration distribution on dendrite growth morphology and dendritic spacing were further investigated. The simulation results are consistent with the melten pool solidification theory.

Keywords: Fe-C alloy;solidification of weld molten pool;phase field method; dendritic morphology

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[P1-48] Phase field simulation of the phase separation in the TiC-ZrC-WC system

○Zelin Luo[1], Hong Ma[1], Sai Tang[1], Yingbiao Peng[2], Yong Du[1], Zikui Liu[3], Qianhui Min[1], Yafei Pan[4] （1.State Key Lab of Powder Metallurgy, Central South University, China, 2.College of Metallurgy and Materials Engineering, Hunan University of Technology, China, 3.Department of Materials Science and Engineering, Pennsylvania State University, United States of America, 4.School of materials science and engineering, Hefei University of Technology, China）

TiC-ZrC-WC system with high hardness is a promising material being widely used in industries like processing and manufacturing. Understanding the microstructural evolution and the mechanism during phase separation process is still a formidable challenge nowadays. Microstructural evolution mechanisms during phase separation process are explained for the first time through the methodology combing our CALPHAD data and two-dimensional Cahn-Hilliard/elastic strain energy model, and we used the parameters in our database of thermodynamics and dynamics. We investigate the effect of elastic strain on lamellar structure, agreeing well with previous results in terms of the variation of the periodicity of the distribution of element composition and the periodicity of regularly lamellar microstructures. It is obvious that phase field method coupled with thermodynamic database is a useful approach to study the microstructure evolution of TiC-ZrC-WC materials and in further speed up the research and development of new materials of TiC-ZrC-WC system.

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[P1-49] Switching of coordinate transformations of a repetitive bar-and-joint framework under uniaxial compression

○Hiro Tanaka[1], Kazutoshi Hamada[1], Yoji Shibutani[1,2] （1.Dept. of Mechanical Engineering, Osaka Univ., Japan, 2.Nanotechnology Program, Vietnam Japan Univ., Viet Nam）

In recent years, a variety of artificial microstructures with multi-functionality have been extensively developed by incorporating specific geometric features. The topic appears in a wide range of fields from geometry to crystallography to engineering, and indeed the mechanical behaviors of many of these structures remain unexplored. Some examples of such behaviors include auxeticity in materials of negative Poisson’s ratio, origami-based folding and deployment, and deformability of hierarchically arranged structures. In this context, we proposed the compressive structural system switching two types of kinematic transformations toward diamond- and square-patterns. To clarify the transition mechanism, we modelled a specific repetitive bar-and-joint framework with the two angular variables specifying the rotation and distortion of the linked square components. Numerically exploring the equilibrium paths then reveals a transition state of the structure at a critical value of the internal stiffness. A simplified formulation of the model with weak nonlinear terms yields an exact solution of its transition state. We further investigated the viscoelastic transition feature of the proposed structure to replace the cell-binding springs inside structure with damping components, and

revealed the interesting transformation characteristics, which depend on the compressive load speeds. The main idea is that our abstract representation might provide an original perspective to nonlinear elastic phenomena in solid state matter.

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[P1-50] Understanding the effect of Residual Stresses in 3D Printed Metals

○Alankar Alankar, BVSS Bharadwaja, Ritam Chatterjee （IIT Bombay, India）

We present phase field and atomistically informed simualtions of 3D printed CP-Ti. In the simulations, the microstructure can be controlled as a function of heat intensity, source velocity and powder size. Also, these process parameters are shown to have direct effect on the preferred crystallographic texture, porosity fraction and residual stresses in the additively created microstructure. This syntheic microstructure is then used as input for crystal plasticity model. In the crystal plasticity model the effect of voids coupled with crystallographic texture is studied as a function of various boundary conditions.

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

[PO-H1] Poster Session 1

Symposium H

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[P1-51] Multi-scale modeling of DNA-dendrimers in electrolyte solutions

○Natasa Adzic[1], Clemens Jochum[2], Gerhard Kahl[2], Christos Likos[1] （1.Faculty of Physics, University of Vienna, Austria, 2.Institute for Theoretical Physics, Vienna University of Technology, Austria）

[P1-52] Structural and dynamical properties 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）

[P1-53] Multiscale simulation of polymeric solids for fracture processes

○Takahiro Murashima[1], Shingo Urata[2] （1.Dept. of Physics, Tohoku Univ., Japan, 2.AGC, Japan）

[P1-54] Quantification and validation of the mechanical properties of DNA nicks

○Jae Young Lee, Jae Gyung Lee, Do-Nyun Kim （Dept. of Mechanical and Aerospace Engineering, Seoul National Univ., Korea）

[P1-55] Investigating the mechanical properties of azobenzene-tethered DNA for controlling self-assembling DNA nanostructures

○Jae Gyung Lee, Chanseok Lee, Do-Nyun Kim （Dept. of Mechanical and Aerospace Engineering, Seoul National Univ., Korea）

[P1-56] FTMP-based Modeling and Simulations of Glassy Polymers.

○Soushi Miyamoto, Tadashi Hasebe （Dept. of Mechanical Engineering, Kobe Univ., Japan）

[P1-57] Shock Wave Induced Damage in Tumor Cells: Experiments and Simulations

○Martin Steinhauser （Fraunhofer Ernst-Mach-Institute, EMI, Germany）

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[P1-51] Multi-scale modeling of DNA-dendrimers in electrolyte solutions

○Natasa Adzic[1], Clemens Jochum[2], Gerhard Kahl[2], Christos Likos[1] (1.Faculty of Physics, University of Vienna, Austria, 2.Institute for Theoretical Physics, Vienna University of Technology, Austria)

We have studied a novel class of macromolecules, the so-called DNA-based dendrimers. They have recently been synthesized from the enzymatic ligation of Y-shaped DNA building blocks. In order to describe such dendrimers of various generations we have performed MD simulations employing two independent models: a bead-spring model and the oxDNA model. The former one models each base-pair of double-stranded DNA as a single charged monomer and the interactions and interaction parameters in the model have been carefully chosen to mimic the structural properties of a single DNA chain. The system was immersed in water, which was modeled as a uniform dielectric and counterions were introduced in the system to preserve electroneutrality. Furthermore, we added salt, treating it explicitly, in order to investigate its influence on conformational characteristics of a single dendrimer molecule. On the other hand, the oxDNA model allowed us to take a closer look into the DNA structure, treating DNA as a string of rigid nucleotides which interact through potentials that depend on the position and orientation of the nucleotides. Equilibrium properties of a single dendrimer-like DNA molecule from the first to the sixth generations obtained from these two models have been investigated and the obtained simulation results have also been compared to the experiments. We have found an excellent agreement between the theoretical and experimental results, which has encouraged us to use the introduced models for theoretical analysis of novel self-assembled structures, such as cluster crystals in the bulk. The study of these charged dendrimer-systems is an important field of research in the area of soft matter due to their potential role in various interdisciplinary applications, ranging from molecular cages and carriers for drug and gene delivery in a living organism to the development of dendrimer-based ultra-thin films in the area of nanotechnology.

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[P1-52] Structural and dynamical properties 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) have been demonstrated to constitute self-assembling building blocks with specific softness, functionalization, shape, and flexibility. In this work, we studied the structural and dynamical behavior of an isolated SBC under a shear flow by means of particle-based multiscale simulations (MD+MPCD) covering a wide range of system parameters, which include the functionality (number of arms of the star), the amphiphilicity degree, and the solvent quality. We systematically analyzed the conformational properties of low-functionality SBC, as well as the formation of attractive patches on their corona as a function of the shear rate. Three mechanisms of patch reorganization under shear were identified, which determine the dependence of the patch numbers and orientations on the shear rate, namely, free arms joining existing patches, a fusion of medium-sized patches into bigger ones, and fission of large patches into two smaller ones at high shear rates [1]. As well as, the dynamics of the SBC was investigated by means of the so-called Eckart’ s frame, which allows separating pure rotational and vibrational motions [2,3]. It is shown that SBCs display a richer structural and dynamical behavior than athermal star polymers in a shear flow [4] and therefore they are also interesting candidates to tune the viscoelastic properties of complex fluids.

Because the conformation and dynamics of single SBCs are expected to be preserved in low-density bulk phases, the presented results are the first step in understanding and predicting the rheological properties of semidilute suspensions of this kind of polymers.

[1] Jaramillo-Cano et al. J. Phys. Chem. B (2018) In press
[2] Sablic et al. Soft Matter 13: 6988 (2017)
[3] Jaramillo-Cano et al. (2018) In preparation
[4] Ripoll et al. Phys. Rev. Lett. 96: 188302 (2006)

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[P1-53] Multiscale simulation of polymeric solids for fracture processes

○Takahiro Murashima[1], Shingo Urata[2] (1.Dept. of Physics, Tohoku Univ., Japan, 2.AGC, Japan)

We have developed a new multiscale simulation technique in order to investigate polymeric solids. Macroscopic features of polymeric solids are described by finite element method and microscopic features are described by molecular dynamics simulation. Each of finite elements has its microscopic simulator instead of using a constitutive equation. Polymers are described by the Kremer-Grest model, namely the bead-spring model. This model is simple but it can consider entanglements of polymers, which cause long time hysteresis. We solve macroscopic continuum mechanics and microscopic molecular dynamics concurrently. We have applied our multiscale simulation technique to fracture processes of polymeric solids under uniaxial tension.

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[P1-54] Quantification and validation of the mechanical properties of DNA nicks

○Jae Young Lee, Jae Gyung Lee, Do-Nyun Kim (Dept. of Mechanical and Aerospace Engineering, Seoul National Univ., Korea)

Understanding the mechanical properties at a nick site of double-stranded DNA is important to precisely design self-assembling DNA nanostructures because they inevitably contain many nicks that are structural discontinuities of DNA backbones. It is, however, difficult to characterize the mechanical properties of DNA nicks experimentally due to its resolution limit while those for normal DNA double helix without nicks have been relatively well measured. Here, we quantitatively studied the sequence-dependent characteristics of DNA nicks at the base-pair scale using the molecular dynamics (MD) simulation. We found that a primary structural role of DNA nicks is the relaxation of torsional constraint by sugar-phosphate backbones and that neighboring base-pair sequences affect the degree of mechanical rigidity changes by a nick. To validate these findings, we designed DNA nanostructures sensitive to torsion where the torsional rigidity at nick sites was regulated by using various sequences of DNA nicks and measured their overall twist angle using the atomic force microscope (AFM). We expect our study for nicks offers a versatile way of fine tuning the shape and properties of DNA nanostructures.

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[P1-55] Investigating the mechanical properties of azobenzene-tethered DNA for controlling self-assembling DNA nanostructures

○Jae Gyung Lee, Chanseok Lee, Do-Nyun Kim （Dept. of Mechanical and Aerospace Engineering, Seoul National Univ., Korea）

Advances in structural DNA nanotechnology have enabled the construction of a nanostructure with various shapes using self-assembling characteristics of DNA strands. Recently, there is an increasingly higher demand for building a dynamic, morphing structure in response to environmental signals so that DNA nanostructures can be used as a functional structure as well.

Azobenzene is one of the representative molecules that change its conformation under the change of light source. It switches from the trans isomer to the cis isomer when absorbing ultraviolet lights, while it is reversibly isomerized under visible lights. Multiple azobenzene molecules can be combined with DNA by intercalated between base-pair steps through threonine linkers and non-planar cis-azobenzenes destabilize the stacking interaction of DNA bases unlike planar trans-azobenzenes. Hence, azobenzene-tethered DNA (AzoDNA) can serve as a structural motif that triggers the conformational change of DNA nanostructures with lights. Nevertheless, its mechanical properties and transition dynamics are rarely known. Here, we investigate the mechanical properties of AzoDNA at its trans and cis states by performing molecular dynamics simulation. To validate, we construct a DNA nanostructure whose bending angles are controlled by the rigidity of AzoDNA at the hinge part.

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).

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[P1-56] FTMP-based Modeling and Simulations of Glassy Polymers.

○Soushi Miyamoto, Tadashi Hasebe （Dept. of Mechanical Engineering, Kobe Univ., Japan）

Multiscale modeling of glassy solids, such as polymers and metallic glasses, will require mathematically rational as well as effective treatments of the glassy states (free volume) responsible for carrying the viscoplastic flow. For amorphous polymers, it is rephrased as “modeling network degrees of freedom (NW-DOFs)” in connection with the orientating polymer chains. The “glassy states” can then be expressed in this context as those with curled and/or entangled chains with no net orientation, whereas the “strength” is attributed to their fully-extended counterparts with the alignments in the load-bearing direction, referred to as orientation hardening. To express the NW-DOFs, we introduce Finslerian geometry for an extended description of FTMP, together with the polymer-slip system-based kinematics proposed by Shizawa, et al. as the framework that allows direct treatments of the orientation change of the consisting polymer chains in a

similar manner to the conventional crystal plasticity. The current extension enables one to deal explicitly with the associated microscopic degrees of freedom of underlying kinds, e.g., cross-linking and unzipping. Targeted material here is PMMA for modeling the early-stage viscoplastic and the attendant softening responses as typical mechanical properties of engineering polymers. By allocating the vecotrial field in the extended Finslerian formalism to the representative direction of the polymer chains, together with the associated fabric tensor field, the study attempts to express the NW-DOFs. Assuming that the NW-DOFs are given as a function of the incompatibility, on the basis of the “flow-evolutionary” perspectives in FTMP, the evolving “free volume” can be effectively expressed, with which both the targeted properties are successfully reproduced. The free volume change, on the other hand, is shown to qualitatively agree with that reported in the literature.

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[P1-57] Shock Wave Induced Damage in Tumor Cells: Experiments and Simulations

○Martin Steinhauser （Fraunhofer Ernst-Mach-Institute, EMI, Germany）

ABSTRACT

Despite the therapeutic success of extracorporeal shock wave therapy in medicine, e.g. for disintegrating concrements, the effects of shock waves on the damage of biological cells and their membranes remain widely unknown. We present experimental results on the destruction of tumor cells using laser-induced shock waves. For the simulation of biological systems such as membranes under highly transient conditions such as external shock wave load, we propose a thermodynamically consistent and energy conserving coupling scheme between the atomistic and the continuum domain. The coupling scheme links the two domains using the DPDE (Dissipative Particle Dynamics at constant Energy) thermostat and is designed to handle strong temperature gradients across the atomistic/continuum domain interface. Using DPDE we investigate the effects of shock-wave impact on the damage of lipid bilayer membranes. A coarse-grained model for the phospholipid bilayer in aqueous environment is employed, which models single lipids as short chains consisting of a hydrophilic head and two hydrophobic tail beads. Water is modeled by mapping four water molecules to one water bead. Using the DPDE method enables us to faithfully simulate the non-equilibrium shock-wave process with a coarse-grained model as the correct heat capacity can be recovered. At equilibrium, we obtain self-stabilizing bilayer structures that exhibit bending stiffness and compression modulus comparable to experimental measurements under physiological conditions. We study in detail the damage behavior of the coarse-grained lipid bilayer upon high-speed shock-wave impact as a function of shock impact velocity and bilayer stability. A single damage parameter based on an orientation dependent correlation function is introduced.

REFERENCES

[1] Martin O. Steinhauser, Computational Multiscale Modeling of Fluids and Solids - Theory and Applications, Springer 2nd ed., Berlin, Heidelberg, New York 2017.

[2] Tanja Schindler, Dietmar Kröner, Martin O. Steinhauser, On the dynamics of molecular self-assembly and the structural analysis of bilayer membranes using coarse-grained molecular dynamics, Biochimica at Biophysica Acta, **1858**, 1955-1963, 2016

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

[PO-I1] Poster Session 1

Symposium I

Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall

[P1-58] Phase-field modeling of anisotropic grain growth with incorporation of Sigma 3 CSL grain boundaries.

○Kunok Chang （Kyung Hee Univ., Korea）

[P1-59] Direct mapping from molecular dynamics to phase-field simulations for accurate prediction of grain growth

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

[P1-60] Density functional theory plus Hubbard U study of the segregation of Pt to the CeO_{2-x} grain boundary

Guoli Zhou, Pan Li, Qingmin Ma, ○Zhixue Tian, Ying Liu （Hebei Normal Univ., China）

[P1-61] **Interfacial charge transfer and enhanced photocatalytic mechanism for Bi_2WO_6/BiOCl heterostructure: A first-principles theoretical study**

○Pan Li （Hebei Normal Univ., China）

[P1-62] Investigation of abnormal grain growth conditions by phase-field method

○Nobuko Mori, Eisuke Miyoshi, Tomohiro Takaki （Kyoto Institute of Technology, Japan）

[P1-63] **Phase Field Crystal Modeling of Mechanism of Strain-Driven for Nucleation and Grain of Deformed-Grain**

○Ying-Jun Gao （Guangxi University, China）

[P1-64] **Diffusion and trapping of hydrogen at grain boundaries scale in fcc polycrystalline nickel: some implications of the atomic volume and the interstitial self-stress**

○xavier Feaugas, jiaqi Li, abdel malek Hallil, abdelali oudriss, arnaud metsue, jamaa bouhattate （university of La Rochelle, France）

(Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall)

[P1-58] Phase-field modeling of anisotropic grain growth with incorporation of Sigma 3 CSL grain boundaries.

○Kunok Chang （Kyung Hee Univ., Korea）

Understanding of grain growth is one of the major on-going challenges of materials science. Since grain growth is complex multi-physics phenomena, it is extremely difficult to describe grain growth phenomenon analytically with the completed theory. Therefore, a number of researchers have tried to investigate grain growth using computational techniques. Among them, the phase-field method has been used one of the efficient and strong tools. So far, 3D grain growth with isotropic grain boundary energy has been intensively studied and their microstructural characteristics have been quantitatively analyzed. On the other hand, since anisotropic 3D grain growth is way more complicated than isotropic phenomena, only a few attemps have been made with simplified assumptions. In this study, we performed anisotropic 3D grain growth with consideration of Sigma 3 CSL grain boundary. To perform the modeling within realistic time window, we implemented OpenMP parallelized technique. We analyzed how degree of anisotropy in grain boundary energy and fraction of CSL boundaries affects growth kinetics and evolution of microstructural characteristics.

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[P1-59] Direct mapping from molecular dynamics to phase-field simulations for accurate prediction of grain growth

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

For numerically predicting grain growth, two different approaches have been used: atomistic simulations typified by molecular dynamics (MD); and continuum-based treatments including the Monte-Carlo, phase-field, and vertex methods. The former can model the spontaneous nucleation process that precedes grain growth. However, due to the large computational cost, it is difficult to simulate grain growth until the late stage using only atomistic methods. On the other hand, continuum-based models allow for relatively efficient computations. In particular, the multi-phase-field (MPF) model [I. Steinbach and F. Pezzolla, Physica D, 134 (1999) 385], which is an extension of the phase-field model to polycrystalline systems, is widely employed in recent years as a prominent tool for simulating grain growth with accuracy and efficiency. Nevertheless, the MPF model cannot directly reproduce the nucleation phenomenon. Considering the strong dependence of grain growth behaviors on the initial structure, there is a pressing need for a means of providing realistic initial structures for MPF simulation.
In this study, we aim to achieve more accurate and efficient prediction of grain growth by exploiting the merits of atomistic and continuum simulations. To this end, we propose a method to convert MD-generated atomic configurations into the MPF interfacial profiles; this enables us to perform MPF grain growth simulations in succession to MD nucleation simulation. Furthermore, using the proposed method, MPF and MD grain growth simulations from the same initial structure are directly compared, via which the difference between each simulation result is quantified. Through the detailed investigation of the causes of the difference, a way to improve the accuracy of the MPF model is discussed.

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[P1-60] Density functional theory plus Hubbard U study of the segregation of Pt to the CeO_{2-x} grain boundary

Guoli Zhou, Pan Li, Qingmin Ma, ○Zhixue Tian, Ying Liu （Hebei Normal Univ., China）

Grain boundaries (GBs) can be used as traps for solute atoms and defects, and the interaction between segregants and GBs is crucial for understanding the properties of nanocrystalline materials. In this study, we have systematically investigated the Pt segregation and Pt-oxygen vacancies interaction at the sigma 3 (111) GB in ceria (CeO_2). The Pt atom has a stronger tendency to segregate to the sigma3 (111) GB thanto the (111) and (110) free surfaces, but the tendency is weaker than to (112) and (100). Lattice distortion plays a dominant role in Pt segregation. At the Pt-segregated-GB (Pt@GB), oxygen vacancies prefer to form spontaneously near Pt in the GB region. However, at the pristine GB, oxygen vacancies can only form under O-poor conditions. Thus, Pt segregation to the GB promotes the formation of oxygen vacancies, and their strong interactions enhance the interfacial cohesion. We propose that GBs fabricated close to the surfaces of nanocrystalline ceria can trap Pt from inside the grains or other types of surface, resulting in the suppression of the accumulation of Pt on the surface under redox reactions, especially under O-poor conditions

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[P1-61] Interfacial charge transfer and enhanced photocatalytic mechanism for Bi_2WO_6/BiOCl heterostructure: A first-principles t heoretical study

○Pan Li （Hebei Normal Univ., China）

First-principles calculations based on density functional theory are used to explore the interfacial structure and properties of the Bi_2WO_6/BiOCl heterojunction aiming at gaining insights into the photocatalytic mechanism of the Bi_2WO_6/BiOCl heterojunction. Bi_2WO_6/BiOCl interface has a good lattice match, with the interface formation energy is -4.67eV. The calculated band alignment between the Bi_2WO_6 and BiOCl reveals that the valence band offset and conduction band offset between BiOCl and Bi_2WO_6 are 0.37 eV and 1.02 eV, respectively. The calculated Mulliken charge population and electron difference density maps reveal that there is a self-induced internal electric field along the perpendicular direction to the layers in the BiOCl and Bi_2WO_6. Based on the obtained work function and band edge positions of BiOCl and Bi_2WO_6, the formation mechanism of the internal electric field at the interface of Bi_2WO_6/BiOCl heterostructure is studied. The existence of band offsets and the internal electric field can facilitate the separation of the photo-generated electron-hole pairs, resulting in the enhanced photocatalytic activities of the heterostructures.

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[P1-62] Investigation of abnormal grain growth conditions by phase-field method

○Nobuko Mori, Eisuke Miyoshi, Tomohiro Takaki （Kyoto Institute of Technology, Japan）

To improve the properties of materials by controlling their textures and grain sizes, it is essential to accurately predict abnormal grain growth, a phenomenon through which a few grains undergo preferential growth. In addition, the abnormal grain growth is considered to be one of the origins for the nucleation of recrystallized grains and, thus, is of great importance for modelling recrystallization processes.
As a prominent theory of abnormal grain growth, that proposed by Humphreys (here referred to as the cellular microstructural stability (CMS) theory) is well known. In this theory, a complicated polycrystalline microstructure, where grain size, boundary energy, and boundary mobility are not uniform, is simplified as a cellular microstructure model. The model consists of two ingredients: a specific grain and its surrounding matrix with uniform grain size and boundary properties. This modelling makes it possible to describe the abnormal grain growth behavior of the specific grain using only three parameters, i.e., its relative size, boundary energy, and boundary mobility normalized by those of the matrix. However, the validity of this theory has not been confirmed yet neither in experiment and simulation.
In this study, we aim to evaluate the applicable range of the CMS theory via systematic two-dimensional numerical simulations. As the numerical model, the multi-phase-field model [2] is employed, enabling accurate treatment of curvature-driven grain boundary migration in polycrystalline systems. Grain growth simulations are performed while varying the size, boundary energy, and boundary mobility of a specific grain in the matrix. By comparing the simulated results with the prediction of the CMS theory, we reveal the validity and applicable range of the theory.

[1] F. J. Humphreys, Acta Mater., 45, (1997), 4231.
[2] I. Steinbach, F. Pezzolla, Physica D, 134, (1999), 385.

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[P1-63] Phase Field Crystal Modeling of Mechanism of Strain-Driven for Nucleation and Grain of Deformed-Grain

○Ying-Jun Gao （Guangxi University, China）

The phase-field-crystal (PFC) method is used to investigate dynamic strain-induced a splitting of grain boundary (GB) to generate a deformed grain with high strain energy and to drive it to grow in two dimensions. The simulated results show that the essence of the splitting process of the original GB is that new deformed grain is nucleated, and results in formation of high-density ensembles of mobile lattice dislocation that is capable of plastic flow localization (deformed banding). The GB migration is the process of the new deformed grain with higher strain energy consuming the original grain to extend. The deformed grain stores the strain energy through climbing of the dislocation, as well as changing the orientation of the original grain. The deformed grain growth (DGG) is the acceleration process of the speed, and its area extension is proportional to the time square. The rule of the time square of the DGG can also be deduced by establishing the dynamic equation of the strain-driven for the dislocation and the deformed grain extension.

(Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall)

[P1-64] Diffusion and trapping of hydrogen at grain boundaries scale in fcc polycrystalline nickel: some implications of the atomic volume and the interstitial self-stress

○xavier Feaugas, jiaqi Li, abdel malek Hallil, abdelali oudriss, arnaud metsue, jamaa bouhattate （university of La Rochelle, France）

The mobility of hydrogen in metals is a key parameter for understanding the basic mechanisms of hydrogen embrittlement (HE). This problem is directly related to the mechanisms of diffusion and trapping of hydrogen within a specific metallurgical state. These mechanisms depend on the various microstructural heterogeneities and in particular the grain boundaries (GBs), triple junction (TJs) and several defects (dislocations, vacancies …). Although a number of theories have been proposed to describe the role of GBs for hydrogen diffusion and segregation, none of them is able to give an exact answer. In present work we report our recent works, which support the investigation of diffusion and trapping of hydrogen in two elementary systems: nickel single crystals and bi-crystals to highlight the impact of GB on hydrogen mobility in polycrystalline fcc metals. We developed a methodology combining experimental tools (electrochemical permeation / TDS, HRTEM, EBSD) and numerical methods (FEM-COMSOL / EAM-LAMMPS). We propose to screen several bi-crystals of pure nickel with different grain boundaries (**Σ11-**50°*30<110>{311},* **Σ11-***129° 30<110>{332},* **Σ3-***70°30<110>{111}* and **Σ5-***37°<100>{310}).*

The results allow us to associate the short-circuit diffusion and trapping phenomena to the grain boundaries and defect characters (excess volume, defects density and distribution …). In each situation, we highlight the importance of the self-stress on the processes of diffusion and segregation. The segregation energy of hydrogen depends on the nature of the site (the local free volume and the elastic energy associated with the incorporation of solute). The diffusion of hydrogen is directly influenced by the nature of the grain boundary (the free volume and the distribution of the segregation sites). Our results, at the atomic scale, show a correlation between the solubility and the free volume of the grain boundary. The grain boundaries with a higher free volume have more favorable diffusion paths for hydrogen than in the crystal lattice and at the same time more segregation sites.

Poster Session | J. Multiscale Modeling of Heterogeneous Layered Media

[PO-J1] Poster Session 1

Symposium J

Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall

[P1-65] Multiscale Model for Interlayer Defects in Heterogeneous Bilayer Material

○Shuyang Dai[1], David Joseph Srolovitz[2], Yang Xiang[3] （1.Wuhan University, China, 2.University of Pennsylvania, United States of America, 3.Hong Kong University of Science and Technology, Hong Kong）

(Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall)

[P1-65] Multiscale Model for Interlayer Defects in Heterogeneous Bilayer Material

○Shuyang Dai[1], David Joseph Srolovitz[2], Yang Xiang[3] （1.Wuhan University, China, 2.University of Pennsylvania, United States of America, 3.Hong Kong University of Science and Technology, Hong Kong）

We present a multiscale model to describe the interlayer defects in bilayer materials. The model incorporates both the anisotropy elasticity of each layer and the first-principle calculation informed interaction between two layers, i.e., the 3-dimensional generalized stacking-fault energy. The force balance between these two contributions determines the structure. We apply this approach to determine the structure and energetics of twisted bilayer material. In twisted bilayer graphene, two distinct, modified Moiré structures are observed. We also study the buckling twisted heterogeneous bilayer material such as bilayer graphene/hexagonal boron nitride. We investigate the structure and corresponding dislocation network due to various misfits and twist angles between two layers. The relaxation of the Moiré structure reduces the symmetry and increases the period of the bilayer material. Our model agrees well with the atomistic results. An analytical description is developed based on the obtained structural features.

Poster Session | L. Structure, Statistics and Mechanics in Crystal Dislocation Plasticity

[PO-L1] Poster Session 1

Symposium L

Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall

[P1-66] Molecular dynamics study on temperature and loading rate dependence of nano-indentation pop-in load

○Yuji Sato[1], Shuhei Shinzato[1], Takahito Ohmura[2], Shigenobu Ogata[1,3] （1.Department of Mechanical Science and Bioengineering, Osaka University, Japan, 2.Research Center for Structural Materials, National Institute for Materials Science, Japan, 3.Center for Elements Strategy Initiative for Structural Materials (ESISM), Kyoto University, Japan）

[P1-67] Geometry of curved surface and energetics of in graphene with defects

○Ako Kihara[1], Xiao-Wen Lei[1], Akihiro Nakatani[2] （1.Dept. of Mechanical Engineering, Univ.of Fukui, Japan, 2.Dept. of Adaptive Machine Systems, Osaka Univ., Japan）

[P1-68] Collective motion of dislocation associated with local plasticity initiation and subsequent behavior in bcc metals

○Takahito Ohmura （National Institute for Materials Science, Japan）

(Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall)

[P1-66] Molecular dynamics study on temperature and loading rate dependence of nano-indentation pop-in load

○Yuji Sato[1], Shuhei Shinzato[1], Takahito Ohmura[2], Shigenobu Ogata[1,3] (1.Department of Mechanical Science and Bioengineering, Osaka University, Japan, 2.Research Center for Structural Materials, National Institute for Materials Science, Japan, 3.Center for Elements Strategy Initiative for Structural Materials (ESISM), Kyoto University, Japan)

Nano-indentation test is commonly used to investigate mechanical properties of materials in nano-scale. In nano-indentation test, a displacement burst behavior of indenter, “pop-in”, can be usually observed. Pop-in is considered to be attributable to dislocation nucleation phenomena, thus pop-in can be associated with incipient plasticity in materials. It is well-known that the pop-in occurs when a shear stress along a slip system beneath the indenter reaches near theoretical shear strength. However, the temperature and loading rate dependency of pop-in load is still unclear. In this study, using atomistic simulation with EAM interatomic potentials, we computed stress dependent activation energy of homogeneous dislocation nucleation event in BCC Fe and Ta under actual complex stress condition beneath a spherical indenter. Based on the computed activation energy and stochastic modeling method, temperature and loading-rate dependent probability distribution of the critical indentation load was successfully predicted. Eventually, we compared the atomistic predictions with experiments, and confirmed validity of our atomistic modeling.

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[P1-67] Geometry of curved surface and energetics of in graphene with defects

○Ako Kihara[1], Xiao-Wen Lei[1], Akihiro Nakatani[2] (1.Dept. of Mechanical Engineering, Univ.of Fukui, Japan, 2.Dept. of Adaptive Machine Systems, Osaka Univ., Japan)

Two-dimensional (2D) materials have attracted attentions as unique functional materials.
Among them, graphene is well-known as a fundamental structure of 2D materials of nano-carbon.
In 2D materials, lattice defects, such as dislocations and disclinations, cause out-of-plane deformation.
For example, carbon nano-cone or nano-horn is formed geometrically by the wedge disclination of graphene sheet (GS).

In this study, we focus on the fundamental mechanism which can explain how the shape of 2D materials with defects is determined.
Typical four structure models of GS with defects are studied, i.e. positive perfect wedge disclination, negative perfect wedge disclination, positive partial wedge disclination, and negative partial wedge disclination.
The partial wedge disclinations are implemented by the array of edge dislocations in which the local structure consists of pentagon-heptagon atomic bonds.
Then the equilibrium configuration is calculated by using large-scale atomic/molecular massively parallel simulator (LAMMPS).

The obtained surfaces are examined by fitting to analytical test functions.
All results of out-of-plane displacement z are organized by a universal form of $z=rf(\theta)$, in a cylindrical coordinate (r, θ, z), in which $f(\theta)$ is an appropriate function of θ.

This result means that the all models of GS are represented as conical surfaces in a broad sense.
From a local viewpoint, according to the distribution of atomic site potential energy, it is observed that the energy values at atoms in pentagon ring are relatively high, but the energy values at atoms in heptagon ring are relatively low.
From a global viewpoint, the energy values decrease with increasing distance r from the core of disclination.
After a detail examination, we found the site potential energy is proportional to the square of curvature.
The fundamental knowledge obtained would be applicable to desgin/control the shape of 2D materials.

(Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall)

[P1-68] Collective motion of dislocation associated with local plasticity initiation and subsequent behavior in bcc metals

○Takahito Ohmura （National Institute for Materials Science, Japan）

Nanoindentation-induced mechanical behavior was investigated for bcc metals. Pop-in event that corresponds presumably to local plasticity initiation was detected on load-displacement curves with major parameters of critical load P_c and corresponding excursion depth *deltah*. In a plot of P_c vs delta*h*, the P_c increases monotonically with the *deltah*, and the slope depends on alloy systems. On the other hand, brittle-to-ductile transition temperature (BDTT) also depends on the alloy systems, and the alloy with higher BDTT shows higher slope in the P_c vs delta*h* plot. Dislocation structures underneath the indenter were observed through TEM before and after a pop-in event. No dislocations were observed before initiation while considerable dislocations were generated right after the event. These results suggest that dislocation nucleation and multiplication occur drastically upon plasticity initiation based on collective dislocation motion. Since the BDTT is closely consistent with pop-in event, crack propagation might be related with plasticity initiation. Statistical analysis of the events suggests physical models of the phenomena. In the case of the first pop-in event, the probability of the event to the P_c is Gaussian distribution, which indicates that a thermally activated process dominates the event. For the second or later cases, the probability to the magnitude of the event shows power law function like Gutenberg-Richter model, which suggests a dislocation avalanche.

Poster Session | M. Time- and History-Dependent Material Properties

[PO-M1] Poster Session 1

Symposium M

Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall

[P1-69] FORMATION OF PHYSICAL GELS BY ARRESTED SPINODAL DECOMPOSITION IN CHARGED COLLOIDS

○Jose Manuel Olais-Govea[1], Alonso Gomez-Canales[1], Leticia Lopez-Flores[2], Martin Chavez-Paez[2], Magdaleno Medina-Noyola[2] （1.Instituto Tecnologico y de Estudios Superiores de Monterrey, Mexico, 2.Universidad Autonoma de San Luis Potosi, Mexico）

[P1-70] How to improve the ductility of CuZr BMGs based on cyclic pre-straining: MD simulations and mechanical testing

○Jonathan Amodeo[1], Oriane Baulin[1], Damien Fabregue[1], David Rodney[2] （1.MATEIS, Univ. Lyon 1, France, 2.ILM, Univ. Lyon 1, France）

[P1-71] Modeling plastic deformation of amorphous solids from atomic scale mechanisms

○Francesca Boioli[1], Tristan Albaret[2], David Rodney[2] （1.LEM, CNRS-ONERA, Chatillon, France, France, 2.ILM, University of Lyon 1, France, France）

[P1-72] Thermally Activated Creep and Constant Shear Rate Deformation in Amorphous Materials

○Samy MERABIA[1], Julien LAM[2], François DETCHEVERRY[1] （1.CNRS and Universite Lyon 1, France, 2.Université de Bruxelles, Belgium）

[P1-73] Numerical analysis of shrinkage process based on the experimental data

○Barbara Kucharczykova[1], Hana Simonova[2], Petr Frantik[2] （1.Brno University of Technology, Faculty of Civil Engineering, Institute of Building Testing, Czech Republic, 2.Brno University of Technology, Faculty of Civil Engineering, Institute of Structural Mechanics, Czech Republic）

(Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall)

[P1-69] FORMATION OF PHYSICAL GELS BY ARRESTED SPINODAL DECOMPOSITION IN CHARGED COLLOIDS

○Jose Manuel Olais-Govea[1], Alonso Gomez-Canales[1], Leticia Lopez-Flores[2], Martin Chavez-Paez[2], Magdaleno Medina-Noyola[2] （1.Instituto Tecnologico y de Estudios Superiores de Monterrey, Mexico, 2.Universidad Autonoma de San Luis Potosi, Mexico）

The general understanding of gelation processes is recognized as a major challenge in soft matter field. Particularly, attractive liquids that suffer a suddenly instantaneous isochoric quench an homogeneous state to thermodynamic instability could form a physical gel. Although, both experimental and simulation advances in understanding gelation phenomenon had led to build a general comprehension about physical gel properties and even had discussed the perform of novel materials as amorphous solids, there is no a clear theoretical approach to explain these class of ubiquitous materials. In recent work, however, the general theory referred to as the non-equilibrium self-consistent generalized Langevin equation (NESCGLE) theory, based on a non-equilibrium extension of Onsager’ s canonical theory of thermal fluctuations, was adequately adapted to describe memory effects, protocol-dependent preparation and irreversible aging processes associated with the glass and the gel transitions in attractive simple liquids. In particular, this theory was capable of predict a glass-glass transition line and propose a glass-gel line in a monocomponent attractive Yukawa simple fluid (HSAY) by arested spinodal decomposition when that system is instantaneously quenched inside spinodal region. In the present work, we extend this analisys in the context of a very specific model system, namely, let us consider an screened restricted primitive model (YRPM), represented as an electroneutral mixture of charged hard spheres embedded in a dielectric medium of uniform dielectric constant. Additionaly we show pertinent comparisons between our theoretical results and the gel formation in a mixture of equally-sized oppositely charged colloids both experimentally and by means of computer simulations.

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[P1-70] How to improve the ductility of CuZr BMGs based on cyclic pre-straining: MD simulations and mechanical testing

○Jonathan Amodeo[1], Oriane Baulin[1], Damien Fabregue[1], David Rodney[2] （1.MATEIS, Univ. Lyon 1, France, 2.ILM, Univ. Lyon 1, France）

Bulk metallic glasses are currently used as technical materials(*e.g.*magnetic transmitters, golf clubs, brazing materials) for their high elastic and strength properties, significantly larger than their crystalline counterparts. However, their use is generally limited to elastic engineering applications due to their quasi-brittle behaviour caused by the early initiation of localized shear bands upon plastic deformation.

In this study, we used a combination of atomistic simulations and compressive mechanical testing to investigate the role of mechanical pre-cycling on the stress response and elementary deformation processes of a CuZr glass. In the experiments, unprestrained $Zr_{52.5}Cu_{17.9}Ni_{14.6}Al_{10}Ti_5$(Vitreloy 105) samples show a plastic strain before failure of about 3% strain and a yield strength of about 1900 MPa. After applying a limited number of cycles with a maximum amplitude of 400 MPa (n=2, 4 or 6), the plastic strain increases up to 15%. It remains however in the same low range for higher pre-cycling amplitudes of 700 and 1200 MPa. MD simulations performed on $Cu_{64.5}Zr_{35.5}$thin films show that (i) unprestrained samples deform due to a local

shear banding process, (ii) pre-cycled samples are characterized by the occurrence of homogeneous deformation zones with a concentration that depends on the cyclic stress amplitude *i.e.*the lower the stress amplitude of the pre-cycles, the higher the proportion of homogeneous deformation. This emphasizes the existence of a critical stress under which the main shearing process of CuZr BMGs changes due to pre-cycling, reducing shear localization and the early occurrence of cracks. These results are confirmed by the statistical analysis of experimental vein patterns on fracture surfaces that show larger cusps (ϕ >3500 m^2), attributed to highly localized plastic events, only in the cases of samples pre-cycled at high stress amplitude.

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[P1-71] Modeling plastic deformation of amorphous solids from atomic scale mechanisms

○Francesca Boioli[1], Tristan Albaret[2], David Rodney[2] （1.LEM, CNRS-ONERA, Chatillon, France, France, 2.ILM, University of Lyon 1, France, France）

Amorphous solids are characterized by high strength and low ductility. The latter property is a consequence of the localization of the plastic deformation in shear bands, which leads to catastrophic failure. As a consequence, understanding the localization of plastic deformation and the formation of shear bands is of utmost importance. Generally, it has been accepted that local irreversible rearrangements of small clusters of atoms, Shear Transformations (STs), are the elementary processes involved in the deformation of amorphous systems and several mesoscale models based on STs have been proposed. Still the fundamental mechanisms underlying ST occurrence and shear bands formation are not yet clear. In this context, atomistic simulations can provide significant details that would otherwise be unavailable.
In this work we characterize shear transformations (STs) at the atomic scale in a model of amorphous silicon using a mapping on Eshelby inclusions. First, by using Nudged Elastic Band calculations, we measure the energy barrier against ST activation. Analyzing different paths leading to either an isolated ST or an avalanche, we show that the barrier is systematically controlled by the first ST with an activation volume equal to the effective volume of the ST at the activated state, which represents only a fraction of the complete ST volume. The activation volume is also found smaller for avalanches, presumably because of accumulated local damage. Furthermore, we investigate the dynamic process of ST formation, determining the characteristic time involved in the development of STs and the influence of the strain rate on the STs distribution and organization. This work provides essential information to build reliable mesoscale models of plasticity.

(Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall)

[P1-72] Thermally Activated Creep and Constant Shear Rate Deformation in Amorphous Materials

○Samy MERABIA[1], Julien LAM[2], François DETCHEVERRY[1] （1.CNRS and Universite Lyon 1, France, 2.Université de Bruxelles, Belgium）

In this contribution, we shall discuss two issues related to the deformation of amorphous materials.
The first issue concerns transient creep also called Andrade creep, characterized by strain slowly increasing algebraically with time, a regime interrupted by fluidization and eventually steady flow. Here we characterize

creep and fluidization on the basis of a mesoscopic viscoplastic model that includes thermally activated yielding events and a broad distribution of energy barriers, which may be lowered under the effect of a local deformation. We relate the creep exponent observed before fluidization to the width of barrier distribution and to the specific form of stress redistribution following yielding events. We show that Andrade creep is accompanied by local strain hardening driven by stress redistribution and find that the fluidization time depends exponentially
on the applied stress, in qualitative agreement with experiments.
The second issue to be discussed concerns constant shear rate deformation of molecular glasses. Recent experiments on polymer glasses [2] have demonstrated enhanced mobility in the preyield regime accompanied by a narrowing of the distribution of segmental relaxation times. Yet, the mechanisms at play remain partially understood.
In the light of the mesoscopic model [1], we characterized the evolution of the distribution of energy barriers during constant shear rate deformation. Our simulation results account for enhanced mobility and the narrowing of the distribution of relaxation times. Good agreement is obtained with the experimental observations of Bending et al., without any adjustable parameter.
All the simulation results are interpreted in the light of a mean-field analysis, and should help in rationalizing the creep and deformation phenomenology as observed in disordered materials.

References

[1] S. Merabia and F. Detcheverry, Thermally activated creep and fluidization in flowing disordered materials, EPL (2016)

[2] B. Bending, K. Christison, J. Ricci, and M. D. Ediger, Measurement of Segmental Mobility during Constant Strain Rate
Deformation of a Poly(methyl methacrylate) Glass, Macromolecules (2014)

(Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall)

[P1-73] Numerical analysis of shrinkage process based on the experimental data

○Barbara Kucharczykova[1], Hana Simonova[2], Petr Frantik[2] (1.Brno University of Technology, Faculty of Civil Engineering, Institute of Building Testing, Czech Republic, 2.Brno University of Technology, Faculty of Civil Engineering, Institute of Structural Mechanics, Czech Republic)

The shrinkage process in cement based materials is still an actual problem of civil engineers and manufacturers of cement based composites, such as concrete, mortars, floor compounds etc. There are many standardized and non-standardized testing techniques which are used for estimation/determination of real value of shrinkage process during the whole time of material ageing, unfortunately the results are often inconsistent, especially because of different measurement equipment, dimensions of the test specimens and initial time of the start or evaluation of measurement. There are also incomplete experimental data of early-age volume changes, which can be used for numerical prediction models. The article focuses on the implementation of the experimentally obtained data to the shrinkage model B4 designed by research group of prof. Z. P. Bazant. The results show that especially the early-age part of real-measured shrinkage process does not correspond with the prediction model. In order to improve the correlation between the measured process and the prediction model, it is necessary to adjust the existing correction factors. The published

results were obtained within the implementation of the research project granted by the Czech Science Foundation - project No. GA17-14302S.

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

[PO-O1] Poster Session 1

Symposium O

Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall

[P1-74] Designing Lubricant Additives for Titanium Carbide Surface: First-principles and Molecular Dynamics Investigations

○Tasuku Onodera, Jun Nunoshige, Hiroshi Kanemoto （Research &Development Group, Hitachi, Ltd., Japan）

[P1-75] Crystal Growth Molecular Dynamics Simulation of alpha-Al_2O_3 Cutting Tools for Realizing Their Best Tribological Properties

○Shandan BAI[1], Hiroya Nakata[1], Jingxiang Xu[2], Nobuki Ozawa[2], Momoji Kubo[2] （1.KYOCERA Cop., Japan, 2.Tohoku Univ., Japan）

[P1-76] Atomistic modeling of polymer friction

○Robin Sam Vacher （SINTEF-NTNU, Norway）

[P1-77] A two degree-of-freedom extension to the Prandtl Tomlinson-model for friction strengthening in layered materials

○David Andersson[1,2], Astrid de Wijn[2] （1.Department of Physics, Stockholm University, Sweden, 2.Department of Mechanical and Industrial Engineering, Norwegian University of Science and Technology, Norway）

[P1-78] Analysis of Friction Characteristics of Steel Powders using Parallelized Discrete Element Method

○Naoki Yashiro[1,2], Kouya Oohira[2], Natsuko Sugimura[1], Hitoshi Washizu[1] （1.Graduate School of Simulation Studies, University of Hyogo, Japan, 2.Advanced Technology R&D Center, NTN Corporation, Japan）

[P1-80] Dynamics of Polymer Under Shear in Confinement Geometry

○Taiki Kawate[1], Soma Usui[1], Hiroaki Yoshida[2], Hitoshi Washizu[1] （1.Univ. of Hyogo, Japan, 2.Toyota Central R&D Labs, Japan）

[P1-81] Dynamics of a Polymer in Bulk Solution under Shear Flow

○Soma Usui[1], Taiki Kawate[1], Hiroaki Yoshida[2], Hitoshi Washizu[1] （1.Univ. of Hyogo, Japan, 2.Toyota Central R&D Labs., Japan）

[P1-82] Mechanochemistry induced atomic wear in chemical mechanical polishing processes

○Jialin Wen, Tianbao Ma, Xinchun Lu （Dept. of Mechanical Engineering, Tsinghua Univ., China）

[P1-83] Adsorption property of a fatty acid on iron surface with grain boundary

○Yuki Uchiyama, Yoshinori Shiihara, Ivan Lobzenko （Toyota Technological Institute, Japan）

(Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall)

[P1-74] Designing Lubricant Additives for Titanium Carbide Surface: First-principles and Molecular Dynamics Investigations

○Tasuku Onodera, Jun Nunoshige, Hiroshi Kanemoto （Research &Development Group, Hitachi, Ltd., Japan）

In order to highly improving performance of industrial products such as automobile, the innovative technology should be strongly required, especially for the fields of surface and interface technology. Several problems on surface fractures, i.e. fatigue, wear, corrosion and erosion have been arisen in a metallic bearing or gear which typically work under the conditions of high temperature, extreme pressure and shear.

One of the technologies for reducing surface fractures is a hard coating on surface. For example, in the field of tribology, diamond-like carbon (DLC) coatings have been strenuously investigated so far. Covering surface with the film leads to low friction and low wear performances, contributing to extending a product lifetime and to reducing a maintenance work of products. However, under the lubrication by engine oil, DLC coating unexpectedly caused wear. This negative effect may be due to existence of organic molybdenum compounds in engine oil as a friction modifier. A novel additive compound has been developed by modifying adsorption property. This story tells us that tailor-made additives have to be required for own hard coating applied to shear parts.

Titanium-based hard coatings are also forcused for extending lifetime of products. Especially, titanium carbides show extremely high hardness and coincidently have anti-wear, anti-corrosion, and anti-oxidant properties. This material has been applied to cutting tools used at high temperature, extreme pressure and shear. Hence, titanium carbide seems to be a suitable surface coating material for extending lifetime.

In the present study reported here, for the purpose of extending lifetime of industrial products, a chemical composition of lubricant oil was optimized for titanium carbide coatings. An optimum molecular structure of additive compounds and its interaction with titanium carbide were theoretically investigated by using a method of density functional theory (DFT). An adsorption energy on TiC(100) was calculated for several additive compounds. The simulation results showed that the amide-type molecule showed high adsorption energy, suggesting that these additives would exhibit a good lubrication performance.

(Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall)

[P1-75] Crystal Growth Molecular Dynamics Simulation of alpha-Al_2O_3 Cutting Tools for Realizing Their Best Tribological Properties

○Shandan BAI[1], Hiroya Nakata[1], Jingxiang Xu[2], Nobuki Ozawa[2], Momoji Kubo[2] （1.KYOCERA Cop., Japan, 2.Tohoku Univ., Japan）

Aluminum oxide (Al_2O_3) as coating materials has been used for cutting tools. It is widely applied on machining metals, because Al_2O_3 films show the tribological properties of high hardness and heat resistance. The Chemical Vapor Deposition (CVD) coating process for Al_2O_3 film is a very effective way to get its excellent tribological properties. $AlCl_3/CO_2/H_2$ gas system is used for the CVD process to obtain the Al_2O_3 coating. At the beginning step of the CVD process, the surface reactions affect the orientation of Al_2O_3 surface. However, the relationship between the surface reactions and Al_2O_3 orientation is difficult to be clarified by the

experiments. In this study, we investigate the details of surface reactions on the alpha-Al_2O_3 (0001) and (11-20) surfaces using computational simulation methods at the molecular scale. The alpha-Al_2O_3 take place through the hydrolysis reactions of $AlCl_3$ and H_2O. In order to clarify the surface reaction mechanism on alpha-Al_2O_3 (0001) and (11-20), we calculate the $AlCl_3$ molecule adsorption on these surfaces using the first principles calculation. GGA-PBE functional is employed. One $AlCl_3$ molecule is placed on various sites atom of alpha-Al_2O_3 (0001) and (11-20), and the system is optimized. The highest adsorption energies are -107.63 and -60.87 kcal/mol, respectively. The result indicates that $AlCl_3$ molecule easily adsorbed on the alpha-Al_2O_3 (0001) surface. After the optimization of the $AlCl_3$ molecule, the 6-coordinated Al and 4-coordinated Al of the $AlCl_3$ molecule are observed on the alpha-Al_2O_3 (0001) and (11-20) surfaces, respectively. It means that 6-coordinated Al shows the stable adsorption state. Furthermore, molecular dynamics simulation is performed to clarify the surface reaction dynamics on the alpha-Al_2O_3 (0001) and (11-20). The details will be discussed on our presentation.

(Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall)

[P1-76] Atomistic modeling of polymer friction

○Robin Sam Vacher （SINTEF-NTNU, Norway）

Polymers are present in our daily life and we are using their tribological properties even without noticing it, walking with shoes is just one example. However, the theoretical understanding of the friction and wear of polymers is still lacking and therefore, development of novel low friction material of solid polymers can only be achieved by trial and error procedures including expensive testing. In this work, the focus is put on the influence of structural properties of solid polymers on the friction and wear. Molecular dynamic simulation is used to capture the crystallization process of PolyVinyl Alcohol (PVA). The coarse grain potential for PVA (CG-PVA) developed by Meyer and Muller-Plathe (” *Formation of chain-folded structures in supercooled polymer melts” , J. Chem. Phys. 2001, 115, 7807*) has been used in order to drastically speed up the simulation. Depending on the cooling rate and the number of monomers per chain, the crystalline domains will have different structural properties (eg. crystallinity level). We create samples of polymers with different crystalline structure, and investigate numerically by simulating the effect of rubbing the surface with an AFM tip the relation between friction, wear, and crystallinity.

Keywords : molecular dynamic, polymers, friction and wear

(Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall)

[P1-77] A two degree-of-freedom extension to the Prandtl Tomlinson-model for friction strengthening in layered materials

○David Andersson[1,2], Astrid de Wijn[2] （1.Department of Physics, Stockholm University, Sweden, 2.Department of Mechanical and Industrial Engineering, Norwegian University of Science and Technology, Norway）

The Prandtl Tomlinson-model model has been exceedingly successful in describing the stick-slip friction response signal observed in atomic systems. However, recently it has been observed in both experiments and MD simulations that layered materials exhibit an initial period of friction strengthening, which is not found

within the Prandtl Tomlinson-model [1][2]. Furthermore, out-of-plane bending has been proposed as a driving mechanism for this friction strengthening regime [2][3]. In this paper we propose an extension to the Prandtl Tomlinson-model to account for friction strengthening. We show that this model successfully exhibits friction strengthening for a wide range of parameters, and that it is consistent with the out-of-plane bending hypothesis as well as previous experiments. Moreover, we make predictions as to the importance of commensurability for friction strengthening in these systems.

[1] Frictional Characteristics of Atomically Thin Sheets, Lee at al, Science 2010, doi: 10.1126/science.1184167
[2] The evolving quality of frictional contact with graphene, Li at al, Nature 2016, doi: 10.1038/nature20135
[3] Flexible graphene strengthens friction, de Wijn, Nature Communication 2016, doi:10.1038/539502a

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(Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall)

[P1-78] Analysis of Friction Characteristics of Steel Powders using Parallelized Discrete Element Method

○Naoki Yashiro[1,2], Kouya Oohira[2], Natsuko Sugimura[1], Hitoshi Washizu[1] (1.Graduate School of Simulation Studies, University of Hyogo, Japan, 2.Advanced Technology R&D Center, NTN Corporation, Japan)

In order to increase the application of sintered metal parts, high dense and less pores parts have to be produced with stable quality. Since sintered metal parts cannot be fully densified during sintering, it is essential to understand the steel powders' characteristics in detail and to densify them in the compaction step. Sufficient powder characteristic data, however, cannot be evaluated by conventional versatile methods, and there are few cases where actual powder characteristics are applied to large scale particle simulation. In this study, we evaluated flowability and friction characteristics of steel powders experimentally in detail, and applied them to parallelized discrete element method (DEM).

We prepared steel powders with different kinds of solid lubricant and addition process. Their characteristics were evaluated by a method using a powder yield locus (PYL). The evaluation indexes are flowability (uniaxial collapse stress), inter-particle friction (internal friction angle), and friction between particles and mold (wall friction angle).

The PYL method, which can measure flowabilities under various vertical loads, enabled collection of powder characteristics corresponding to the actual powder behavior in the mold. Furthermore, inter-particle and wall friction coefficients were calculated using the friction angles obtained from these experiments. These coefficients were higher than those which were applied in previous DEM simulation reports.

We created a parallelized DEM code for powder behavior simulation, using FDPS (Framework for Developing Particle Simulator) developed by Iwasawa *et al.*[1] in order to develop into large scale parallelization in the future. FDPS is designed to reduce the calculation load at the time of region division and interaction calculation by constructing a tree structure. In this code, we evaluated flowabilities and friction characteristics by changing the model of the contact force between particles, especially the tangential component.

In the conference presentation, we will show the flowabilities and the friction characteristics of steel powders, which are evaluated by this parallelized DEM code.

[1] Iwasawa *et al.*, *Publ. Astron. Soc. Japan*, 68, 54 (2016)

(Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall)

[P1-80] Dynamics of Polymer Under Shear in Confinement Geometry

○Taiki Kawate[1], Soma Usui[1], Hiroaki Yoshida[2], Hitoshi Washizu[1] （1.Univ. of Hyogo, Japan, 2.Toyota Central R&D Labs, Japan）

In lubricants, a small amount of polymer named viscosity index improver (VII) is used to control temperature dependence of viscosity. When VII is confined in small space, such as space between piston ring and cylinder bore in combustion engine, the dynamics of the solution changes due to the confinement. Here we simulate the dynamics of polymer under shear flow in confinement geometry. Polymer segment is modeled as sphere Brownian particle. The motion of the particle is tracked by the Langevin equation, whereas the Navier-Stokes equation governing the behavior of the base oil is analyzed by using the lattice Boltzmann method. The two equations are coupled through the friction between the particle and the fluid. The friction force is in proportion to the velocity of a particle relative to the host fluid, which is evaluated locally based on the velocity difference at the position of the point particle. The friction force acting on a particle is estimated by fitting the analytical solution or the flow around a Stokes-let to the flow field obtained numerically. The reaction force acts on the position of the particle, which realizes two-way coupling between the particle and fluid motions. The lattice Boltzmann method is employed for the flow simulation, which is compatible with massive parallel computing, and is easy to apply various types of boundary conditions. In order to describe confined system, periodical boundary is adopted in x, y (flow and transverse) direction, and non-slip boundary is adopted in bottom plate in z direction and moving wall is set in top plate of it. During the simulation, the polymer is pulled to upper layer where the shear field is large. To show the orientation of the molecule, order parameter is calculated. The orientation of the polymers changed to the direction of the external shear force.

(Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall)

[P1-81] Dynamics of a Polymer in Bulk Solution under Shear Flow

○Soma Usui[1], Taiki Kawate[1], Hiroaki Yoshida[2], Hitoshi Washizu[1] （1.Univ. of Hyogo, Japan, 2.Toyota Central R&D Labs., Japan）

This study describes dynamics of viscosity index improver (VII) in bulk lubricants under shear flow. Small amount of polymer named VII is added in basis oil to control viscosity index (VI) which is a parameter to express temperature dependence of viscosity. Controlling VI is one of the commonly used methods to improve the fuel consumption of motor vehicles. Here we simulate the dynamics of polymer under shear flow in Bulk Solution. Polymer segment is modeled as sphere Brownian particle. The motion of the particle is tracked by the Langevin equation, whereas the Navier-Stokes equation governing the behavior of the base oil is analyzed by using the lattice Boltzmann method. The two equations are coupled through the friction between the particle and the fluid. The friction force is in proportion to the velocity of a particle relative to the host fluid, which is evaluated locally based on the velocity difference at the position of the point particle. The friction force acting on a particle is estimated by fitting the analytical solution or the flow around a

Stokes-let to the flow field obtained numerically. The reaction force acts on the position of the particle, which realizes two-way coupling between the particle and fluid motions. The lattice Boltzmann method is employed for the flow simulation, which is compatible with massive parallel computing, and is easy to apply various types of boundary conditions. In order to simulate the system, the computational domain has three-dimensions and Periodic boundary condition. External forces are introduced to form simple shear flow. The dynamics of polymer in shear flow is examined by using two computational methods.

(Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall)

[P1-82] Mechanochemistry induced atomic wear in chemical mechanical polishing processes

○Jialin Wen, Tianbao Ma, Xinchun Lu （Dept. of Mechanical Engineering, Tsinghua Univ., China）

Chemical mechanical polishing (CMP) is widely applied in the semiconductor industry to achieve ultra-high precision manufacturing of surfaces (such as Si and Cu), however, its mechanisms remain elusive because of interaction between chemical effects (such as the chemical reactions with the existence of H_2O_2 and glycine) and mechanical effects (such as the tribology process). By using molecular dynamics simulations based on the ReaxFF reactive force field, we have explored the CMP mechanisms at the atomic level and have revealed the importance of mechanochemistry induced atomic wear during the CMP processes.

(Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall)

[P1-83] Adsorption property of a fatty acid on iron surface with grain boundary

○Yuki Uchiyama, Yoshinori Shiihara, Ivan Lobzenko （Toyota Technological Institute, Japan）

Reducing the coefficient of boundary friction on steel surfaces is one of key technologies to improve the efficiency of machines such as automotive engines. It has been shown that the boundary friction on nanostructured steel surfaces in the sliding test using particular lubricant is smaller than the friction of normal steel surfaces [1]. This difference between the nanostructured and a normal surfaces lies in the density of the grain boundary as a surface defect. The surface defect can attract lubricant molecules and enhance lubricating film formation on metal surfaces. This can be one of the mechanism that induces the friction reduction on the nanosructured steel surface. In this work, using first principles calculations, the adsorptivity of a lubricant molecule, a fatty acid, on iron surfaces has been studied.The chemical adsorption of fatty acids is expected to be enhanced at the site near the crystal grain boundary which may have high chemical activity. Adsorption energy calculations were preformed for acetic acids as the simplest fatty acids. Adsorbability of a Fe (110) surface with symmetrical tilt Σ3 (111)grain boundarywas compared to clean Fe(100), (110) and (111) surfaces. As a result, we found that the molecule can adsorb on the particular site on grain boundary more strongly than that on Fe surfaces without grain boundary. [1]

Yoshikazu Todaka, Kenichi Toda, Motohiro Horii, Minoru Umemoto, Tetsu-to-Hagané 101, 10 (2015)

Poster Session | A. Advances in Materials Theory for Multiscale Modeling

[PO-A2] Poster Session 2

Symposium A

Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall

[P2-01] Multiscale model of solid state amorphization during processing of pharmaceutical materials

Chunyu Li[1], Yifei Zeng[1], Lorena Alzate-Vargas[1], Pilsun Yoo[1], Rachel Frocino[2], Jeff Brum[2], Peilin Liao[1], Marisol Koslowski[1], ○Alejandro Strachan[1] （1.Purdue University, United States of America, 2.GlaxoSmithKline, Analytical Sciences and Development, United States of America）

[P2-02] FTMP-based Modeling and Simulations of HCP Mg Single Crystal

○Takahiro Kitano, Tadashi Hasebe （Dept. of Mechanical Engineering, Kobe Univ., Japan）

[P2-03] Nonlinear elasticity on Riemannian manifold and its application to general surface development

○Yuto Horikawa[1], Ryuichi Tarumi[2], Yoji Shibutani[1] （1.Dept. of Mechanical Engineering, Osaka Univ., Japan, 2.Grad. Sch. of Engineering Science, Osaka Univ., Japan）

[P2-04] The challenge of achieving quantitative phase field models for microstructure evolution in irradiated solids - the case of voids

○Anter El-Azab （Purdue University, United States of America）

[P2-05] A Molecular-Dynamics Study of Surface Tension: From Alloy Droplets to Bubbles in Molten Alloy

○Xiangming Ma, Hongtao Liang, Yang Yang （East China Normal Univercity, China）

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-01] Multiscale model of solid state amorphization during processing of pharmaceutical materials

Chunyu Li[1], Yifei Zeng[1], Lorena Alzate-Vargas[1], Pilsun Yoo[1], Rachel Frocino[2], Jeff Brum[2], Peilin Liao[1], Marisol Koslowski[1], ○Alejandro Strachan[1] （1.Purdue University, United States of America, 2.GlaxoSmithKline, Analytical Sciences and Development, United States of America）

Processing of active pharmaceutical ingredients and excipients to reduce and control particle size involve milling and micronization which result in severe plastic deformation and fracture. The increase in free energy of the crystal during deformation can result in polymorphic transformations and amorphization and affect the physical properties of the product, including bioavailability.

In order to predict how materials properties and processing conditions affect plastic deformation and phase transitions in pharmaceutical materials we developed a multiscale model that combines electronic structure using density functional theory, large-scale molecular dynamics simulations and a phase field modeling. At the finer scale, we use DFT to predict elastic constants of the crystals and amorphous systems of interest and validate the force fields used with MD. MD simulations provide insight into the process of amorphization and enables the characterization of the difference in enthalpy between the crystal and amorphous phase and their interfacial energy, critical to describe the nucleation and growth of the amorphous phase. Finally, the materials properties from DFT and MD calculations are used to inform a phase field model that describes, self-consistently, plastic deformation, including the nucleation of crystal defects informed by dislocation dynamics, with phase transformations.

Using the multiscale model, we investigate the effect of deformation, shear, impact and particle surface roughness on the evolution of the crystallite size and the nucleation and growth of an amorphous phase in molecular crystals of interest for pharmaceutical applications.

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-02] FTMP-based Modeling and Simulations of HCP Mg Single Crystal

○Takahiro Kitano, Tadashi Hasebe （Dept. of Mechanical Engineering, Kobe Univ., Japan）

Extended usages of Mg and Mg alloys have been widely promoted to date, attempting to make the best use of their attractive properties, such as light weight, high specific strength, superior recyclability and excellent bio-compatibility. Modeling attempts of Mg and Mg alloys, however, often meet difficulty in the treatments of the complex plasticity, mainly stem from their highly anisotropic slip systems and intricate activities of twinning. The present study aims at enhancing the feasibility of the recently-proposed model for deformation twinning based on FTMP (Field Theory of Multiscale Plasticity) toward extended applications to HCP Mg single crystal. The major updates of the model are two fold: one is the extension to efficient 3D simulations by introducing special computational schemes, while the other is to apply modified lattice rotation based on the rotational part of the incompatibility tensor. The twinning model with the modified lattice rotation is introduced in the hardening law in the FTMP-based crystalline plasticity framework, and is further implemented into a finite element code accommodated with the above new scheme. Deformation analyses are performed based on 2D/3D FEM for pure single crystal magnesium with HCP (hexagonal close-packed) structure, and critical comparisons are made with experimental data obtained under plain-strain

compression in multiple orientations by Kelly and Hosford, particularly, with those exhibiting the unique stress-strain responses induced by deformation twinning, i.e., orientations A, E and F. Natural expression of twin-induced lattice rotation is attempted by introducing a modification based on the pure rotation part of the incompatibility tensor, spontaneously evolved during deformation. The modification is shown to allow autonomic transitions between slip and twinning modes, e.g., from twin-dominant stress response to that carried by slip, as in the orientations E and F by Kelly-Hosford.

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-03] Nonlinear elasticity on Riemannian manifold and its application to general surface development

○Yuto Horikawa[1], Ryuichi Tarumi[2], Yoji Shibutani[1] （1.Dept. of Mechanical Engineering, Osaka Univ., Japan, 2.Grad. Sch. of Engineering Science, Osaka Univ., Japan）

This study aims to develop a theoretical framework to construct a three-dimensional curved surface from pieces of an elastic sheet which is embedded in two-dimensional Euclidean space. Our formulation is based on the standard nonlinear elasticity within the framework of differential geometry. We first introduce the Riemannian manifolds which equip the metrics, g[0] and g[t], for reference and current configurations. The strain energy density is defined as a quadratic form of Green strain tensor under the assumption that elastic medium is isotropic in the reference configuration g[0]. Then, the surface development problem ends up with a variational problem such that to find an embedding mapping which minimizes the strain energy functional. We solve the variational problem numerically using the isogeometric analysis (IGA). To this end, we first derive a weak form equilibrium equation from the first variation of the functional. The embedding mapping is approximated by a linear combination of non-uniform rational B-spline (NURBS) functions with the coefficients ξ. Consequently, the equilibrium equation yields a system of nonlinear algebraic equations for ξ and which is solved iteratively around a linearized solution by the Newton method. It should be noted here that present method consider in-plane deformation of the elastic sheet exclusively. It implies that two-dimensional isometric deformation, such as out-of-plane bending deformation, produces no strain energy in the medium. In this regards, present method is a fair generalization of conventional surface development method which is frequently used in the paper craft such as origami. Numerical analysis for a one-dimensional system demonstrates that present method converges to an exact solution within a sufficient accuracy.

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-04] The challenge of achieving quantitative phase field models for microstructure evolution in irradiated solids - the case of voids

○Anter El-Azab （Purdue University, United States of America）

We present a thermodynamics-consistent formalism of a phase field model of void growth in irradiated solids, along with its sharp interface counterpart. Asymptotic matching of the two models was performed to yield all phase field model parameters in terms of real materials properties. In this presentation, the results of a first quantitative simulations of void growth driven by irradiation using our phase field approach will be reported. This work was performed in collaboration with Srujan Rokkam, Thomas Hochrainer, and Karim Ahmed.

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-05] A Molecular-Dynamics Study of Surface Tension: From Alloy Droplets to Bubbles in Molten Alloy

○Xiangming Ma, Hongtao Liang, Yang Yang （East China Normal Univercity, China）

We present a substantial atomistic simulation study of the equilibrium surface tension for liquid-state binary alloy systems. Four types of spherical surface/interfaces are investigated: liquid Pb droplet embedded in bulk liquid Al, liquid Al droplet in bulk liquid Pb, a bubble in liquid state Pb-Bi eutectic (LBE) and a LBE droplet. The surface tension for these non-planar surfaces are calculated based on the calculation of the local pressure tensor in spherical coordinates. Several thermodynamics property (droplet size, temperature, capillary pressure, mutual miscibilities) dependencies of surface tension are obtained. Our results provide useful input data for the mesoscale simulations of the selective laser melting, advanced welding and bubble formation in nuclear coolants.

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

[PO-B2] Poster Session 2

Symposium B

Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall

[P2-06] Effects of rhenium on the mechanical behavior of irradiated tungsten: a molecular dynamics study using neural-network potential

○Ryo KOBAYASHI （Nagoya Institute of Technology (NITech), Japan）

[P2-07] Diffusion behavior and temperature dependence of hydrogen in tungsten and molybdenum under isotropic strain state

○QuanFu Han[1], Yue-Lin Liu[2], Ying Zhang[1], Guang-Hong Lu[1] （1.Beihang University, China, 2.Yantai University, China）

[P2-08] **Diffusion of Point Defects on Tungsten Surface**

Jiannan Hao[1], ○Shuo Jin[1], Haixuan Xu[2], Xiaolin Shu[1], Guanghong Lu[1] （1.School of Physics and Nuclear Energy Engineering, Beihang University, China, 2.Department of Material Science and Engineering, The University of Tennessee, Knoxville, United States of America）

[P2-09] Influence of anisotropic strain and temperature on hydrogen dissolution in tungsten

○Ying zhang[1], Quan Fu Han[1], Yue lin Liu[2], Guang Hong Lu[1] （1.Beihang University, China, 2.Yantai University, China）

[P2-10] Screw dislocation-interstitial solute coevolution in W-O alloys using atomistically-informed kinetic Monte Carlo simulations

○Yue Zhao[1], Lucile Dezerald[3], Jaime Marian[1,2] （1.Dept. of Materials Science and Engineering, University of California, Los Angeles, United States of America, 2.Dept. of Mechanical Engineering, University of California, Los Angeles, United States of America, 3.Institut Jean Lamour, University of Lorraine, France）

[P2-11] 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）

[P2-13] **Dynamics of Magnetism in Neutron Irradiated Iron-Chromium Steels**

○Jacob B. J. Chapman, Pui-Wai Ma, Sergei L. Dudarev （Culham Centre for Fusion Energy (CCFE), UK）

[P2-14] **Atomistic insights into the grain boundaries interaction with radiation-induced point defects in bcc Fe-Cr alloys**

○Marcin Roland Zemla, Jan Stanislaw Wrobel, Tomasz Wejrzanowski （Faculty of Materials Science and Engineering, Warsaw University of Technology, Woloska 141, 02-507 Warsaw, Poland）

[P2-15] Production and Process of Cascade Development in Irradiated Pure α-Zr from Molecular Dynamics Simulations

○Rongjian Pan[1], Lu Wu[1], Xiaoyong Wu[1], Aitao Tang[2], Bang Wen[1], Wen He[1], Y.R. Ovcharenko[3], D.O. Kharchenko[3] （1.The First Sub-Institute, Nuclear Power Institute of China, China, 2.College of Materials Science and Engineering, Chongqing University, China, 3.Institute of Applied Physics, National Academy of Science of Ukraine, Ukraine）

[P2-16] Microstructure evolution of cascade annealing in irradiated pure α-Zr from molecular dynamics simulations

○Bang Wen[1], Rongjian Pan[1], Wei Zhang[1], Lu Wu[1], Xiaoyong Wu[1], Aitao Tang[2], Wen He[1], Y.R. Ovcharenko[3], D.O. Kharchenko[3] （1.The First Sub-Institute, Nuclear Power Institute of China, China, 2.College of Materials Science and Engineering, Chongqing University, China, 3.Institute of Applied Physics, National Academy of Science of Ukraine, Ukraine）

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-06] Effects of rhenium on the mechanical behavior of irradiated tungsten: a molecular dynamics study using neural-network potential

○Ryo KOBAYASHI （Nagoya Institute of Technology (NITech), Japan）

Tungsten (W) is considered as a promising candidate for the plasma facing wall material at divertor in nuclear fusion reactors. In order to assess the lifetime of the divertor for safe operation of the nuclear fusion reactors, mechanical response to the irradiation of high energy neutrons and helium atoms should be precisely understood from atomistic scale. Under the irradiation of high energy neutrons, not only defects are formed but also transmutation occurs, which will produce a few percent of rhenium (Re) concentration within several-year operation of nuclear fusion reactor. Thus the effect of solute Re atoms on the mechanical behavior of host material, W, should be taken into account, such as recovering rate after cascading damage, H/D/T retention, He bubble formation, or dislcation mobility. In this study, we create a neural-network (NN) potential for quarternary system, W-Re-H-He, combined to an EAM potential for W-Re binary system. It is known that machine-learning (ML) potentials such as NN can well reproduce DFT energies of wide variety of atomic configurations, but it requires big data to learn a lot of free parameters and it is usually much slower than the classical potentials such as EAM. By combining the NN with EAM potentials, we can construct a potential with smaller number of referece data and make it much faster than fully NN potential. The properties of the potential and the effect of Re on the recovering rate after cascading damage, He bubble formation/growth rate, and dislocation punching will be discussed.

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[P2-07] Diffusion behavior and temperature dependence of hydrogen in tungsten and molybdenum under isotropic strain state

○QuanFu Han[1], Yue-Lin Liu[2], Ying Zhang[1], Guang-Hong Lu[1] （1.Beihang University, China, 2.Yantai University, China）

The interaction between hydrogen and metal exhibits a great scientific and technological importance so that it has a direct impact on the design and operation of metallic materials. Here, we have carried out first-principles calculations to investigate interstitial hydrogen diffusion behaviors in tungsten and molybdenum by considering double effects of temperature and strain. The temperature and strain effects are reflected by the vibration Helmholtz free energy in the quasi-harmonic approximation and isotropic loading, respectively. The hydrogen diffusion is analyzed through two nearest neighbor tetrahedral sites. At a ground state (0-K) condition, the hydrogen diffusion activation energy can increase and decrease notably with rising compressive and tensile strain, respectively. While at each compressive/tensile strain case, the hydrogen diffusion activation energy depends distinctly on the temperature and increases with rising temperature. This is mainly originated from the contribution of vibration Helmholtz free energy induced by the larger vibration frequency of hydrogen in two metals. With the increasing temperature, the hydrogen diffusivity is shown to be dependent on the compressive/tensile strain alteration. The present study demonstrates a remarkable influence of “temperature and strain” on the hydrogen diffusion behaviors in tungsten and molybdenum.

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[P2-08] Diffusion of Point Defects on Tungsten Surface

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Hydrogen (H) / helium (He) retention in tungsten (W) and can significantly reduce the thermal conductivity and sputtering threshold of W, and at the same time, continuous bombardment with 14.1 MeV neutron can introduce Frenkel defects (composed of self-interstitial atoms (SIAs) and vacancies), which lead to a high concentration of W impurity. The surface deformation and blisters are observed experimentally in W, in which the surface morphology is relevant to the plasma fluence and surface directions [1-2]. The near-surface atomistic configuration is changed via diffusion of frenkel defects which is driven by heat and/or bubble loop punching process. Therefore, revealing the evolution mechanism of point defects on the W surfaces under H/He irradiation is crucial for W application in future fusion reactors.

We employ the first-principles and molecular dynamics simulation to calculate the energy barriers of single adatom (AD) and vacancy (VA) diffusion on the W (100), (110) and (111) surface. The diffusion paths of defects is determined by the dimmer method built in the SEAKMC code [3]. At least three diffusion paths with high energy barriers are found for both AD and VA on the (100) surface. However, only one path with low energy barrier of both AD and VA on the (110) surface are dominated throughout the diffusion process. Moreover, the diffusion of AD and VA on the (111) surface is investigated, in which the formation energies of different surface defects are biased. Nonetheless, the symmetry of the (111) surface will break spontaneously at the certain temperature and concentration of impurity through the thermodynamic calculation, and the morphology is in good agreement with the SEM images [1]. The work will help to understand the early stage of surface morphology evolution under irradiations or in the annealing process.

Keywords: tungsten, point defects, diffusion, surface

References

[1] H. Y. Xu, Y. B. Zhang, Y. Yuan, B. Q. Fu, A. Godfrey, G. De Temmerman, W. Liu, and X. Huang, J. Nucl. Mater. 443, 452 (2013).

[2] F. W. Meyer, H. Hijazi, M. E. Bannister, K. A. Unocic, L. M. Garrison, and C. M. Parish, Phys. Scr. T167, 14019 (2016).

[3] H. Xu, Y. N. Osetsky, and R. E. Stoller, J. Phys. Condens. Matter 24, 375402 (2012).

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[P2-09] Influence of anisotropic strain and temperature on hydrogen

dissolution in tungsten

○Ying zhang[1], Quan Fu Han[1], Yue lin Liu[2], Guang Hong Lu[1] （1.Beihang University, China, 2.Yantai University, China）

Tungsten (W) is an alternative candidate for a plasma facing material in the future fusion reactor due to its high melting point, high thermal conductivity and low plasma sputtering yield. The solubility of hydrogen in tungsten is a basic and crucial factor to influence the formation of hydrogen bubbles. In this work, we have investigated the effects of anisotropic strain and temperature on the dissolution of H in tungsten via the first-principles calculation in combination with thermodynamic models. The temperature and strain effects are reflected by the vibration Helmholtz free energy in the quasi-harmonic approximation and uniaxial/biaxial strain loading, respectively. It is found that the solubility of hydrogen can be enhanced by both compressive and tensile anisotropic strain, independent with of the sign of strain. This is different from the influence of isotropic strain, where the solubility of hydrogen in tungsten responds to the isotropic strain monotonically. Besides, the difference of the dissolution energy between hydrogen dissolves in tetrahedral and octahedral site constantly changes in the anisotropic strain range of -4%-4%. Further, under same anisotropic strain condition, the solution energy of hydrogen in tungsten increases with the increasing of the temperature from 300-1800 K, which can be mainly contributed to the vibration Helmholtz free energy. Our finding suggests that the local anisotropic strain and temperature can significantly influence the dissolution of hydrogen in tungsten, which may play a key role on hydrogen bubble formation.

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[P2-10] Screw dislocation-interstitial solute coevolution in W-O alloys using atomistically-informed kinetic Monte Carlo simulations

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The interaction of interstitial impurities with in-grown dislocations in metals can lead to various processes, including solute solution hardening and/or dynamic strain aging. The coevolution of solutes and dislocations occurs on length and time scales that are very challenging to resolve experimentally. The interaction of interstitial solutes with dislocation segments is highly local, however, and models must be capable of resolving the fine details of the interaction if we are to gain any understanding from the process. Here we develop a kinetic Monte Carlo model of dislocation motion in the presence of diffusing solutes. We focus on the W-O solid solution, such that the subject of our study is screw dislocations, as they control plastic flow at low temperatures in body-centered cubic metals and alloys. Solute diffusion is affected by dislocation strain fields, which we study via the elastic dipole tensor using electronic structure calculations. As well, we calculate binding energies of O atoms to screw dislocation cores, and discuss the joint structures formed, the implications of the calculated energetics, and show the effect on the dislocation velocity of solute diffusion at several temperatures.

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[P2-11] Kinetic Monte-Carlo Simulations of Radiation Damage in W(Re,Os) Alloys

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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.

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[P2-13] Dynamics of Magnetism in Neutron Irradiated Iron-Chromium Steels

○Jacob B. J. Chapman, Pui-Wai Ma, Sergei L. Dudarev （Culham Centre for Fusion Energy (CCFE), UK）

Ferritic-martensitic (F/M) steels, with a high chromium content, are critical materials for magnetic confinement fusion technology due to high temperature stability and corrosion resistance, facilitating the thermal efficiency necessary for fusion power plant operation. To predict the evolution of the steel microstructure and mechanical properties when subjected to sustained high doses of radiation at elevated temperatures, we must understand how radiation damage affects magnetic properties of the materials, which strongly influence phase stability and chromium solubility.

We investigate the effect of neutron irradiation on the magnetic properties of F/M steel alloys, relating experimentally observed [1] concentrations, radii and number densities of Cr precipitates within a Fe-Cr matrix to the dynamics and degradation/enhancement of magnetism across a broad range of temperatures. The Curie temperature is shown to vary, strongly dependent upon microstructure, increasing significantly with Cr precipitation observed at high doses and ageing times. These large-scale non-collinear calculations are performed using a method implementing magnetic cluster expansion (MCE), parameterised using a

database of DFT-generated observables [2], with spin-dynamics (SD) incorporating both transverse and longitudinal spin fluctuations [3]. SD simulations provide valuable insight into the ageing of alloys under realistic magnetic confinement conditions to inform material choices and construction strategy for fusion power plant design.

This work has been carried out within the framework of the EUROfusion Consortium and has received funding from the Euratom research and training programme 2014-2018 under grant agreement No 633053. The views and opinions expressed herein do not necessarily reflect those of the European Commission.

[1] E.R.Reese *et al.*, JNM **500**, 192 (2018); [2] M.Y.Lavrentiev *et al.*, JAP **109**, 07E123 (201); [3] P.-W.Ma *et al.* , PRB **81**, 184202 (2017)

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[P2-14] Atomistic insights into the grain boundaries interaction with radiation-induced point defects in bcc Fe-Cr alloys

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Grain boundaries (GBs) are an immanent components of crystal structure of the structural materials, such as e.g. Fe-Cr steels. Moreover, they have considerable influence on the materials properties, especially on the mechanical one. As a consequence of that, is necessary to investigate effect of radiation-induced defects on the GBs in order to a deeper understanding of the radiation damage.

In current study, we investigated characteristics of bcc-Fe and Fe-Cr based tilt GBs interacting with point defects such as vacancy, self-interstitial (SIA, dumbbell-type), and interstitial atoms (He impurities). Several tilt GBs with the rotation axis along [100] and [110] directions were modelled with He impurities, vacancy, and SIA in Fe-Cr. Molecular dynamics (MD) simulations using the interatomic Fe-Cr-He embedded atom model potential were conducted, for twelve GBs, in order to investigate GBs energies, He segregation energies, and the weakening effect of He impurity for several Cr and He concentrations. Furthermore, spin-polarized density functional theory (DFT) calculations focused at two GBs, Σ3(111) and Σ5(210), allowed to deeper insights into GBs properties. For example, the DFT results show that the presence of He significantly influences the magnetic properties of the system in the relatively distant neighbourhood [1]. The fluctuation of magnetic moments, chemical potentials, formation and migration energies of point defects were studied as a function of distance from GB’ s plane. Representative structures of GBs, with Cr content ranging 6-10%, generated using DFT-based Monte Carlo simulations [2] were used to analyse how parameters, such as alloy short-range ordering or local environment, effects on defects properties.

[1]. M. R. Zemla, J. S. Wrobel, T. Wejrzanowski, D. Nguyen-Manh, K. J. Kurzydlowski, Nuclear Instruments and Methods in Physics Research Section B Beam Interactions with Materials and Atoms 393:118 (2017).

[2]. J.S. Wrobel, D. Nguyen-Manh, M.Y. Lavrentiev, M. Muzyk, S.L. Dudarev, Physical Review B 91 (024108) 2015.

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[P2-15] Production and Process of Cascade Development in Irradiated Pure α-Zr from Molecular Dynamics Simulations

○Rongjian Pan[1], Lu Wu[1], Xiaoyong Wu[1], Aitao Tang[2], Bang Wen[1], Wen He[1], Y.R. Ovcharenko[3], D.O. Kharchenko[3] （1.The First Sub-Institute, Nuclear Power Institute of China, China, 2.College of Materials Science and Engineering, Chongqing University, China, 3.Institute of Applied Physics, National Academy of Science of Ukraine, Ukraine）

The formation and development of cascade in pure α-Zr crystals at sample temperatures *T*=300K and *T* =500K, energy of 2, 6 and 10 keV and initially driving directions and of primary knock atoms (PKA) are investigated by molecular dynamics. The simulation results show that when crystals temperature is *T*=300K and 500K and initial direction of motion for PKA is the cascades volume is greater than for the initial direction at same all other parameters. The largest size of cascade is found after 0.4 ps, which regardless of crystal temperature, energy and initial direction of primary knock-on atom (PKA). The formation of crowdions is caused by channeling during cascade development.

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[P2-16] Microstructure evolution of cascade annealing in irradiated pure α-Zr from molecular dynamics simulations

○Bang Wen[1], Rongjian Pan[1], Wei Zhang[1], Lu Wu[1], Xiaoyong Wu[1], Aitao Tang[2], Wen He[1], Y.R. Ovcharenko[3], D.O. Kharchenko[3] （1.The First Sub-Institute, Nuclear Power Institute of China, China, 2.College of Materials Science and Engineering, Chongqing University, China, 3.Institute of Applied Physics, National Academy of Science of Ukraine, Ukraine）

The microstructure evolution of cascade annealing in α-Zr crystals at *T*=300K, 400K, and 500 K for energy of 2, 6 and 10 keV with initially driving directions <0001> and <01-10> of primary knocked atoms (PKA) are investigated by using molecular dynamics simulations. The results show that the relaxation time (τ_r) of cascades can play a role of an effective parameter for describing radiation damages during molecular dynamics simulations. of cascade with the larger surface area but with the same volume is much smaller, which promotes faster recombination of defects during cascade annealing. Energy is a crucial factor in the formation of cascade displacements of atoms and appearing of defects compared with temperature and direction of movement for initially knocking atoms.

Poster Session | C. Crystal Plasticity: From Electrons to Dislocation Microstructure

[PO-C2] Poster Session 2

Symposium C

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[P2-18] **Prediction of Biaxial Tensile Deformation Behavior of Aluminum Alloy Sheets using Crystal Plasticity Finite Element Method and Machine Learning**

○Kota Koenuma[1], Akinori Yamanaka[1], Ikumu Watanabe[2], Toshihiko Kuwabara[1] （1.Tokyo University of Agriculture and Technology, Japan, 2.National Institute of Materials Science, Japan）

[P2-19] MobiDiC: A 3-D Dislocation Dynamics Simulation

○Ronan MADEC[1], Laurent COLOMBET[1], Ladislas KUBIN[2] （1.CEA, DAM, DIF, France, 2.LEM, UMR 104 CNRS-ONERA, Université Paris Saclay, France）

[P2-20] Temperature dependence of fatigue crack growth in Ti-6Al-4V

○Bhargavi Rani Anne, Masaki Tanka, Tatsuya Morikawa （Dept. of Materials Science and Engineering, Kyushu University, Japan）

[P2-21] Parametric model of discrete dislocation dynamics based on mathematical theory of moving curves

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

[P2-22] On Visualization of Multiscale Information Transfer/Exchange Processes via FTMP-based Duality Diagram Representation Scheme

○Takuya Takagi, Tadashi Hasebe （Dept. of Mechanical Engineering, Kobe Univ., Japan）

[P2-23] **Rotational Field Evolutions based on Field Theory of Multiscale Plasticity (FTMP)**

○Tadashi Hasebe[1], Yasutaka Matsubara[2] （1.Kobe Univ., Japan, 2.Graduate School of Kobe Univ., Japan）

[P2-24] **A 2D MESOSCALE STUDY OF DISLOCATIONS, CRACKS AND MARTENSITIC PHASE TRANSFORMATIONS**

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

[P2-25] Effects of Stress Distribution on the Plastic Deformation of Metallic Glasses under Different Geometries

○Chih-Jen Yeh[1], Hsuan-Teh Hu[1], Chang-Wei Huang[2], Yu-Chieh Lo[3] （1.National Cheng Kung University, Taiwan, 2.Chung Yuan Christian University, Taiwan, 3.National Chiao Tung University, Taiwan）

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-18] Prediction of Biaxial Tensile Deformation Behavior of Aluminum Alloy Sheets using Crystal Plasticity Finite Element Method and Machine Learning

○Kota Koenuma[1], Akinori Yamanaka[1], Ikumu Watanabe[2], Toshihiko Kuwabara[1] (1.Tokyo University of Agriculture and Technology, Japan, 2.National Institute of Materials Science, Japan)

Aluminum alloy sheets are used for automotive body parts to reduce the weight of automotive. However, because the formability of aluminum alloy sheets is much lower than that of steel sheets, the plastic deformation behavior of aluminum alloy sheets during plastic forming processes has been predicted by sheet metal forming simulations based on the finite element method. In order to predict the plastic deformation behavior of an aluminum alloy sheet subjected to a biaxial stress state in a sheet metal forming process, we proposed the numerical biaxial tensile test (NBT) methodology using the crystal plasticity finite element method (CPFEM) and the mathematical homogenization method. The NBT method has been already applied to predict the contour of equal plastic work of a 5000-series aluminum alloy sheet. The results demonstrated that the contour of equal plastic work (the yield locus) calculated by the NBT method shows a good agreement with that measured by the experimental biaxial tensile test using a cruciform specimen. Unfortunately, because we need to perform multiple NBTs to calculate the contour of equal plastic work, the disadvantage of the NBT method is its high computational cost. In this study, in order to predict the biaxial tensile deformation behavior of aluminum alloy sheets more efficiently, we propose a new numerical material testing methodology by combining the NBT method with machine learning methods. The deformation behavior of aluminum alloy sheets predicted by the proposed method is verified by experimental multi-axitial material tests.

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[P2-19] MobiDiC: A 3-D Dislocation Dynamics Simulation

○Ronan MADEC[1], Laurent COLOMBET[1], Ladislas KUBIN[2] (1.CEA, DAM, DIF, France, 2.LEM, UMR 104 CNRS-ONERA, Université Paris Saclay, France)

In 3D lattice-based dislocation dynamics (DD) codes, dislocation segments are discretized on an underlying lattice in which they move by discrete jumps. The first version of such codes goes by the name of microMegas and dates back to the beginning of the 1990s [1]. It makes use of a line model in which dislocations are discretized in their slip planes into a succession of straight segments with edge and screw characters. Two more sophisticated versions of the initial code are currently in use, Tridis, which retains the 'screw-edge' line model [2] and an evolved version of microMegas with two additional mixed line directions [3].

MobiDiC (for 'Mobile Dislocation Colony') derives from this last version of microMegas and is devoted to mass mesoscopic simulations involving a large number of perfect dislocations. It is designed to overcome some limitations of the parent code in order to provide an improved and efficient framework for DD simulations that can further evolve.

The specificities of this code will be presented, in particular the ability to handle complex crystallographic structures and dislocation reactions. Indeed, MobiDiC is considerably more flexible than other lattice-based

DD codes because there is no limitation to the number of vectors per slip system. In addition a semi-nodal approach is used. For instance, the movements of segments connected to a high connectivity node, like triple nodes of a junction, are coordinated to move the node with the adequate degree of freedom.

Examples of applications will be given as well as results obtained with OpenMP and hybrid parallelisms using many-core processors.

[1] L. P. Kubin, G. Canova, M. Condat, B. Devincre, V. Pontikis and Y. Bréchet, Solid State Phenomena., 23-24, 455 (1992).
[2] M. Verdier, M. Fivel and I. Groma, Model. Simul. Mater. Sci. Eng. 6, 755-770 (1998).
[3] B. Devincre, R. Madec, G. Monnet, S. Quereau, R. Gatti, L. Kubin, Modeling crystal plasticity with dislocation dynamics simulations: the 'microMegas' code, in Mechanics of Nano-Objects, O. Thomas, A. Ponchet, S. Forest, (Eds.), Presses des Mines, Paris 2011, pp. 81-89.

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[P2-20] Temperature dependence of fatigue crack growth in Ti-6Al-4V

○Bhargavi Rani Anne, Masaki Tanka, Tatsuya Morikawa （Dept. of Materials Science and Engineering, Kyushu University, Japan）

Fatigue properties of dual phase (α+ß and primary α) Ti-6Al-4V were studied with respect to the range of temperatures and stress intensity range. Fatigue tests were conducted with both high and low stress intensity ranges in the temperature range between room temperature and 550K. Micro crack propagation was observed. Crack growth rate (da/dN) was measured where a is a crack length and N is a number of cycles, changing temperature. It was found that da/dN was increased with temperature. It is assumed that da/dN is the Arrhenius type of equation as it shows temperature dependence. Activation energy calculations were attained from Arrhenius plot between the logarithm of da/dN and the reciprocal of temperature. The dependence of activation energy on stress intensity range was also obtained, which provides the information on the dislocation mobility controlling the fatigue crack growth. The comparison of fatigue crack growth rate with the temperature dependence of dislocation motion was also studied in detail.

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[P2-21] Parametric model of discrete dislocation dynamics based on mathematical theory of moving curves

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

In this contribution we present the comprehensive model of discrete dislocation dynamics based on the mathematical theory of moving curves. The purpose of our model is the precise and mathematically rigorous description of the dynamics of dislocations, which are represented as smooth curves evolving in their respective slip planes.

Dislocations are described by parametric curves and their motion is governed by the curvature driven flow.

The parametric model is coupled with the model of tagential velocity for increased stability, and with algorithms for topological changes which allow modeling of complex effects as merging, splitting, self-replication or interaction with obstacles.
The numerical algorithm is based on the flowing finite volume method.

We present qualitative and quantitative results of our numerical simulations. We demonstrate the capabilities of our model in the predicting of dipole formation and consequent estimation of the endurance limit, in the modeling of several interacting dislocations, and in the application of our method on complex scenarios involving moving dislocations interactiong with several obstacles.

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[P2-22] On Visualization of Multiscale Information Transfer/Exchange Processes via FTMP-based Duality Diagram Representation Scheme

○Takuya Takagi, Tadashi Hasebe （Dept. of Mechanical Engineering, Kobe Univ., Japan）

It may safely be said that one of the critical issues about multiscale polycrystalline plasticity modeling are ultimately consolidated into those about “information transfer and exchange” concurrently taking place among plural scales of spontaneously evolving kinds. In tackling these, we make an attempt here to introduce the duality diagram-based scheme of FTMP into multi-grained models under tension, where FTMP stands for Field Theory of Multiscale Plasticity. The model used is composed of systematic combinations of representative crystallographic orientations, i.e., three multi-slip [100], [110] and [111], and two single-slip [123] and [125]. Strongly orientation-dependent intragranular substructure evolutions, successfully reproduced solely via FTMP-based finite element analyses, result in distinct overall deformation/fracture modes, including, e.g., local instability-induced brittle-like fracture modes. Corresponding duality diagrams, i.e., the spatial trace of the incompatibility tensor versus fluctuation of the elastic strain energy, are drawn and are compared with their rate versions. Found first is a similarity between the two diagrams, i.e., the normal and their rate forms, when they are constructed via grain-wise net sum basis, without taking the absolute values as we have done so far. Phase space diagrams are newly introduced both for the incompatibility and strain energy fluctuation to further examine those similarities in general. Demonstrated thereby is the models yielding “in-phase” responses roughly correspond to the cases that exhibit relatively stable and ductile deformation/fracture modes. The phase shifts, on the other hand, are shown to be closely related to instability outset, based on which the construction of a possible measure of the “degree” of instability is also attempted.

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[P2-23] Rotational Field Evolutions based on Field Theory of Multiscale Plasticity (FTMP)

○Tadashi Hasebe[1], Yasutaka Matsubara[2] （1.Kobe Univ., Japan, 2.Graduate School of Kobe Univ., Japan）

FTMP-based modeling and simulations have revealed its prominent descriptive capability of deformation-induced evolving inhomogeneities, e.g., band-like dislocation substructures, which are generally accompanied by misorientation across them. Three representative cases are examined in detail, i.e., (a)spontaneously evolved dislocation substructures, (b)eigenstrain-driven misorientation development for modeling lath martensite block structures, and (c)alternative degrees of freedom-driven lattice rotations enriched by incompatibility-based modified spin. For (a), we discuss deformation-induced spontaneous evolution of misoriented dislocation substructures, comparing dislocation density contours for BCC and FCC models, while, for (b), comparison is made of the eigenstrain-driven misoriented lath block structures among three incompatibility conditions, where screw dislocation networks are commonly evolved, yielding twisted lath boundaries. For (c), we examine emerging “kink-like” patterns associated with tensile twining assisted by incompatibility-based modification of rotation, comparing component-wise contributions of incompatibility tensor on evolving rotation fields with “kink-like” morphology for Mg single crystal under c-axis tension. In addition to these, “crystallization-like” patterns evolved in single crystal sample are extensively examined, where initially-prescribed laminated misorientation distributions and/or hardening moduli are introduced to the model used in (c).

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[P2-24] A 2D MESOSCALE STUDY OF DISLOCATIONS, CRACKS AND MARTENSITIC PHASE TRANSFORMATIONS

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

TRIP-Steels are of commercial interest due to their exceptional strength. This is a result of the microstructure; a matrix of both austenite and martensite that when plastically strained, exhibits strain hardening behavior. Plastic deformation arises from the presence of dislocations and the martensitic phase transformations (MT) that take place inside the metal. To understand the macroscopic properties of TRIP-Steels, it is necessary to understand the underlying dynamics occurring at the mesoscale.

Most models do not take into account the interactions between martensitic phase transformations and dislocations, and therefore are missing the impact that these two phenomena exert on each other. While MD simulations can resolve both phenomena naturally, they are prohibitively expensive for larger crystal sizes or time scales. On the contrary, continuum models cannot resolve the motion of dislocations inside the material.

We combine dislocation dynamics and martensitic phase transformations to study the interplay between the two phenomena. For the dislocation problem we use a continuum dislocation dynamics (CDD) model, allowing us to reduce computational cost and increase the system size. CDD is coupled with a Phase Field approach, which we use to model martensitic phase transformations. This allows us to study how dislocation motion can be influenced in the presence of an MT. Additionally, simple crack geometries can also be modeled as special dislocation configurations, which helps to understand how cracks and voids may trigger or inhibit MT.

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[P2-25] Effects of Stress Distribution on the Plastic Deformation of Metallic Glasses under Different Geometries

○Chih-Jen Yeh[1], Hsuan-Teh Hu[1], Chang-Wei Huang[2], Yu-Chieh Lo[3] （1.National Cheng Kung University, Taiwan, 2.Chung Yuan Christian University, Taiwan, 3.National Chiao Tung University, Taiwan）

Metallic glasses (MGs) generally have diverse mechanical properties, such as high strength and poor ductility. The deformation behaviors of MGs, to a large extent, depend on the ambient conditions. For example, the deformation of MGs is homogenous at high temperature and low stress. On the other hand, the deformation of MGs is inhomogeneous at low temperature and high stress. However, the inhomogeneous deformation further causes the shear band which is an accumulation of local plastic deformation. The formation of shear band always leads to a catastrophic failure with the increasing plastic deformation. In order to study the generation of shear band, a multiscale model which considers the microscopic shear transformation in macroscopic deformation is inevitable. In this paper, a mesoscale model combines the finite element method and the kinetic Monte Carlo method is used to investigate the properties of the metallic glasses. More mechanical properties and deformation behaviors of the MGs can be explored through the proposed model. In addition, the geometries of pores in composite MGs are investigated. Stress concentration and redistribution due to the different shapes and sizes of pores in composite MGs are discussed. These results can improve the design of the MGs and prevent MGs from catastrophic failure.

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

[PO-D2] Poster Session 2

Symposium D

Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall

[P2-26] Generalized nano-thermodynamic model for predicting size-dependent surface segregation in multi-metal alloy nanoparticles from smaller particles

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

[P2-27] Development of thermodynamic database of Nd-Fe-B-based permanent magnet alloys

○Jiang Wang, Lei Xu, Kaicheng Yang, Qingrong Yao, Guanghui Rao, Huaiying Zhou （School of Material Science and Engineering, Guilin University of Electronic Technology, China）

[P2-28] Design of proteins and biopolymers: role of directional interactions and of water.

○Valentino Bianco[1], Ivan Coluzza[2] （1.University of Vienna, Austria, 2.CIC biomaGUNE, center for cooperative research in biomaterials, Spain）

[P2-29] Aquatic pollutant removal by adsorption in zeolite structures: An experimental and molecular simulation study

○Mate Erdos[1], Nan Jiang[2], Sebastian G. J. Heijman[2], Othonas A. Moultos[1] （1.Process &Energy Department, Faculty of Mechanical, Maritime and Materials Engineering, Delft University of Technology, Netherlands, 2.Department of Water Management, Faculty of Civil Engineering and Geosciences, Delft University of Technology, Netherlands）

[P2-30] Optimizing elastic moduli of the silicate glasses through high-throughput atomistic modeling and machine learning techniques

Yong-Jie Hu[1], Ge Zhao[2], Tyler Del Rose[1], ○Liang Qi[1] （1.Dept. of Materials Science and Engineering, University of Michigan, United States of America, 2.Department of Statistics, Pennsylvania State University, United States of America）

[P2-31] High pressure phase transition and structural stability of transition metal compounds

○Fanyan Meng[1], Wandong Xing[1,2], Rong Yu[2] （1.Dept. of Physics, University of Science and Technology Beijing, China, 2.School of Materials Science and Engineering, Tsinghua University , China）

[P2-32] Development of artificial neural network model for prediction of electronic density of states in atomistic systems

○Atsushi Kubo, Yoshitaka Umeno （Institute of Industrial Science, the University of Tokyo, Japan）

[P2-33] Development of First-principles Platform Technology for Energy Research

○Kanghoon Yim[1], Chan-Woo Lee[1], Jehyun Lee[1], Incheol Jeong[2], Yong Youn[3], Seungwu Han[3] （1.R&D Platform Center, Korea Institute of Energy Research, Korea, 2.Dept. of Energy Science and Engineering, Daegu Gyeongbuk Institute of Science &Technology, Korea, 3.Seoul National University, Korea）

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-26] Generalized nano-thermodynamic model for predicting size-dependent surface segregation in multi-metal alloy nanoparticles from smaller particles

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

Multi-metal alloy nanoparticles (NPs) offer new avenues for exploration and design of nanoscale-properties, e.g., catalytic, electronic and optical, by virtue of their tunable composition. Unfortunately, a method that can aid such exploration by accurately predicting the size-, shape- and composition-dependent elemental distribution associated with nanomaterials is crucially missing. A nano-thermodynamic model based on distribution coefficients Δ is introduced to fill this gap. Δ is employed to predict surface segregation in NPs as a function of the NP size and composition. Interestingly, we find Δ to be independent of size for NPs beyond 2 nm. This key finding motivates the construction of thermodynamic tables for distribution coefficients using segregation observed with one or more NP sizes. The tables can enable accurate prediction of phase diagrams for nanomaterials across a wide-range of sizes. Key concepts of this new theory are demonstrated with Au-Pt-Pd, Ag-Au-Pd and Ni-Pt-Pd, which are found to exhibit complex size-dependent segregation behavior for 2-6 nm NPs and relatively weaker size-dependence beyond 6 nm. Numerically well-converged values of Δ are calculated for small NPs using Monte Carlo simulations in the canonical ensemble. Simulations are based on an embedded atom method (EAM) potential for metal alloys.
[1] S Divi, A Chatterjee, RSC Advances 8, 10409, 2018.

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-27] Development of thermodynamic database of Nd-Fe-B-based permanent magnet alloys

○Jiang Wang, Lei Xu, Kaicheng Yang, Qingrong Yao, Guanghui Rao, Huaiying Zhou （School of Material Science and Engineering, Guilin University of Electronic Technology, China）

Nd-Fe-B permanent magnets with excellent magnetic properties have been used in the industrial applications including medical apparatus and instruments, electrical machinery, aerospace, permanent magnet motor and wind power. In order to fully balance the application of rare-earth resource in magnetic materials and reduce the costs, it is a promise way to introduce high abundant rare earth (RE) metals (e.g. La, Ce, Y) into Nd-Fe-B permanent magnets [1-3]. Phase diagrams and thermodynamic information of the RE-Fe-B alloys are necessary to understand the effect of the abundant rare earth metals on phase formation, microstructure and magnetic properties of Nd-Fe-B permanent magnets.

In this work, the RE-Fe, RE-B and Fe-B sub-binary systems were reviewed firstly in the published literature. After that, the RE-Fe-B (RE=La, Ce, Pr, Nd) ternary systems were assessed using CALPHAD method on the basis of thermodynamic data and phase equilibria data, which is fundamental to obtain the thermodynamic database of multi-component RE-Fe-B alloy systems. The calculated results including liquid projects, isothermal sections and vertical sections as well as the solidification path of some alloys were compared with the experimental results using the thermodynamic database obtained. The thermodynamic database of the Nd-Fe-B-based permanent magnet alloy systems with high abundant rare earth elements is developed finally, which is necessary to design alloy composition and heat treatments of novel Nd-Fe-B permanent magnets

with good magnetic properties and low costs.

References

[1] X.J. Cao, L. Chen, S. Guo, J.H. Di, G.F. Ding, R.J. Chen, A.R. Yan, K.Z. Chen, Aip Adv. 8 (2018) 056222.
[2] L. Liu, H. Sepehri-Amin, T. Ohkubo, M. Yano, A. Kato, T. Shoji, K. Hono, J. Alloy. Comp. 666 (2016) 432-439.
[3] J.Y. Jin, T.Y. Ma, M. Yan, Y.J. Zhang, B.X. Peng, Y.S. Liu, F.H. Cao, J. Alloy. Comp. 735 (2018) 2225-2235.

Acknowledgements

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(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-28] Design of proteins and biopolymers: role of directional interactions and of water.

○Valentino Bianco[1], Ivan Coluzza[2] (1.University of Vienna, Austria, 2.CIC biomaGUNE, center for cooperative research in biomaterials, Spain)

The design of a (bio-)polymer is a rational scheme allowing to transfer the one-dimensional information contained in the polymer sequence into the three-dimensional information contained in the polymer folded conformation.
Proteins are an example of designable heteropolymers able to fold in unique target structures. The stability of the native conformation depends on the protein sequence and on the thermodynamic conditions of temperature and pressure.
In our work we use a multiscale approach to investigate how the geometry of the polymer backbone and the properties of the surrounding water affect the selection and the stability of proteins and, more in general, of artificial heteropolymers.
We find that the key actors are: i) the directional interactions along the backbone and ii) the hydrophilic/hydrophobic composition of the surface and core of the folded structure.

References:

V. Bianco, G. Franzese, C. Dellago, I. Coluzza, Phys. Rev. X 7, 021047, 2017.
V. Bianco, N. Pagès-Gelabert, I. Coluzza, G. Franzese, J. Mol. Liq. 245, 129, 2017.
C. Cardelli, V. Bianco, L. Rovigatti, F. Nerattini, L. Tubiana, C. Dellago, I. Coluzza, Sci. Rep. 7, 4986, 2017.
V. Bianco, G. Franzese, Phys. Rev. Lett. 115, 108101, 2015.
V. Bianco, S. Iskrov, G. Franzese, J. Biol. Phys. 38, 27, 2012.

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-29] Aquatic pollutant removal by adsorption in zeolite structures: An experimental and molecular simulation study

○Mate Erdos[1], Nan Jiang[2], Sebastian G. J. Heijman[2], Othonas A. Moultos[1] （1.Process &Energy Department, Faculty of Mechanical, Maritime and Materials Engineering, Delft University of Technology, Netherlands, 2.Department of Water Management, Faculty of Civil Engineering and Geosciences, Delft University of Technology, Netherlands）

Water contamination with micropollutants poses a serious threat to public health and the ecosystem. Technologies based on adsorption are widely used to remove micropollutants (inorganic and organic) from wastewater. Zeolites show a promising potential as adsorbents in these applications. Zeolites are crystalline, microporous aluminosilicates with well-defined 3-dimensional structure, composed of tetrahedral SiO_4 and AlO_4 clusters connected to each other by shared oxygen atoms. To compensate the charge imbalance caused by the aluminum content of the framework, exchangeable cations (usually alkali and alkaline earth cations) are located in the cavities of the structure. By removing the aluminum content of the framework the hydrophobicity of the zeolite can be increased, providing favorable adsorption characteristic to organic molecules. In this study, the effect of aluminium content of zeolite structures for aquatic pollutant removal are investigated. To that end, molecular simulations using Monte Carlo method are performed. In comparison with experimental methods, these simulation techniques can provide fundamental understanding of the nano scale behavior of the system which is crucial for designing new materials.
In this study, two types of zeolites (FAU, BEA) with different aquatic pollutants (2,4,6-trichlorophenol, triclosan) are investigated experimentally and with simulations. The simulated and experimentally measured results show qualitative agreement. To obtain insights into the adsorption mechanisms, radial distribution functions, and the distribution of adsorbates are calculated for each structure. The preferred adsorption sites and configuration of adsorbates (e.g., pi-pi stacking, H-bonding) are identified for each adsorbates and structures. Based on the simulation and experimental results the relationship of aluminium content and adsorption affinity can be determined and the performance of the different zeolites can be evaluated.

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-30] Optimizing elastic moduli of the silicate glasses through high-throughput atomistic modeling and machine learning techniques

Yong-Jie Hu[1], Ge Zhao[2], Tyler Del Rose[1], ○Liang Qi[1] （1.Dept. of Materials Science and Engineering, University of Michigan, United States of America, 2.Department of Statistics, Pennsylvania State University, United States of America）

Chemical design of the silicate glass with high elastic moduli is of great interest. However, it is difficult to find a universal expression to predict the elastic moduli according to the glass composition before synthesis since the elastic moduli are a complex function of several material properties at different length scales. This work presents a computational framework to efficiently predict the elastic moduli of the silicate glass across a multicomponent compositional design space, including 11 types of additive oxides, by integrations of high-throughput molecular dynamic (MD) calculations and machine learning (ML) techniques. Our newly developed ML model can predict the elastic moduli for k-nary silicate glass systems, using the learning datasets generated from MD calculations for only binary and ternary systems. The usefulness of our model is

illustrated by identifying the most relevant materials descriptors that determine the elastic moduli and screening for the silicate glasses with high stiffness.

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-31] High pressure phase transition and structural stability of transition metal compounds

○Fanyan Meng[1], Wandong Xing[1,2], Rong Yu[2] （1.Dept. of Physics, University of Science and Technology Beijing, China, 2.School of Materials Science and Engineering, Tsinghua University , China）

The lattice, charge, spin and other degrees of freedom in transition metal compounds couple to one another, giving these materials rich physics and properties. The extreme conditions of high pressure and high temperature provide a new way to create new structures that do not exist at ambient pressure, which has become an important way for the discovery of novel transition metal compounds. In recent years, important progress has been made in the theoretical prediction and high pressure synthesis of new structures. First, this work suggests a lot of new materials to be investigated by changing stoichiometry in phase diagrams. Taking the V-C binary system as an example, here we report the first-principles prediction of a new type of vanadium carbide, V_5C_3, which has an unprecedented stoichiometry in the V-C system. It is demonstrated that the new phase is mechanically stable, and is energetically favorable than known phases under high pressures. We believe that this work opens a door to materials design by changing stoichiometry. And the relationship between the crystal structure, electronic structure and physical properties are discussed. Secondly, the phase transition under high pressure will be analyzed to understand the structural stability of materials at high temperatures and high pressures, providing important theoretical basis for optimizing high-pressure synthesis conditions.

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-32] Development of artificial neural network model for prediction of electronic density of states in atomistic systems

○Atsushi Kubo, Yoshitaka Umeno （Institute of Industrial Science, the University of Tokyo, Japan）

Recently, the artificial neural network (ANN) model has been intensively applied to interatomic potentials for atomistic simulations. ANN-based potential functions possess basic characteristics; i.e., (1) they do not have any physical background besides the least geometrical conditions, e.g., physical quantity conservation against any coordinate transformation; (2) theoretically they can mimic any continuous functions. These features make ANN potentials applicable to complex atomistic systems, where various crystal structures and phases are relevant.
Since an ANN potential can be simply regarded as a mapping from atomistic structure to a real number, it is found that the application of ANNs does not have to be limited only for prediction of potential energy; i.e., ANNs are applicable to prediction of other physical quantities or material properties of the atomistic systems, e.g., electronic density of states (DoS), magnetic moment, etc. However, to the best of our knowledge, there has been no attempt to apply ANNs to prediction of physical quantities beside potential energy in atomistic systems. It will be of great impact if we can evaluate physical quantities such as electric or magnetic properties in huge atomistic structures using ANNs with the accuracy of the first-principles calculation.

In this study, we developed an ANN model to predict the DoS, as an exemplified case of prediction of general physical quantities in atomistic systems with ANNs. The ANN was optimized to reproduce the DoS in various crystal structures of silicon-carbon system that was obtained by first-principles calculations based on the density functional theory.

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-33] Development of First-principles Platform Technology for Energy Research

○Kanghoon Yim[1], Chan-Woo Lee[1], Jehyun Lee[1], Incheol Jeong[2], Yong Youn[3], Seungwu Han[3] (1.R&D Platform Center, Korea Institute of Energy Research, Korea, 2.Dept. of Energy Science and Engineering, Daegu Gyeongbuk Institute of Science &Technology, Korea, 3.Seoul National University, Korea)

As future energy technologies such as high-capacity energy storage and renewable energy applications require exceptional functionalities of host materials, the importance of employing a novel material is getting bigger and bigger. However, discovering a new superior material is very hard to success though it requires large costs and manpower. Recently, many researchers attempt to use an informatics technology such as machine learning in materials screening to overcome the realistic limitations of conventional trial and error method. The key to successive research using informatics technology largely depends on the quantity and quality of the considered database rather than technical details of informatics model. Since property data from experiments are usually sparse or biased to favorable materials in industry, it is hard to obtain a practical database for the informatics research. In that point of view, first-principles calculation is an excellent tool for generating systematic and reliable data of materials properties. However, first-principles calculation itself also requires considerable computational resources and many practical properties are hard to obtain by simple calculations. Therefore, a decent automation of first-principles calculation can do a significant role to establish a successive database. In this talk, I’ ll introduce the first-principles platform of Korea Institute of Energy Research aiming at providing a practical computing platform for various researchers with different backgrounds. After introducing the importance of well-defined automation procedure in former materials design studies such finding novel high-k dielectrics and p-type transparent oxides, I'll introduce the automated platform technology for surface-adsorption reactions which have great importance in most energy applications.

Poster Session | E. Deformation and Fracture Mechanism of Materials

[PO-E2] Poster Session 2

Symposium E

Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall

[P2-34] Dynamics of a solidification front made by invasion of fluid with a different temperature

○So Kitsunezaki, Chika Yamanaka （Nara Women's Univ., Japan）

[P2-35] Strengthening through solid solution in $W_{1-x}Ta_xB$ system

○lijuan liu[1], Wandong Xing[2], Fanyan Meng[1], Rong Yu[2] （1.Dept. of Applied Physics, University of Science and Technology Beijing, China, 2.School of Materials Science and Engineering, Tsinghua University , China）

[P2-36] Desiccation crack patterns based on phase-field modeling and their statistical properties

○Shin-ichi Ito[1], Satoshi Yukawa[2] （1.The Univ. of Tokyo, Japan, 2.Osaka Univ., Japan）

[P2-37] Ce-terminated (111) surface of CeO_2

○YaNan Zhao[1], Wandong Xing[2], Fanyan Meng[1], Rong Yu[2] （1.Dept. of Applied Physics, University of Science and Technology Beijing, China, 2.School of Materials Science and Engineering, Tsinghua University , China）

[P2-39] Numerical analysis of elasto-plastic behavior of metallic architectured materials

○Filip Siska[1], Ivo Dlouhy[1], Jan Cizek[2], Hanus Seiner[3] （1.Institute of Physics of Materials, Czech Academy of Sciences, Czech Republic, 2.Institute of Materials Science and Engineering, Brno University of Technology, Czech Republic, 3.Institute of Thermomechanics, Czech Academy of Sciences, Czech Republic）

[P2-40] Automatic analysis and numerical prediction of flow stress curves for aluminium alloys

○Evgeniya Kabliman, Johannes Kronsteiner, Ana-Helena Kolody （Light Metals Technologies Ranshofen, Center fo Low-Emission Transport, Austrian Institute of Technology, Austria）

[P2-41] Comparison of different alkali activated mortars with hemp fibres response during fracture test by acoustic emission method

Libor Topolar[1], ○Hana Simonova[1], Barbara Kucharczykova[1], Zbynek Kersner[1], Jelena Dragas[2], Ivan Ignjatovic[2], Miroslav Komljenovic[3], Violeta Nikolic[3] （1.Brno University of Technology, Faculty of Civil Engineering, Czech Republic, 2.University of Belgrade, Faculty of Civil Engineering, Serbia, 3.University of Belgrade, Institute for Multidisciplinary Research, Serbia）

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-34] Dynamics of a solidification front made by invasion of fluid with a different temperature

○So Kitsunezaki, Chika Yamanaka （Nara Women's Univ., Japan）

When fluid flows into another hotter or colder fluid, solidification often occurs in narrow regions at the vicinity of the interface. Such interfaces exhibit peculiar patterns in the growth process because of accompanying solidification fronts. Similar phenomena are observed in soft membranes created by chemical reactions of two fluid, as reported by H.˜Wagatsuma et al.(Physical Review E, 2017). In geological scales, we could also see examples of such phenomena in pillow lava and growth of a volcanic island.
We carried out experiments by pouring ice-cold water into paraffin melt in a Hele-Shaw cell and found that solidification of paraffin causes fingering patterns with large meandering. The melting temperature of paraffin we used is about 56-58 degrees C, but the rheological measurements indicated that paraffin behaves as a soft viscoelastic material under the temperature. We infer that precipitous increase of the viscosity of paraffin is mainly responsible for large meandering of fingering growth.
A simple two-dimensional mathematical model is considered to find an interface dynamics in such phenomena theoretically. Although a standard method of the center-manifold reduction can not be used for solidification fronts growing in time, we develop a similar systematic method to derive the equations of interface motion.

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-35] Strengthening through solid solution in $W_{1-x}Ta_xB$ system

○lijuan liu[1], Wandong Xing[2], Fanyan Meng[1], Rong Yu[2] （1.Dept. of Applied Physics, University of Science and Technology Beijing, China, 2.School of Materials Science and Engineering, Tsinghua University , China）

The elastic properties, electronic structures and the energy barriers in slip processes of $W_{1-x}Ta_xB$ system have been studied using first-principles calculations. It was found that the (110) plane is the easiest slip plane in tungsten monoboride. By substituting tungsten with tantalum, slipping on the (110) plane can be hindered through dislocation pinning, resulting in the increase of overall hardness of tungsten monoboride Strengthening of the easiest planes is an effective approach to creating new hard materials in more metallic materials.

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-36] Desiccation crack patterns based on phase-field modeling and their statistical properties

○Shin-ichi Ito[1], Satoshi Yukawa[2] （1.The Univ. of Tokyo, Japan, 2.Osaka Univ., Japan）

We investigate morphological properties on desiccation crack patterns through numerical simulations of a phase-field (PF) model. Since our PF model does not require any assumptions related to crack nucleations and numerical lattice configurations, we can investigate the pattern formations that purely depend on material/external parameters. Our PF model showed us various pattern formations depending on a drying

speed and material constants. We discovered, in particular, the difference of the drying speed provides a significantly qualitative difference in the pattern formations. Cellular patterns resulting from sequential fragmentations of straight cracks can be observed when using a slow drying speed, while random network patterns resulting from connections of micro cracks that appear simultaneously can be observed when using a rapid drying speed. We quantify the difference of the pattern formations statistically, and explain the origin of the difference on the basis of a simple continuum theory of a thin layer of viscoelastic material.

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-37] Ce-terminated (111) surface of CeO_2

○YaNan Zhao[1], Wandong Xing[2], Fanyan Meng[1], Rong Yu[2] （1.Dept. of Applied Physics, University of Science and Technology Beijing, China, 2.School of Materials Science and Engineering, Tsinghua University , China）

Surface structure and properties of ceria are closely related to the applications of ceria in catalysis. Here, the atomic structures of the (111) surface of CeO_2 nanoparticles have been studied combining aberration-corrected transmission electron microscopy and first-principles calculations. Besides the oxygen termination that have reported extensively previously, the cerium termination has also been revealed by direct atomic imaging, which can be viewed as the simultaneous loss of surface and subsurface oxygen. The stabilization mechanism, electronic structure and magnetism of the surface, and the behavior of oxygen vacancies have been discussed.

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-39] Numerical analysis of elasto-plastic behavior of metallic architectured materials

○Filip Siska[1], Ivo Dlouhy[1], Jan Cizek[2], Hanus Seiner[3] （1.Institute of Physics of Materials, Czech Academy of Sciences, Czech Republic, 2.Institute of Materials Science and Engineering, Brno University of Technology, Czech Republic, 3.Institute of Thermomechanics, Czech Academy of Sciences, Czech Republic）

Architectured materials is a class of materials that is characteristic by the ordering of constituents in specific geometrical manner. Such geometry provides an extra degree of freedom which allows reaching combinations of properties that cannot be obtained by standard materials. Metallic architectured materials are especially attractive because metals are important structural materials and adding internal architecture can enhance their performance in particular applications.
Our study is focused on a numerical investigation of an elasto-plastic response of different planar architectured patterns under the basic types of loading (tension-compression, bending). These patterns are made by different combinations of basic metals (for example: Al, Fe, Ti). The objective is to find the relation between the geometry and the resulting properties like stiffness, strength, hardening, ductility, buckling resistance. These relations will help to find optimal internal structure geometries for given materials combinations and loadings. The results from FE simulations will be further used for the production of the real structures using cold spray technology which is very well suited for a fabrication of structures and materials made of metals with different mechanical and physical properties.

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-40] Automatic analysis and numerical prediction of flow stress curves for aluminium alloys

○Evgeniya Kabliman, Johannes Kronsteiner, Ana-Helena Kolody （Light Metals Technologies Ranshofen, Center fo Low-Emission Transport, Austrian Institute of Technology, Austria）

In present work, we develop a toolkit for automatic analysis of experimental flow stress curves as well for their numerical prediction by a combined approach of physics based and data driven modelling. By using a single environment it is possible to filter measured raw data, account for temperature increase during a deformation process, extract the mechanical properties such as yield and ultimate strength, obtain the processing maps for the optimization of deformation conditions, as well as to predict the flow stress curves by using a dislocation density based model in combination with algorithms of machine learning. It is possible to account for processes such as work hardening and recovery due to spontaneous annihilation of dislocations and their climb. For testing purposes we choose a conventional AA6082 alloy and perform a series of hot compression tests by using a deformation and quenching dilatometer DIL805A/D of TA Instruments. In order to choose the most suitable algorithm of machine learning, different approaches found in literature for the prediction of flow stress curves are compared. A modified version of a flow stress model is formulated and implemented into a finite element framework, as a result.

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-41] Comparison of different alkali activated mortars with hemp fibres response during fracture test by acoustic emission method

Libor Topolar[1], ○Hana Simonova[1], Barbara Kucharczykova[1], Zbynek Kersner[1], Jelena Dragas[2], Ivan Ignjatovic[2], Miroslav Komljenovic[3], Violeta Nikolic[3] （1.Brno University of Technology, Faculty of Civil Engineering, Czech Republic, 2.University of Belgrade, Faculty of Civil Engineering, Serbia, 3.University of Belgrade, Institute for Multidisciplinary Research, Serbia）

In last decades, natural fibres are increasingly used as reinforcements for the production of low-cost composites in civil engineering. The benefits of natural fibers include non-abrasive nature, high specific properties, and biodegradability. However, their disadvantages are the bad moisture absorption, poor wettability and large scattering in mechanical properties. The aim of this paper is contribute to the better understanding of mechanical behaviour and failure modes of alkali activated materials reinforced by hemp fibers. Two different mortars based on alkali activated fly ash and slag were investigated. The paper includes the results of acoustic emission measurement captured during the three-point bending fracture test of specimens made of mentioned composites. Acoustic emission method is proving useful for the capability of real-time monitoring of materials over the whole volume and with high sensitivity to any processes generating stress waves. The effect of different mix composition and amount of hemp fibers on the acoustic signal features such as the energy, counting and amplitude is including in this research. The obtained acoustic emission results together with mechanical fracture parameters can serve as input values of material models used for modelling of structure response.

This outcome has been achieved with the financial support of the Czech Science Foundation, project No. 18-12289Y and the results obtained within the project DS-2016-0060, which belongs to Multilateral Scientific and Technological Cooperation Project in Danube Region between Technische Universität Wien, Brno

University of Technology and University of Belgrade, are presented in this paper.

Poster Session | F. From Microstructure to Properties: Mechanisms, Microstructure, Manufacturing

[PO-F2] Poster Session 2

Symposium F

Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall

[P2-43] Design of spontaneous formation-based 3D plasmonic optical structure, using multyphysics modeling

○Jihwan Song[1], Inhee Choi[2], Yonghee Shin[3], SoonGweon Hong[5], Younggeun Park[5], Dongchoul Kim[4], Taewook Kang[3], Luke Lee[5] （1.Dept. of Mechanical Engineering, Hanbat National University, Korea, 2.Dept. of Life Science, University of Seoul, Korea, 3.Dept. of Chemical and Biomolecular Engineering, Sogang University, Korea, 4.Dept. of Mechanical Engineering, Sogang University, Korea, 5.Dept. of Bioengineering and Berkeley Sensor and Actuator Center, University of California, Berkeley, United States of America）

[P2-44] **Characterization of $K_xNa_{1-x}NbO_3$ powders and ceramics prepared by hydrothermal synthesis**

○Jing Yang, Aifen Tian, Xuan Xi, Huiling Du （Dept. of Materials Science and Engineering, Xi An Univ. of Science and Technology, China）

[P2-45] Numerical and experimental investigation of liquid metal dealloying of Cu-Ni alloy in liquid silver.

○Pierre-Antoine Geslin[1,2,3], Takumi Suga[2], Takeshi Wada[2], Hidemi Kato[2] （1.INSA Lyon/CNRS, France, 2.Institute for Materials Research, Tohoku University, Japan, 3.Frontier Research Institute for Interdisciplinary Sciences, Tohoku University, Japan）

[P2-46] **Application of DLVO theory to predict dispersion stability of ZrO_2 submicron particles in electrolyte solutions**

○Ming-Hong Chiueh, Tien-Jung Huang （Industrial Technology Research Institute, Taiwan）

[P2-47] Multi-GPU large-scale phase-field lattice Boltzmann simulation of dendrite growth with thermal-solutal convection

○Shinji Sakane[1], Tomohiro Takaki[1], Munekazu Ohno[2], Yasushi Shibuta[3], Takayuki Aoki[4] （1.Kyoto Institute of Technology, Japan, 2.Hokkaido University, Japan, 3.The University of Tokyo, Japan, 4.Tokyo Institute of Technology, Japan）

[P2-48] Stress analysis of 4H-SiC power devices via FEM and Raman spectroscopy

○Hiroki Sakakima[1], Asuka Hatano[1], Akihiro Goryu[2], Kenji Hirohata[2], Satoshi Izumi[1] （1.The Univ. of Tokyo, Japan, 2.Toshiba, Japan）

[P2-49] A Functionally Graded Multi-Phase Micromechanical Model for Carbon Nanotube - Polymer Composites

○Vahidullah Tac[1,2], Ercan Gurses[1] （1.Middle East Technical University, Turkey, 2.Turkish Aerospace Industries, Turkey）

[P2-50] **Atomic surface treatment of copper nanowires by electron beam irradiation simulated by first principle calculation**

○Shih Kuang Lee （National Chiao Tung University, Taiwan）

[P2-51] Molecular-Dynamic Simulation of Rapid Solidification of Dipolar Molecular Crystal from Its Melt

○Xianqi Xu, Yang Yang （East China Normal University, China）

[P2-52] Intrinsic Analysis of Structural Order Parameter at Equilibrium Crystal-Melt Interfaces

○Wenliang Lu, Hongtao Liang, Yang Yang （EAST CHINA NORMAL UNIVERSITY, China）

[P2-53] Multiscale Modelling of Indirect-to-Direct Band Gap Transition in Silicon Nanosheets

○Byung-Hyun Kim[1], Chan-Woo Lee[1], Mina Park[2], Gyubong Kim[2], Kersti Hermansson[3], Peter Broqvist[3], Heon-Jin Choi[4], Kwang-Ryeol Lee[2] （1.R&D Platform Center, Korea Institute of Energy Research, Korea, 2.Computational Science Research Center, Korea Institute of Science and Technology, Korea, 3.Dept. of Chemistry-Ångström Laboratory, Uppsala University, Sweden, 4.Dept. of Materials Science and Engineering, Yonsei University, Korea）

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-43] Design of spontaneous formation-based 3D plasmonic optical structure, using multyphysics modeling

○Jihwan Song[1], Inhee Choi[2], Yonghee Shin[3], SoonGweon Hong[5], Younggeun Park[5], Dongchoul Kim[4], Taewook Kang[3], Luke Lee[5] （1.Dept. of Mechanical Engineering, Hanbat National University, Korea, 2.Dept. of Life Science, University of Seoul, Korea, 3.Dept. of Chemical and Biomolecular Engineering, Sogang University, Korea, 4.Dept. of Mechanical Engineering, Sogang University, Korea, 5.Dept. of Bioengineering and Berkeley Sensor and Actuator Center, University of California, Berkeley, United States of America）

Oil droplets in water or water droplets in oil have been generated fascinating science and utilized in enormous applications from medicine to energy harvesting. However, the creation of integrated three-dimensional architectures by liquid droplet and immiscible liquid interface is relatively less investigated. Here we report interfacial energy-driven and spontaneous formation of plasmonic cavity at room temperature without an external force. With the multiphysics approach considering the densities and interfacial energies of two different liquids, we simulated the spontaneous formation of cavity when a liquid water droplet meets immiscible liquid interface. At the interface, the metal ions in the liquid droplet are automatically reduced and they form the interfacial plasmonic layer onto the cavity surface. Due to the both optical cavity and integrated plasmonic structure, the significantly enhanced fluorescence is obtained by 1000 times. We believe our findings could offer a new avenue and advance in a variety of photonic and plasmonic materials and devices.

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-44] Characterization of $K_xNa_{1-x}NbO_3$ powders and ceramics prepared by hydrothermal synthesis

○Jing Yang, Aifen Tian, Xuan Xi, Huiling Du （Dept. of Materials Science and Engineering, Xi An Univ. of Science and Technology, China）

There is an increasing demand to replace $Pb(Zr,Ti)O_3$-based piezoelectric materials with lead-free alternatives, because of the toxicity of lead oxide which is largely used during the production process. $K_xNa_{1-x}NbO_3$ (KNN) is considered as one of the most promising candidates for lead free piezoelectric ceramics due to its high Curie temperature and good electrical properties.

$K_xNa_{1-x}NbO_3$ ceramics can be used for several applications such as high frequency transducers, ultra-sonic diagnostics and tunable micro-wave components. However, it is well known that dense and well-sintered $K_{0.5}Na_{0.5}NbO_3$ ceramics are very difficult to obtain by the ordinary sintering process owing to the high volatility of alkali elements at high temperatures. The major strategy to overcome this problem is simply to synthetized KNN powders at low temperature. One method of making dense $(K_xNa_{1-x})NbO_3$ ceramics is to use refined powder with improved sintering activity, prepared in the molten salt process, sol-gel routine or hydrothermal process. In this work, $(K_xNa_{1-x})NbO_3$ powders and ceramics were prepared by hydrothermal synthesis. X-ray diffraction and scanning electron microscope were performed to investigate the structure and surface morphology of the $(K_xNa_{1-x})NbO_3$ powders and ceramics. The results showed that all the KNN powders possessed the pervoskite structure and a handful of second phases. The $K_{0.7}Na_{0.3}NbO_3$ ceramic prepared by the powders exhibits relatively good properties (relative dielectric constant ε = 416 and piezoelectric coefficient d_{33}=40 pC/N).

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-45] Numerical and experimental investigation of liquid metal dealloying of Cu-Ni alloy in liquid silver.

○Pierre-Antoine Geslin[1,2,3], Takumi Suga[2], Takeshi Wada[2], Hidemi Kato[2] （1.INSA Lyon/CNRS, France, 2.Institute for Materials Research, Tohoku University, Japan, 3.Frontier Research Institute for Interdisciplinary Sciences, Tohoku University, Japan）

Liquid metal dealloying has emerged as a promising technique to produce finely porous structures of various nature (non-noble metals, refractory metals or semi-conductors) presenting a high surface area, valuable in a numerous applications (catalysis, battery materials, sensors,...). This process consists in emerging a binary precursor alloy (i.e. Cu-Ni) in a liquid metal (Ag) chosen such that only one element of the precursor alloy (Cu) dissolves into the metallic melt while the other element (Ni) reorganizes into a porous structure. We investigated the formation of this microstructure based on the ternary phase diagram of the Ni-Cu-Ag system. First, we developed a quantitative phase-field model to investigate the initiation of this dealloying process. The phase-field method is particularly adapted to investigate this kind of free-boundary problem and the complex morphogenesis of the structures, but is enable to reach the experimental time and size-scales. In a multi-scale approach, we use phase-field results and experimental observations to develop a macroscopic diffusion model able to reproduce the kinetics and the composition profiles obtained experimentally. Also, based on this work on the Cu-Ni-Ag model system, we were able to generalize our findings to other systems and assess the potential of other systems to form finely porous microstructures upon dealloying.

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-46] Application of DLVO theory to predict dispersion stability of ZrO_2 submicron particles in electrolyte solutions

○Ming-Hong Chiueh, Tien-Jung Huang （Industrial Technology Research Institute, Taiwan）

In the manufacturing process of multi-layer ceramic capacitors (MLCC), electronic components often used in modern mobile phones, dispersion stability of ZrO_2 submicron particles can be improved by altering the pH of electrolyte solution. In this study we used the DLVO theory to predict the energy barriers of interaction forces between two ZrO_2 particles in various electrolyte solutions at different pH. The electrolyte solutions may be strong basic, weakly acidic, or strong acidic. The distance-dependent potentials of van der Walls force and electrical double layer force were calculated. The calculation results show that weakly acidic solution induces larger energy barrier between ZrO_2 particles, because of stronger electrical double layer force. This larger energy barrier can prevent aggregation of ZrO_2 particles and lead to dispersion stability.

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-47] Multi-GPU large-scale phase-field lattice Boltzmann simulation of dendrite growth with thermal-solutal convection

○Shinji Sakane[1], Tomohiro Takaki[1], Munekazu Ohno[2], Yasushi Shibuta[3], Takayuki Aoki[4] （1.Kyoto Institute of Technology, Japan, 2.Hokkaido University, Japan, 3.The University of Tokyo, Japan, 4.Tokyo Institute of Technology, Japan）

Thermal-solutal convection, that inevitably occurs during terrestrial solidification of an alloy, drastically changes the dendrite morphology and microsegregation. Although phase-field method is the most powerful computational tool for predicting the dendrite morphology and microsegregation, we need many computational costs in the phase-field simulation taking the thermal-solutal convection into account. In this study, we enable a large-scale simulation for phase-field lattice Boltzmann model, which can express the dendrite growth with the transport of solute and heat and the fluid flow. Here, to reduce the computational cost, we employ a multi-level mesh and multi-level time step when solving phase-field equation, advection-diffusion equations for heat and solute, and lattice Boltzmann equation for computing the fluid flow. In addition, to accelerate the large-scale simulation, we implement the parallel computation using multiple graphics processing units (GPU). By employing the developed scheme, we perform the dendrite growth simulation during directional solidification of a binary alloy with thermal-solutal convection and investigate the effects of thermal-solutal convection on the dendrite morphology.

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-48] Stress analysis of 4H-SiC power devices via FEM and Raman spectroscopy

○Hiroki Sakakima[1], Asuka Hatano[1], Akihiro Goryu[2], Kenji Hirohata[2], Satoshi Izumi[1] （1.The Univ. of Tokyo, Japan, 2.Toshiba, Japan）

We developed a scheme to analyze the stress distribution of 4H-SiC power devices by FEM and Raman spectroscopy. Raman spectroscopy is widely applied as a method for evaluating stress distribution of semiconductor devices. However, the relationship between phonon frequency, which is measured by Raman spectroscopy, and stress tensor is not clarified for 4H-SiC. In addition, it is impossible to evaluate the distribution of the stress tensor having six components only by Raman spectroscopy since the phonon frequency is a scalar quantity. To solve these problems, we detected phonon deformation potentials, which are the relationships between phonon frequency and stress tensor, and developed the analysis method combining FEM and Raman spectroscopy. Firstly, phonon deformation potentials were detected by first principle calculation. The phonon frequency of the strained crystal is calculated. All components of the phonon deformation potential constants were obtained from the relationship between the magnitude of stress and the phonon frequency shift. The calculated deformation potential constants were validated by previous experimental results. Secondly, multi-step thermal-stress FEM analysis which reproduces actual fabrication process was conducted for a pin diode. Young's modulus, linear expansion coefficient and intrinsic stress of thin films formed on SiC substrates were measured. The obtained stress distribution was converted into the distribution of the phonon frequency shift and validated through comparison with the result of the micro Raman spectroscopy. The obtained stress distribution and its origin will be presented. This work was supported by Council for Science, Technology and Innovation(CSTI), Cross-ministerial Strategic Innovation Promotion Program (SIP), “Next-generation power electronics/Consistent R&D of next-generation SiC power electronics” (funding agency: NEDO)

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-49] A Functionally Graded Multi-Phase Micromechanical Model for Carbon Nanotube - Polymer Composites

○Vahidullah Tac[1,2], Ercan Gurses[1] （1.Middle East Technical University, Turkey, 2.Turkish Aerospace Industries, Turkey）

Carbon nanotubes (CNT) are widely known for their superior stiffness as well as strength since their discovery in 1991. While our current level of understanding of carbon nanotubes prevent us from using them in structural parts per se, embedding them in polymers for strengthening and stiffening purposes shows a great potential. However practical efforts towards designing, manufacturing and employing such nanocomposite materials have not yet fully culminated largely due to a lack of understanding of the bonding between the nanotube and the polymer.

Latest experimental and molecular mechanical observations of the region around a carbon nanotube embedded inside a polymer indicate the presence of at least four distinct “phases” in nanocomposites; the CNT, the thin interfacial gap between the CNT and the polymer, a large portion of polymer around the CNT with linearly varying properties, and the bulk polymer phase.

Hence, to accurately model nanocomposite material the varying nature of polymer in the proximity of the CNT has to be taken into account, among other things.

We adopt a multi-phase micromechanical model that allows gradual degradation/upgradation of the constituent phases to study the mechanical properties of CNT-Polymer composites. Using this model the mechanical properties of the polymer is gradually enhanced in the vicinity of the CNT. We also study the effect of the gap between the CNT and the polymer and the role it plays in such nanocomposites. The results of our analyses are then compared to experimental data and discussed in detail.

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-50] Atomic surface treatment of copper nanowires by electron beam irradiation simulated by first principle calculation

○Shih Kuang Lee （National Chiao Tung University, Taiwan）

Atomic surface treatment of copper nanowires by electron beam irradiation simulated by first principle calculation

Alex Lee [a],Ting-Yi Lin [a], Yu-Chieh Lo [a], and Wen-Wei Wu [a]

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Recently, the techniques of atomic surface treatment by electron beam etching has developed vigorously. However, the improvement and more details should be understood specially in atomic scale. In the experiment when we applied the electron beam on copper nanowires with copper oxide (111) surface without heating, it was found the reduction reaction and the following Cu clusters slip on Cu (111) surface. For further complete the mechanism, we provide the Vienna ab initio simulation package (vasp) to perform the GGA calculation with PAW pseuodopotentials. For reduction reaction, we compare the energy between the theoretical structure of Cu with oxide surface and Cu (111) surface to predict the binding energy of oxygen. For the slip of Cu clusters, we calculate the energy mapping of slip path on Cu (111) surface to find the most probable routine of slip. The calculation data should help us control the intensity of electron beam radiation when we do the surface treatment of material and be the complement of slip observation.

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-51] Molecular-Dynamic Simulation of Rapid Solidification of Dipolar Molecular Crystal from Its Melt

○Xianqi Xu, Yang Yang （East China Normal University, China）

We present results of molecular dynamics (MD) simulations of crystal growth from the melt. The work focuses on a face-centered-cubic molecular crystal consist with molecules modeled by an extended point dipole model. We will present results of non-equilibrium MD growth simulations as a function of temperature and molecular dipole moment. An analysis of the interfacial position as the function of simulation time was employed to extract the steady-state, and the data of the kinetic coefficients vs. molecular dipole moments and their anisotropies were calculated and will be presented. Values of the kinetic coefficient for the (100), (110) interfaces are compared quantitatively to the prediction of Mikheev-Chernov (MC) theory. Our study suggest that incorporating a second relaxation time due to the dipolar fluctuation beside the relaxation time of density waves, is necessary for extending MC theory to be applicable for molecular crystals.

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-52] Intrinsic Analysis of Structural Order Parameter at Equilibrium Crystal-Melt Interfaces

○Wenliang Lu, Hongtao Liang, Yang Yang （EAST CHINA NORMAL UNIVERSITY, China）

We present atomistic simulations of precisely equilibrated crystal-melt interface under ambient pressure, for pure Ni and Fe. We demonstrate the capillary waves roughen the surface, but the intrinsic interfaces can be sharply defined. We use different types of local structural order-parameter together with a reference lattice to characterize the intrinsic interface. The statistical analysis on the structural order-parameters for the interfacial solid and interfacial liquid atoms represents universal scaling behavior, nearly independent of the order parameter type, crystal structure and interface orientations. We will discuss the potential application of such intrinsic analysis to the investigations of crystal nucleation and steady-state crystallization from melt.

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-53] Multiscale Modelling of Indirect-to-Direct Band Gap Transition in Silicon Nanosheets

○Byung-Hyun Kim[1], Chan-Woo Lee[1], Mina Park[2], Gyubong Kim[2], Kersti Hermansson[3], Peter Broqvist[3], Heon-Jin Choi[4], Kwang-Ryeol Lee[2] （1.R&D Platform Center, Korea Institute of Energy Research, Korea, 2.Computational Science Research Center, Korea Institute of Science and Technology, Korea, 3.Dept. of Chemistry-Ångström Laboratory, Uppsala University, Sweden, 4.Dept. of Materials Science and Engineering, Yonsei University, Korea）

Two-dimensional (2D) nanomaterials such as graphene, boron nitride (BN), and MoS_2 have attracted great attention owing to their exceptional and tuneable properties, which are distinguishable from those of their bulk phases. Recently, Si nanosheets (Si NSs) have been synthesized by various experimental techniques. Compared to other materials, Si-based nanostructures have great advantages when it comes to commercialization, as Si is compatible with the conventional device manufacturing processes in the microelectronics industry.

In experiments, (111) Si NSs showed thickness-dependent light emissions in the visible wavelength regime, originating from quantum confinement effects. This observation indicates that thin (111) Si NSs have a direct band gap, whereas bulk Si normally has an indirect band gap. However, the question of the physical origin behind this nano-effect of Si left unanswered.

The effect of biaxial strain on the band structure of 2D Si NSs with (111), (110), and (001) exposed surfaces was investigated by means of a multiscale modelling approach combining molecular dynamics simulations with a reactie force field and the density functional theory. For all the considered Si NSs, an indirect-to-direct band gap transition occurs as the lateral dimensions of Si NSs increase, i.e. increasing lateral biaxial strain from compressive to tensile always enhances the direct band gap characteristics. Further analysis revealed the mechanism of the transition which is caused by preferential shifts of the conduction band edge at a specific *k*-point due to their bond characteristics. Our results explain a photoluminescence result of the (111) Si NSs [U. Kim *et al.*, *ACS Nano* **2011**, *5*, 2176-2181] in terms of the plausible tensile strain imposed in the unoxidized inner layer by the surface oxidation.

Poster Session | G. Modeling Mechanical Behavior of Materials under Harsh Environments

[PO-G2] Poster Session 2

Symposium G

Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall

[P2-54] **Component-wise Effect of Incompatibility Tensor on Misorientation Development in Lath Block Structure Model based on FTMP**

○Yuta Amano, Tadashi Hasebe, Yasutaka Matsubara （Dept. of Mechanical Engineering, Kobe Univ., Japan）

[P2-55] Construction of virtual ITZ specimens using extended stochastic optimization and evaluation of their permeability

○Se-Yun Kim, Tong-Seok Han （Dept. of Civil and Environmental Engineering, Yonsei Univ., Korea）

[P2-56] Estimation for probabilistic distribution of material response according to microstructural characteristics

○JI-SU KIM, Tong-Seok Han （Yonsei Univ., Korea）

[P2-57] **Hypervelocity impact and shock behavior of pillared graphene foams**

○Stefano Signetti, Seunghwa Ryu （Department of Mechanical Engineering, Korea Advanced Institute of Science and Technology (KAIST), Korea）

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-54] Component-wise Effect of Incompatibility Tensor on Misorientation Development in Lath Block Structure Model based on FTMP

○Yuta Amano, Tadashi Hasebe, Yasutaka Matsubara （Dept. of Mechanical Engineering, Kobe Univ., Japan）

Modeling complex microstructures, e.g., those like lath martensite structures in high Cr ferritic heat resistant steels, are one of the critical issues in multiscale modeling of materials, although neither conventional schemes exist nor effective methodologies have been developed to date. In the present study, FTMP (Field Theory of Multiscale Plasticity)-based Di-CAP (Deformation-induced Context-dependent Autonomic Pluripotency) concept is applied to computationally fabricate complex microstructured samples to be further utilized in various deformation analyses based on, e.g., FEM. Here, we focus on the process of modeling single lath-block structures, which can be obtained in preliminary bi-axial compression analyses, provided the corresponding eigenstrain distributions based on the Bain lattice correspondence is initially introduced. One of the keys for the lath-block modeling is the development of misorientation across the lath boundaries, roughly satisfying K-S variant, together with the attendant internal stress fields. FTMP-based approach exhibits spontaneous evolution of such misorientation when substantial contribution of the incompatibility tensor is introduced in the hardening law. Here we decompose the incompatibility tensor into (a)pure deformation and pure rotation, (b)edge and screw, and (c)spherical (isotropic) and deviatoric components, respectively, to examine the mechanisms for the misorientation developments. Analyses are conducted using two basic models for a single lath block structure, i.e., vertical and horizontal models, where lath sub-blocks are aligned vertically and horizontally to the [111] axis, respectively. Demonstrated for (a) is that the pure deformation part shows relatively larger contributions to the misorientation developments, while, for (b), dominant contributions of the screw component are confirmed. For (c), on the other hand, the weighted spherical part is shown to have weak but basically the same contribution.

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-55] Construction of virtual ITZ specimens using extended stochastic optimization and evaluation of their permeability

○Se-Yun Kim, Tong-Seok Han （Dept. of Civil and Environmental Engineering, Yonsei Univ., Korea）

The external substance penetrates into an interfacial transition zone (ITZ) that is located between an aggregate and bulk cement paste and has a relatively high porosity than the bulk cement paste. However, it is difficult to confirm the 3-D microstructure of the ITZ with the functionally graded void distribution to evaluate its permeability. In this study, 3-D microstructures of bulk cement pastes with three kinds of porosities and the void gradient of the ITZ obtained from 2-D SEM image are used to construct the virtual 3-D microstructures of the ITZ. Based on the two information, the phase distribution characteristics of the ITZ are generated, and they are used for constructing the virtual ITZ specimen using a stochastic optimization. The stochastic optimization is an appropriate method to construct a random heterogeneous material [1], but the ITZ has the functionally graded void distribution, which depends on the distance from the aggregate. To construct the functionally graded microstructure, an extended stochastic optimization is proposed. In addition, an efficient iteration method for stochastic optimization is proposed and utilized for construction of the virtual ITZ specimens, which improved the computational cost. The permeability of the virtual ITZ

specimens are evaluated by a finite element method. The effect of the ITZ from the penetration of the external substances is confirmed by the permeability analysis using the virtual ITZ specimen. This study shows that the proposed extended stochastic optimization process is effective for constructing functionally graded phase distribution, while the real 3-D microstructure is difficult to obtain from experimental techniques. This study also confirms that the virtual experiment procedure can be synergistically used with the real experimental approaches.

[1] S. Torquato, Random Heterogeneous Materials: microstructure and macroscopic properties, vol. 16, Springer Science &Business Media, Berlin, 2013.

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[P2-56] Estimation for probabilistic distribution of material response according to microstructural characteristics

○JI-SU KIM, Tong-Seok Han （Yonsei Univ., Korea）

There is a strong correlation between the material microstructure and its response [1]. It is expected that the statistical distribution of material response has a relation with that of the microstructure characteristics, so that the effect of the microstructure to the response can be investigated. In this study, the sensitivity of the material responses due to microstructural characteristics is investigated using a first-order second moment (FOSM) method [2]. The FOSM method is a probabilistic method, which determines the mean and deviation of a function of responses with random input variables. For applying the FOSM method, specimens with certain microstructure characteristics might have to be reconstructed. For this reason, the reconstruction process [3] to generate the target specimens are needed. The area of lineal-path function and porosity of cement paste specimens are selected as random input variables, and the stiffness and strength evaluated by phase field fracture model are selected as output variables. The result of sensitivity analysis from the FOSM method is compared to the simulation results using whole specimens. From this result, the sensitivity of material response to microstructure is estimated using two reconstructed specimens, and the FOSM method is confirmed to reduce the time and cost for evaluating the probabilistic distribution of properties.

[1] Mindess, S., Young, J. F., and Darwin, D. Concrete. 2nd ed. Prentice Hall U.S.A. (2003) 57-80.

[2] Lee, T.-H. Probabilistic Seismic Evaluation of Reinforced Concrete Structural Components and Systems. University of California, Berkeley (2005).

[3] Chung, S.-Y., Han, T.-S., Kim, S.-Y., and Lee, T.-H. Investigation of the permeability of porous concrete reconstructed using probabilistic description methods. Construction and Building Materials (2014) 66:760-770.

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-57] Hypervelocity impact and shock behavior of pillared graphene foams

○Stefano Signetti, Seunghwa Ryu （Department of Mechanical Engineering, Korea Advanced Institute of Science and Technology (KAIST), Korea）

The effectiveness of graphene as material for impact protection has been confirmed both by atomistic simulations [1] and microscale experiment [2] obtaining unprecedented impact toughness up to ~50 MJ/kg at the nanoscale [1]. However, specific energy absorption could be, in principle, further increased by tailoring inter-layer interaction [3] via interface structuring or functionalization. In this study we present a modified graphene nanoarmor concept obtained by the introduction of pillar structures in the form of carbon nanotubes [4] of variable spatial density, aspect ratio, and size which allow the realization of stable graphene multilayers with variable spacing. Impact strength and shock behavior of such structures are investigated via molecular dynamics (MD) simulations and the effect of foam geometry on the specific energy absorption capability is evaluated across different size-scales.

References

[1] S. Signetti, S. Taioli, N.M. Pugno. 2D Materials Armors Showing Superior Impact Strength of Few Layers. *ACS Applied Materials &Interfaces* 8:40820-40830, 2017.
[2] J. Lee, P.E. Loya, J. Lou, E.L. Thomas. Dynamic mechanical behaviour of multilayer graphene via supersonic projectile penetration. *ACS Applied Materials &Interfaces* 346(632):1092-1096, 2014.
[3] S. Signetti, N.M. Pugno. Evidence of optimal interfaces in bio-inspired ceramic-composite panels for superior ballistic protection. *Journal of the European Ceramic Society* 34:2823-2831, 2014.
[4] S. Lee, D. Kang, I. Oh. Multilayered graphene-carbon nanotube-iron oxide three-dimensional heterostructure for flexible electromagnetic interference shielding film. *Carbon* 111:248-257, 2017.

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

[PO-H2] Poster Session 2

Symposium H

Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall

[P2-58] Studying the kinetics of a self-propelled cruiser in 2D granular media under gravity

○Guo-jie Jason Gao （Dept. of Mathematical and Systems Engineering, Shizuoka Univ., Japan）

[P2-59] A Discrete Tetris model showing two flow regimes for hard particles exiting a hopper with an adjustable obstacle

○Tomoya Yasuno[1,2], Guo-jie Jason Gao[1] （1.Dept. of Mathematical and Systems Engineering, Shizuoka Univ., Japan, 2.Dept. of Complex Systems Science, Nagoya Univ., Japan）

[P2-60] Effect of water molecules on polymer chain motion in dense chain ensembles of nafion membrane

○Isamu Riku, Ryoma Oka, Koji Mimura （Osaka Prefecture Univ., Japan）

[P2-61] A Coarse-Grained Model for Competitive Adsorption on the Surface of Inorganic Nanomaterials

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

[P2-62] Molecular Dynamics of Inorganic and Organic Interfaces with Force-Field Parameters Based on DFT Simulations

○Kosuke Ohata, Hiroya Nitta, Kenta Chaki, Taku Ozawa （JSOL Corporation, Japan）

[P2-63] Molecular dynamics screening for developing compounds of electrolytes with high performance in lithium ion batteries

○Yoshihiro Takai[1], Ken-ichi Saitoh[2], Masanori Takuma[2], Yoshimasa Takahashi[2], Tomohiro Sato[2] （1.Graduate school of Science and Engineering, Kansai Univ., Japan, 2.Faculty of Engineering Science, Kansai Univ., Japan）

[P2-64] Molecular dynamics study on transmission mechanism of torsional deformation in cellulose nanofibers with hierarchical structure

○Kentaro Takada[1], Ken-ichi Saitoh[2], Masanori Takuma[2], Yoshimasa Takahashi[2], Tomohiro Sato[2] （1.Graduate School of Science and Engineering, Kansai Univ., Japan, 2.Faculty of Engineering Science, Kansai Univ., Japan）

[P2-65] Bubble dynamics of foam flow around an obstacle

○Antti Puisto, Juha Koivisto, Leevi Viitanen, Mikko J Alava （Aalto University, Department of Applied Physics, Finland）

[P2-66] Shape Deformation and Mechanical Relationship of Ionic Droplet Under An Electric Field

Bo-Yu Shih[1], ○Wei-Chun Lin[1], Alice Hu[2], Hsuan-Teh Hu[1], Yu-Chieh Lo[3] （1.Department of Civil Engineering,National Cheng Kung University, Taiwan, 2.Department of Mechanical and Biomedical Engineering, City University of Hong Kong, Hong Kong, 3.Department of Materials Science and Engineering, National Chiao Tung University, Taiwan）

[P2-67] Multiscale modeling of surface functionalized graphene/polymer nanocomposites: insight into the effect of covalent grafting

○Jeong-ha Lee[1], Seunghwa Yang[2] （1.Dept. of Energy Engineering, Chung-Ang Univ., Korea, 2.Dept. of Energy Systems Engineering, Chung-Ang Univ., Korea）

[P2-68] Durability analysis on the environmental aging of epoxybased nanocomposite

○Sunyong Kwon[1], Man Young Lee[2], Seunghwa Yang[3] （1.Dept. of Energy Engineering, Chung-Ang Univ., Korea, 2.Agency for Defense Development, Korea, 3.Dept. of Energy Systems Engineering, Chung-Ang Univ., Korea）

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-58] Studying the kinetics of a self-propelled cruiser in 2D granular media under gravity

○Guo-jie Jason Gao （Dept. of Mathematical and Systems Engineering, Shizuoka Univ., Japan）

Experimentally and numerically, it has been shown that placing an obstacle near the orifice of a hopper can locally enhance the flow rate for hard discs leaving the hopper under gravity. Besides, the enhanced flow rate happens regardless the interparticle friction, the obstacle geometry, or particle dispersity. In this study, we propose a Tetris model to further clarify the physics behind this phenomenon. The model sequentially moves one particle at a time towards the hopper orifice, governed by Gaussian displacement functions. A particle can move as long as the movement creates no overlap between the particle and the others, the obstacle, or the boundaries of the hopper. Our model reduces the dynamics in the system to its minimal and allows no interparticle collaborative motion due to Newtonian dynamics. Using this model, we successfully reproduce the locally enhanced flow rate, which can be explained by a flow rate difference between its value near the obstacle and its maximal value without an obstacle. Our results show that the flow rate difference is the fundamental reason causing this phenomenon - universal with minimal dynamics involved.

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-59] A Discrete Tetris model showing two flow regimes for hard particles exiting a hopper with an adjustable obstacle

○Tomoya Yasuno[1,2], Guo-jie Jason Gao[1] （1.Dept. of Mathematical and Systems Engineering, Shizuoka Univ., Japan, 2.Dept. of Complex Systems Science, Nagoya Univ., Japan）

Placing an obstacle near the orifice of a hopper has been shown experimentally and numerically to locally enhance the flow rate for hard particles leaving the hopper under gravity. A flow rate difference between its value near the obstacle and its maximal value without an obstacle can explain this phenomenon with minimal dynamics involved. When the obstacle sits close to the hopper orifice, the flow rate near the obstacle is smaller than the maximal value, which corresponds to a fluidized flow regime. On the other hand, when the obstacle is placed further from the orifice, the flow rate near the obstacle becomes larger than the maximal value and a clogging flow regime appears. In this study, we employ a Tetris model in 2D discretized space and successfully demonstrate the two flow regimes. Without creating overlap between any objects in the system, our model sequentially relocates one particle at a time into its von Neumann or Moore neighborhood closer to the hopper orifice. Our results show that in the fluidized regime, where flow rate is low, the Moore protocol, which allows higher freedom to move particles, gives higher flow rate than the von Neumann protocol. The trend reverses in the clogging regime, where higher freedom to move particles renders lower flow rate.

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[P2-60] Effect of water molecules on polymer chain motion in dense chain ensembles of nafion membrane

○Isamu Riku, Ryoma Oka, Koji Mimura （Osaka Prefecture Univ., Japan）

Because of the high power density, high efficiency, fast start-up, and zero emission at the point of use, proton exchange membrane fuel cells (PEMFCs) are the most promising candidates for replacing internal combustion engines in automobiles, and are also being developed for portable and distributed stationary power generation applications.
However, the life of PEMFCs is currently limited by the mechanical endurance of polymer electrolyte membranes (PEMs). The failure of PEM is believed to be the result of a combined chemical and mechanical effect acting together. Recently, it is found that cyclic hydration of the membrane during the operation cycles (start/shut down) of the fuel cell may cause mechanical degradation of the membrane.
Therefore, in this paper, to investigate such mechanical degradation of the membrane subjected to fuel cell cycles, we perform a series of molecular dynamic simulations for the membrane made from the sulfonated tetrafluoroethylene copolymer with the trade name Nafion. The effect of the water molecules on the polymer chain motion in dense chain ensembles of nafion membrane is to be clarified.

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-61] A Coarse-Grained Model for Competitive Adsorption on the Surface of Inorganic Nanomaterials

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

The increased use of nanoparticles (NP) and nanomaterials is pushing scientific research into trying to understand the mechanisms governing interactions between biomolecules and inorganic materials. It is known that, once a NP is in contact with a biological medium, a protein corona forms on its surface, and that the nature of the corona is what regulates the interaction between the NP and the other biomolecules.
In this work we propose a method to coarse grain the interactions of inorganic nanomaterials in contact 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 NP surface is described a potential of mean force from atomistic simulations [2]. The NP is represented by a two-layer model where the surface interacts with the molecule beads by using the beads PMF with a slab of the material, corrected by a geometric factor, while the core interacts with via van der Waals forces calculated using Lifshitz theory. This model can describe the kinetics of competitive adsorption of biomolecules on the surface of a NP.
We have studied the kinetics of adsorption and the corona composition of Au NPs in a biological environment with the typical composition of lung lining fluid and blood plasma. This methodology can then be combined with adverse outcome pathway analysis to build mechanism-based predictive schemes for toxicity assessments.

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[1] M. Rahman, S. Laurent, N. Tawil, L. Yahia, and M. Mahmoudi, Protein-Nanoparticle Interactions, volume 15 of Springer Series in Biophysics. Springer-Verlag, 2013
[2] E. Brandt and A. P. Lyubartsev. Molecular dynamics simulations of adsorption of amino acid side chain analogues and a titanium binding peptide on the TiO_2 (100) surface. J. Phys. Chem. C, 119:18126, 2015.

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-62] Molecular Dynamics of Inorganic and Organic Interfaces with Force-Field Parameters Based on DFT Simulations

○Kosuke Ohata, Hiroya Nitta, Kenta Chaki, Taku Ozawa （JSOL Corporation, Japan）

Nanocomposites are important in the engineering field. However, the controlling of the properties of interfaces between inorganic solid fillers and organic molecules is one of the key issues. We have investigated the interaction between solids and polymers with a combination of Density Functional Theory (DFT) and Molecular Dynamics (MD) simulations. DFT is a reliable method for calculating potential energy surface (PES). The force field parameters for MD simulations were determined by using our scheme for interfacial systems based on the DFT simulation. Then the scheme was applied to a solid-polymer interface. Utilizing the determined coarse-grained and full-atomistic force field parameters, the MD simulations were conducted. In this study, we utilized SIESTA for the QM simulation and J-OCTA for the system modeling and the MD simulation.

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[P2-63] Molecular dynamics screening for developing compounds of electrolytes with high performance in lithium ion batteries

○Yoshihiro Takai[1], Ken-ichi Saitoh[2], Masanori Takuma[2], Yoshimasa Takahashi[2], Tomohiro Sato[2] （1.Graduate school of Science and Engineering, Kansai Univ., Japan, 2.Faculty of Engineering Science, Kansai Univ., Japan）

Recently, there is great interest in development of electric vehicles, so it demands improvement in performance of Lithium-ion Battery (LIB). For higher performance, it is important to develop new substances used for electrolyte or electrode. In particular, electrolyte is an important chemical factor for moving lithium ions between positive and negative electrodes in the battery. When the amount of ions moving is enhanced, the performance of the battery will be effectively improved. But there are hundreds of thousands of compounds as candidates for electrolytes, so we need to screen and choose ones from these many compounds. In this research, we perform atomistic evaluation about various characteristics of possible compounds of electrolyte (such as viscosity, ionic conductivity, degree of dissociation and diffusion coefficient) by mainly using molecular dynamics (MD) simulations. In evaluating at a molecular level, we can understand how the molecular level structure and properties affect the behavior of electrolyte. Molecule models we are using are ethylene carbonate (EC), fluoro ethylene carbonate (FEC), propylene carbonate (PC), butylene carbonate (BC), γ-butyrolactone (GBL), γ-valerolactone (GVL), dimethyl carbonate (DMC), ethyl-methyl carbonate (EMC), diethyl carbonate (DEC), and lithium hexafluorophosphate ($LiPF_6$). An electrolytes system in which 1 mol of $LiPF_6$ is mixed per 1 L of single solvent (solvent + 1M-$LiPF_6$) is simulated. The results suggest that we can determine a criterion for the screening of superior compounds based on information about molecular structures and properties of electrolyte. It is found that the smaller solvent molecules that easily diffuse contribute to the higher ionic conductivity of electrolytes. This is because diffusion coefficient of Li cation is greatly affected by that of solvent molecules. It is also found that solvation structure and size around Li cation take large effect on its diffusivity.

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[P2-64] Molecular dynamics study on transmission mechanism of torsional deformation in cellulose nanofibers with hierarchical structure

○Kentaro Takada[1], Ken-ichi Saitoh[2], Masanori Takuma[2], Yoshimasa Takahashi[2], Tomohiro Sato[2] （1.Graduate School of Science and Engineering, Kansai Univ., Japan, 2.Faculty of Engineering Science, Kansai Univ., Japan）

Cellulose nanofiber (CNF) has high strength comparable to steel, and it shows low environmental load during a cycle of production and disposal. Beside it has many excellent properties and functions such as high rigidity, light-weight, flexibility and shape memory effect, so it is expected as a next-generation new material. CNF is a fibrous and nano-sized substance produced by decomposition of bulk-type cellulose which is a main component of plants. Usually it is constituted by many cellulose micro fibrils (CMFs) in which molecular chains of cellulose are aggregated in a crystal structure. It is also possible to make composite material of CNF together with other components, and then a new material with lightweight as well as high strength and high toughness will be realized. In such case, knowledge of mechanical properties for each CMF units is important. Since actual fibrils are complicatedly intertwined, it is also crucial to elucidate the transmission mechanism of force and deformation not only in one fibril but also in between fibrils. Indeed, how the dynamic and hierarchical structure composed of CMFs responds to bending or torsion, which includes gradient of stress and strain, is an interesting issue. However, little is known on torsional characteristics (shear modulus, torsional rigidity, etc.) concerning CMF. In general, in a wire-like structure, it is difficult to enhance torsional rigidity and strength, compared with tensile ones. Therefore, in this study, we try to build a hierarchical model of CNF by multiplying CMF fibers and to conduct molecular dynamics simulation for torsional deformation, by using a hybrid modeling between all-atoms and united-atoms models. First, shear modulus was estimated for one CMF fibril and it showed a value close to the experimental values. In addition, it is revealed that intermolecular hydrogen bonds (HBs) are dynamically changed and the HB mechanism is likely to work as strong resistance in torsional deformation.

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[P2-65] Bubble dynamics of foam flow around an obstacle

○Antti Puisto, Juha Koivisto, Leevi Viitanen, Mikko J Alava （Aalto University, Department of Applied Physics, Finland）

Foams are one of the rare examples of simple yield stress fluids. Formed of bubbles embedded in liquid they are often studied in the context of jamming [1]. Foam flow is interesting not only because the start-up requires a dynamical unjamming transition (yielding), but also due to novel technological applications related to forming technologies [2].

Here, we study a foam flow through a 2D Hele-Shaw shell with an obstacle, forming a constriction. For this purpose, we use bubble scale dynamics model (the Durian bubble model), which we extend with the appropriate descriptions for the boundary effects coming from the walls and the top and bottom plates. We

observe a negative wake behind the obstacle, analogous to the one observed in gas bubble motion in a viscoelastic medium. There, the medium is succesfully described by an Oldroyd-B model. This suggests that in the present conditions, the foam acts as a typical viscoelastic fluid, rather than the expected elastoviscoplasticity [3]. We compare the simulations data against experiments, foam intruder experiments, where we find a similar flow pattern. We find a reasonable agreement in the flow dynamics and the overshoots between the experimental data and the bubble model. Finally, we identify a viscoelastic timescale, which determines the magnitude of the velocity overshoot.

[1] G. Katgert, B. P. Tighe, M. van Hecke, Soft Matter 9, 9739 (2013).
[2] A. M. Al-Qararah, T. Hjelt, A. Koponen, A. Harlin, J. A. Ketoja, Colloids Surf. A 467, 97 (2015).
[3] S. Bénito, C. -H. Bruneau, T. Colin, C. Gay, F. Molino, Eur. Phys. J. E 25, 225 (2008)

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-66] Shape Deformation and Mechanical Relationship of Ionic Droplet Under An Electric Field

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Nano-sized symmetric double Taylor cone forms a capillary liquid bridge while electric field applied on Ionic liquids (2-dimethyl-3-propylimidazolium- bis(trifluoromethylsulphonyl)imide). This ionic liquid bridge size is around 20 nm. We attempt to understand the critical dimensions and stability criteria for nano-bridge forming mechanism. Therefore, we conduct molecular dynamics simulation under electric field to investigate ionic droplets electrohydrodynamic behavior with different structures and potential functions. Factors that affect liquid bridge size through extensive parameter are studied thoroughly in this work. We also investigate the influence of changing velocity field and shape deformation under different electric field conditions. The mechanical relationship between electric stress, Coulomb electrostatic force and the intermolecular interactions are analyzed. Through this complete studies, surface tension coefficient and ionic liquid viscosity are obtained. Results show that shape deformation and size of liquid bridge are mainly controlled by surface tension coefficient and viscosity.

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[P2-67] Multiscale modeling of surface functionalized graphene/polymer nanocomposites: insight into the effect of covalent grafting

○Jeong-ha Lee[1], Seunghwa Yang[2] （1.Dept. of Energy Engineering, Chung-Ang Univ., Korea, 2.Dept. of Energy Systems Engineering, Chung-Ang Univ., Korea）

Polymer nanocomposites is applied in various industries to improve their mechanical, electrical, thermal properties instead of using pure polymer. In view of improving mechanical properties of polymer nanocomposites, graphene nanosheets is typical reinforcement due to its excellent properties. However, agglomeration of graphene nanosheets in polymer reduces their mechanical and thermal properties. Besides,

weak cohesive energy between graphene and polymer by poor van der waals interaction causes slip condition in their interfacial region. To improve their intrinsic weak interfacial strength and dispersion properties between graphene and polymer nanocomposites, surface treatment of graphene such as covalent grafting or functionalization on graphene nanosheets have been generally used in graphene/polymer nanocomposites.
In this study, multiscale modeling approach for pristine and covalently functionalized graphene included polypropylene nanocomposites is implemented. Representative unit cell consists single-layered graphene and polypropylene matrix is modeled with three-dimensional periodic boundary conditions. Different number of covalent grafting on graphene is considered to investigate effect of grafting density. In molecular dynamics simulations, reactive forcefield for hydrocarbon structure is used to describe carbon-carbon bond breakage in graphene. Through statistical ensemble simulations, thermoelastic behavior of graphene/polypropylene nanocomposites are determined with grafting density differences at single-layered graphene interface. For equivalent continuum modeling to account for covalent grafting, the mean field micromechanics model is supplemented to characterize interfacial and interphase properties of nanocomposites in accordance with number of covalent grafting. In heat of vaporization perspective, correlation of covalent grafting and dispersion inside the polymer matrix is examined.

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[P2-68] Durability analysis on the environmental aging of epoxybased nanocomposite

○Sunyong Kwon[1], Man Young Lee[2], Seunghwa Yang[3] (1.Dept. of Energy Engineering, Chung-Ang Univ., Korea, 2.Agency for Defense Development, Korea, 3.Dept. of Energy Systems Engineering, Chung-Ang Univ., Korea)

Aging is a slow and steady process which occurs by various environmental factors including moisture, uv light, changes in temperature and pressure. Hygroscopic aging of polymer nanocomposite occurs by consistent exposure to moisture in service condition. As bounded water in the material causes microscopic changes in chemical and physical structure of the composite material, it eventually leads to swelling, plasticization, degradation of mechanical and interfacial properties. Thus, to properly examine the long-time process of aging, correlation between aging time-structure-corresponding properties should be developed. Therefore, in this study, multiscale bridging method incorporating atomistic approach of molecular dynamics (MD) simulation and continuum modeling is presented.
To define the relationship between aged structure and corresponding properties, MD simulation is firstly adopted. Different crosslinking ratio of 30% to 70% is established by crosslinking reaction between bisphenol F type epoxy (EPON862®) resin and triethylenetetramine (TETA) curing agent. A single layered defect-free graphene is added as fiber reinforcement in the nanocomposite structure. Also, to observe the hygroelastic behavior of nanocomposite, weight fraction of 0, 2, 4wt% water is included in the nanocomposite unit cell. After isobaric-isothermal (NPT) ensemble simulation, diffusion coefficient of water, coefficient of moisture expansion (CME), elastic modulus and cohesive zone law of epoxy/graphene nanocomposite models are predicted. Based on the results of MD simulation, equilibrium hygroelastic constitutive models incorporating interfacial properties between epoxy and graphene are used to accurately measure the nanoscale effect observed in MD simulations with moisture.

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

[PO-I2] Poster Session 2

Symposium I

Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall

[P2-69] Topological evolution of the microstructures of thin films during grain growth

○Ahu Oencue[1], Thorsten Halle[2], Dana Zoellner[3] (1.Institute of Experimental Physics, Otto-von-Guericke University Magdeburg, Germany, 2.Institute of Materials and Joining Technology, Otto-von-Guericke University Magdeburg, Germany, 3.B CUBE Center for Molecular Bioengineering, TU Dresden, Germany)

[P2-70] Molecular dynamics simulations of phase transformations in nanocrystalline NiTi shape-memory alloys

○Won-Seok Ko (University of Ulsan, 93 Daehak-ro, Nam-gu, Ulsan, 44610, Korea)

[P2-71] An attempt to connect migration of grain boundaries to their atomic structures with help of Molecular Dynamics

Zakaria El Omari, ○Sylvain Queyreau, Charlie Kahloun, Brigitte Bacroix (Universite Paris XIII, Sorbonne Paris Cite, Laboratoire des Sciences des Procedes et des Materiaux, LSPM UPR 3407, France)

[P2-72] Disconnection interaction in Cu grain boundaries

○Christian Brandl (Karlsruhe Institute of Technology, Germany)

[P2-73] Phase-field Approach to Thermo-mechanical Behavior of Through-silicon Vias

Wooju Lee, ○jaekeun yoon, Dongchoul Kim (Sogang Univ., Korea)

[P2-74] Grain-Growth in Nanocrystalline Metals under Ion Irradiation: A Thermal Spike Model

○Djamel Kaoumi[1], Robert Birtcher[2], Arthur Motta[3] (1.North Carolina State University, United States of America, 2.Argonne National Laboratory, United States of America, 3.Penn State University, United States of America)

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-69] Topological evolution of the microstructures of thin films during grain growth

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Historically, metallography has been the two-dimensional characterization of materials microstructures by optical microscopy. Consequential problems have long been known: A two-dimensional section through a three-dimensional object gives us only a very poor idea about size and form of the object. The same holds for the complex grain boundary networks of various kinds of polycrystalline materials. Therefore, many attempts have been made to gain three-dimensional information experimentally. Nevertheless, in simulations and analytical theories thin films are commonly still treated as two-dimensional objects making comparisons with three-dimensional experimental data rather hard.

In the present work, based on experimental measurements, grain growth in metallic thin films is investigated in detail by three-dimensional Monte Carlo Potts model simulations focusing particularly on the transition from bulk-like growth to columnar microstructures. Changes not only in average growth behaviour from a linear increase of the average grain area with annealing time to near-stagnation, but particularly temporal changes in local topology and individual growth kinetics, e.g., in terms of the Lewis-law as well as of the von Neumann-Mullins-law are discussed.

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[P2-70] Molecular dynamics simulations of phase transformations in nanocrystalline NiTi shape-memory alloys

○Won-Seok Ko （University of Ulsan, 93 Daehak-ro, Nam-gu, Ulsan, 44610, Korea）

Molecular dynamics simulations are performed to investigate temperature- and stress-induced phase transformations in nanocrystalline nickel-titanium shape-memory alloys. Our results provide detailed insights into the origins of the experimentally reported characteristics of phase transformations at the nanoscale, such as the decrease of the transformation temperature with grain size and the disappearance of the plateau in the stress-strain response. The relevant atomic scale processes, such as nucleation, growth, and twinning are analyzed and explained. We suggest that a single, unified mechanism--dominated by the contribution of a local transformation strain--explains the characteristics of both temperature- and stress-induced phase transformations in nanocrystalline nickel-titanium.

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[P2-71] An attempt to connect migration of grain boundaries to their atomic structures with help of Molecular Dynamics

Zakaria El Omari, ○Sylvain Queyreau, Charlie Kahloun, Brigitte Bacroix （Universite Paris XIII, Sorbonne Paris Cite, Laboratoire des Sciences des Procedes et des Materiaux, LSPM UPR 3407, France）

Grain Boundary (GB) migration is at the origin of microstructure evolutions in a large variety of crystalline materials. One of the many challenges to fully understand GB motion has to do with the GB vast panel of atomic configurations and existence of several motive forces or impacting parameters. In this context, atomistic simulations have proven to be particularly useful since GB migration can be investigated under well defined conditions, and large scale systematic investigations are now possible (i.g. [1]).
In this work we report a Molecular Dynamics investigation of the migration of a large panel of CSL GB in fcc Ni. In order to construct lesser known GB with mixed tilt+twist or asymmetric character, we orient and constrain the simulation domain to the CSL lattice defined by the two crystal orientations, in a fashion very similar to the approach proposed in [2]. GB motion may be initiated by a synthetic driving force as defined in [3]. As a result, very different temperature behaviour are observed ranging from athermal, to thermally activated and non monotonous thermal behaviour. Different behaviours are sometimes observed for very similar GBs, confirming the important of the GB atomic structure over the macroscopic geometrical parameters describing GB.
In an attempt to rationalise these results we developed an automated post-processing of the atomic configurations into a discrete modelling of GB in terms of intrinsic dislocations and disconnections when present. This analysing tool is applied to a dozen of simple GB and a correlation is made when possible between elementary migration mechanisms -atomic shuffling or disconnection motion- and discrete structure of GB.

[1] DL Olmsted, EA Holm, SM Foiles, Acta Mater. 57, 3704 (2009).
[2] AD Banadaki, S Patala. J. Appl. Cryst. 48, 585 (2015).
[3] K.G.F. Janssens, D. Olmsted, E.A. Holm, S.M. Foiles, S.J. Plimpton, P.M. Derlet, Nat. Mater. 5, 124 (2006).

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-72] Disconnection interaction in Cu grain boundaries

○Christian Brandl （Karlsruhe Institute of Technology, Germany）

Recent molecular dynamics (MD) simulations and transmission electron microscopy indicate that the grain boundary (GB) migration in asymmetric GB plane orientation is mediated by the nucleation and migration of disconnections in the GB plane. The collective motion and reaction of disconnections also initiates the formation of facets as the agglomeration of disconnections into a disconnection arrays.

In MD simulations we address the interaction of disconnection and disconnection dipoles at zero stress in S3 and S7 GBs. The diffusive rearrangement at finite temperate is analyzed in terms of one-dimensional random walks and the drift signatures are used to deduce the interaction strength and the disconnection core interaction. The implications of the disconnection-interaction on the collective migration of asymmetrical GBs is discussed in context of grain coarsening in fcc metals at elevated temperatures and the transition to stress-driven grain coarsening in nanocrystalline metals.

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-73] Phase-field Approach to Thermo-mechanical Behavior of Through-silicon Vias

Wooju Lee, ○jaekeun yoon, Dongchoul Kim （Sogang Univ., Korea）

Three-dimensional stacking of silicon chips via *Through-silicon vias (TSVs)* is an innovative technique for electronic devices due to the drastically shortened electrical path which leads to the faster operation. When TSVs are exposed to high temperature, the higher coefficient of thermal expansion (CTE) of Cu generate the out-of-plane extrusion of Cu from TSV, so-called Cu pumping, which may damage the above lying silicon chip. Furthermore, the thermal expansion is irreversible because the Cu grains are coarsened during the annealing. The comprehensive understanding of Cu pumping mechanism according to the geometry of TSV and annealing conditions is indispensably required to ensure the reliability of electronic devices. A finite element analysis has been used to predict the Cu pumping. However, the finite element method does not incorporate the grain coarsening mechanisms that reduce the elastic energy generated by the thermal expansion. Here, we propose a phase field model that is modified to consider the thermal expansion of Cu polycrystalline during annealing process. The phase field model is the most suitable method to model the evolution of microstructures, since it has benefits for incorporating multiple mechanisms simultaneously. In this study, the significant mechanisms of Cu pumping, including grain boundary migration, thermal expansion, and interfacial characteristics, are considered into the free energy functional of the phase field model

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[P2-74] Grain-Growth in Nanocrystalline Metals under Ion Irradiation: A Thermal Spike Model

○Djamel Kaoumi[1], Robert Birtcher[2], Arthur Motta[3] （1.North Carolina State University, United States of America, 2.Argonne National Laboratory, United States of America, 3.Penn State University, United States of America）

Grain growth was observed in nanocrystalline metallic foils in situ in a transmission electron microscope in a wide range of irradiation doses, temperature (from 20K to 773K) for four different pure metals (Zr, Pt, Cu and Au). The average grain size increased monotonically with ion fluence and similarly to thermal grain growth, the ion-irradiation induced grain growth curves could be best fitted with curves of the type:. With respect to temperature, the experimental results showed the existence of a low-temperature regime (below about 0.15-0.22Tm), where grain growth is independent of the irradiation temperature, and a thermally assisted regime where grain growth is enhanced with increasing irradiation temperature. A model is proposed to describe grain growth under irradiation in the temperature-independent regime, based on the direct impact of the thermal spikes on grain boundaries. In the model, grain-boundary migration occurs by atomic jumps, within the thermal spikes, biased by the local grain-boundary curvature driving. The experimental results will be presented as well as the model proposed to describe grain-growth kinetics in the low-temperature regime (cryogenic temperatures).

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

[PO-N2] Poster Session 2

Symposium N

Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall

[P2-75] **Why the structure-property relationship in metallic glasses should be established beyond short-range order: Insight from potential energy landscape**

○Dan Wei[1,2], Yunjiang Wang[1,2], Lanhong Dai[1,2] （1.University of Chinese Academy of Sciences, China, 2.Institute of Mechanics, Chinese Academy of Sciences, China）

[P2-76] Vacancy segregation analysis near grain boundaries in metallic systems by long-time atomistic simulations

○Shotaro Hara （Dept. of Mechanical Engineering, Chiba Institute of Technology, Japan）

[P2-77] **EXPERIMENTAL AND DENSITY FUNCTIONAL THEORY STUDIES OF PRECIPITATE INTERFACES IN ALUMINIUM ALLOYS, WITH FOCUS ON β" & β**

○Haris Rudianto, Deni Hariadi, Andriansyah Andriansyah （Gunadarma University, Indonesia）

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-75] Why the structure-property relationship in metallic glasses should be established beyond short-range order: Insight from potential energy landscape

○Dan Wei[1,2], Yunjiang Wang[1,2], Lanhong Dai[1,2] （1.University of Chinese Academy of Sciences, China, 2.Institute of Mechanics, Chinese Academy of Sciences, China）

For crystals, structures provide all information needed for predicting material properties. However, what determines non-crystalline solids properties remains elusive for many years. Extensive work has been performed to identify structures playing an important role in glass, but a key question arises that what is the hidden rule of structural feature that can predict properties. Here we calculate an atom’s activation energy (the system’s long-time property) for thermally activated relaxation with the Activation-Relaxation Technique (ART) and correlate the searched local potential energy landscape with several of the successful structural predictors. We find a common nature in the successful structural predictors that spatial correlation of structural information matters a lot once they tend to determine an atom’s properties. There exists a critical correlation length of about sub-nanometer which is corresponding to the second shell of the pair correlation function of glassy structures. We further demonstrate this concept by manipulating the cutoff distance of local structural entropy - one of the successful structural feature - that only if this local structure is defined beyond the short-range order it can predict activation of local atom rearrangement in the model metallic glass. In this way, we question the prevailing approach of materials science aimed at identifying simple structural motifs responsible for metallic glass properties.

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-76] Vacancy segregation analysis near grain boundaries in metallic systems by long-time atomistic simulations

○Shotaro Hara （Dept. of Mechanical Engineering, Chiba Institute of Technology, Japan）

Long-term degradation phenomena in metallic systems under a high temperature, such as creep voiding, are governed by the vacancy diffusion, accumulation and growth processes at an atomistic scale around the material heterogeneities like grain boundaries. However, the basic properties such as the equilibrium vacancy concentrations and the kinetics near grain boundaries are not still understood because a molecular dynamics simulation often suffers from tracking thermally-activated processes due to its limited time scale. In this study, the vacancy segregation behavior at grain boundary has been analyzed using diffusive molecular dynamics simulations, which is a novel approach for exploring the atomic level mass action along the chemical potential gradient at diffusive time scale. The equilibrium vacancy concentrations and the chemical potential distributions at grain boundaries are computed for the different grain boundary character. The correlation between the grain boundary energies and their concentrations have also been considered. Furthermore, the kinetic nature of grain boundary sliding was investigated using this new scheme and the effect of stress on the sliding was discussed.

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[P2-77] EXPERIMENTAL AND DENSITY FUNCTIONAL THEORY STUDIES OF PRECIPITATE INTERFACES IN ALUMINIUM ALLOYS, WITH FOCUS ON β" &β

○Haris Rudianto, Deni Hariadi, Andriansyah Andriansyah （Gunadarma University, Indonesia）

Aluminium is the third most abundant element in the Earth’ s crust, after oxygen and silicon. Before the start of the last century, aluminium started to come into wide use as a structural material. Since then, it has reached the position of being the second most used metal in the world, with only steel beating it to the throne. One important structural limitation of aluminium is their fatigue strength. Precipitation hardening is utilized to strengthen a wide variety of alloy systems especially for Aluminum Alloys. An example is the class of commercially important Al-Mg-Si based alloys which are strengthened by a number of metastable precipitate phases, where the needle-shaped β’ ’ -Mg5Si6 precipitates are often the main contributor to hardening. Beginning with the supersaturated solid solution (SSS), the generic precipitation sequence in Al-Mg-Si alloys is generally believed to be :

SSS -> Mg/Si clusters -> Guinier-Preston zones -> β’ ’ -> β’ ->β

In practice, the sequence can be even more complex and a number of other metastable phases, depending on alloy composition and the heat treatment time and temperature. In this research, interface energy was calculated by Quantum Espresso with super cells designed on VESTA. For comparison, in this research, experimental was also carried out to determine effects of strengthening precipitates on mechanical properties. T6 heat treatment was done starting from solid solution treatment, quenching and finished my artificial aging. Hardness was done to determine mechanical properties and SEM-EDS and XRD were done to characterize the materials.

Keywords; Aluminum Alloys, DFT, Strengthening Precipitates, Heat Treatment

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

[PO-O2] Poster Session 2

Symposium O

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[P2-78] Adsorption of Volatile Organic Compounds (VOCs) on Silicene by Density Functional Theory Calculations

○Thi Viet Bac Phung[1], Trong Lam Pham[1], Van An Dinh[1,2] (1.Nanotechnology Program, Vietnam Japan University - Vietnam National University, Viet Nam, 2.Center for Atomic and Molecular Technologies, Graduate School of Engineering, Osaka University, Japan)

[P2-79] Atomistic insights into defect formation mechanism in single crystal SiC based on molecular dynamics simulation

○Kenji Nishimura[1], Koji Miyake[1], Ken-ichi Saitoh[2] (1.AIST, Japan, 2.Kansai Univ., Japan)

[P2-80] Potential cathode material Na_xVOPO_4 for rechargeable Sodium - ion batteries: DFT investigation

○Duc Huu Luong[1], An Van Dinh[1,2], Yoshitada Morikawa[3], Yoji Shibutani[2,1] (1.Nano Technology Program, Vietnam Japan University, Viet Nam, 2.Center for Atomic and Molecular Technology, Graduate School of Engineering, Osaka University, Japan, 3.Department of Precision Science and Technology, Graduate School of Engineering, Osaka University, Japan)

[P2-81] Two-dimensional Na_xSiS as a promising anode material for rechargeable Sodium-based batteries: Ab initio material design.

Thi Dung Pham[1], ○Van An Dinh[1,2], Kazunori Sato[3], Yoji Shibutani[1,2] (1.Nanotechnology Program, Vietnam Japan University, Viet Nam, 2.Center for Atomic and Molecular Technology, Graduate School of Engineering, Osaka University, Japan, 3.Division of Materials and Manufacturing Science, Graduate School of Engineering, Osaka University, Japan)

[P2-82] Modelling and analysis of SiO2 interfaces of non-firing solids

○Tomohiro Sato[1], Ken-ichi Saitoh[1], Masayoshi Fuji[2], Chika Yamashita Takai[2], Hadi Razavi[2], Masanori Takuma[1], Yoshimasa Takahashi[1] (1.Dept. of Mechanical Engineering, Kansai Univ., Japan, 2.Advanced Ceramics Reserch Center, Nagoya Institute of Technology, Japan)

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Cancer can be regarded as a rising threat towards modern societies. Detecting cancer at an early stage significantly improves the curability of the disease [1]; unfortunately, currently available methods for early diagnosis of cancer are scarce and inefficient. In fact, the concentration of VOCs in cancer patients in the breath is different from that in normal people [2]. Therefore, development of new sensors that can detect VOCs at low concentrations, corresponding to the early stage of cancer, is desirable. 2D materials are expected as attractive materials for these sensors due to their large surface area to volume ratio. In this work, we investigated the adsorption mechanism of some small-to-medium VOCs on the surface of silicene by the quantum simulation method. The images of the potential energy surfaces for different positions of the adsorbate on the silicene surface were explored by *Computational DFT-based Nanoscope* [3] for determination of the most stable configurations and diffusion possibilities. The adsorption energy profiles were calculated by three approximations of van der Waals interation: revPBE-vdW, optPBE-vdW, and DFT-D2. It is found that the adsorption energies of the VOCs in question vary in the range of 0.6-1.0 eV, which indicates that silicene is considerably sensitive with these VOCs. The charge transfer between the substrate and VOCs and the effect of an electric field on the adsorption configurations, energies, and band structures were also addressed.

References

[1] M. Hakim, Y. Y. Broza, O. Barash, N. Peled, M. Phillips, A. Amann, H. Haick Chem. Rev. 2012, 112, 11, 5949-5966.

[2] E. M. Gaspar, A. F. Lucena, J. D. da Costa, and H. C. das Neves. Journal of Chromatography A 2009, 1216, 14, 2749-2756.

[3] Developed by V. A. Dinh, Vietnam Japan University.

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[P2-79] Atomistic insights into defect formation mechanism in single crystal SiC based on molecular dynamics simulation

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Silicon carbide (SiC) is a promising next-generation semiconductor for high-power, high-temperature, and high-voltage devices because of its wide bandgap, high breakdown field, and high thermal conductivity. However, the efficient and smooth machining of SiC is technically difficult due to its intrinsic nature of high hardness and brittleness as well as strong anisotropy. It is still a great challenge to understand machining

processes in which damage layers caused by stress-induced phenomena such as plastic deformation and fracture are introduced beneath grinding surface. In this study, we perform one million-atom molecular dynamics simulations of nanoindentation tests on cubic SiC single crystal using a nano-sized spherical indenter to clarify the plastic deformation mechanism and defect formation criteria in SiC. An analytical bond-order Tersoff-type interatomic potential for SiC developed by Erhart *et al.*, which reproduces the elastic, defect, and thermal properties, is adopted. The load-displacement curves of the nanoindentation tests obtained by our simulations demonstrate transition from elastic deformation to plastic deformation so-called “pop-in” event. Our results also predict the decrease of the CRSS (critical resolved shear stress) of single crystal SiC with increasing temperature from 300 K to 2000 K for both (001) and (111) indent, which means less energy is required to activate slip systems at higher temperature. These results are similar to the feature of ductile materials such as metals, although SiC is known as brittle materials. In addition, we identify crystalline slips and defects generated beneath the indenter after the pop-in event by means of a novel type of structural analysis method using sub-lattice of Si or C which is based on common neighbor analysis. The structural analysis we propose reveals that dislocation loops in {111} planes which correspond to the slip plane of SiC are developed with increasing indenter depth. Furthermore, we find that for lower temperature perfect dislocations are dominantly formed, while for higher temperature partial dislocations together with stacking faults are superior to the perfect dislocations, resulting in the dramatic increase of the partial dislocations.

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Using the density functional calculations, we investigated the crystal and electronic structures, electrochemical properties and ion diffusion mechanism of Sodium - polaron complex in Sodium Vanadyl phosphate $NaVPO_5$. A calculated voltage of 3.77 V (GGA+U) and 3.58 V (HSE06) corresponding to a redox reaction of potential couple $V^{4+/}V^{5+}$ were in good agreement with experimental result [1]. The diffusion mechanism of charge carriers was explored using GGA+U. In the charge process, a Sodium ion is removed from the crystal structure so that the Sodium vacancy appears and a positive small polaron forms at one the two first nearest VO_6 octahedron. The diffusion of Na+ ion which is accompanied by a positive small polaron is described by three elementary diffusion processes, including single, crossing and parallel diffusions [2]. With the smallest activation energy of 395 meV, the pathway of Sodium diffusion along the [010] direction is the most favorable diffusion pathway and it is significantly higher than previous calculation which did not mention the small polaron formation. In the discharge process, Sodium ion is intercalated to structure of β-$VOPO_4$, then the negative small polaron forms at one of the nearest neighbour VO_6 octahedron. In addition, the elementary diffusion process of sodium ion is more favorable in the [010] direction. However, because of about 10% smaller volume, the diffusion activation energy (627 meV) is significantly higher than those required in the charge process. Compared with the other materials, it is obviously that this material would perform as well as some common materials for cathode such as Olivine.

[1] G. He, A. Huq, W. H. Kan, and A. Manthiramm, Chem. Mater. 2016, **28**, 1503−1512
[2] V. A. Dinh *et al.* App. Phys. Express, 2012, **5**, 045801

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The rapidly rising demand of energy storage system for electronic devices presents an imperative need to develop sodium-ion batteries with high energy density, high conductivity, and low barrier energy. In this work, we present the density functional study on properties of the two-dimensional (2D) Na_xSiS as a promising anode material for rechargeable sodium ion batteries (SIBs). Energetically stable structures of Na-adsorbed *Silicene sulfide* Na_xSiS were explored. It is found that *silicene sulfide* has an adsorption energy to sodium atom about of -0.4 eV, which is large enough to ensure a good stability for sodium inserting into SiS during sodiate process. The electronic structure and capacity of Na_xSiS were calculated. The electronic structure of pristine SiS monolayer and Na adsorbed layer shows the distinction of a semiconductor material. The fully sodiated phase of SiS is $Na_{0.5}SiS$ corresponding to a highest theoretical capacity of 187.2 mAh/g per one side layer. The diffusion mechanism of Na ions was also investigated by using NEB method. Two possible elementary processes are explored: one is along *a*-and the other is along *b*-direction. Most importantly, *Silicene sulfide* shows a good sodium mobility with an energy barrier along two dimension is only 183 meV, which is much smaller than that in Li_xSiS (430meV), 2D TiS_2 (220meV), and 2D MoS_2 (280-680 meV). Our investigations also reveal that SiS exhibits the better electrochemical performance as an anode in the SIBs than in the LIBs. All these characteristics suggest that 2D SiS can expected to be a promising anode material for sodium batteries.

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Generally, ceramics are manufactured by using sintering process. However, this process needs high temperature and loss a lot of fuels. CO2 emission in the process is also need to improve. So, non-fire process is focused to make ceramics products.

For non-fire process, surfaces of SiO2 particles are polished and put hydrogen on the activate surfaces. These SiO2 particles are compressed and put into water that is non-fire process of ceramics. In this study, SiO2 interface models were constructed for molecular dynamics simulation. Interactions between SiO2 and H2O were presented by using ReaxFF potential. At first, SiO2 interfaces model without OH as end groups were conducted. By put water molecules between SiO2 interfaces, some atoms were changed their combinations. Some of them achieved lower potential energy through the simulation. It is seemed that a part

of non-fire process was reproduced. For example, hydrogen atom connected the oxygen atom of SiO2. However, connection of SiO2 did not observed over SiO2 interfaces.

Then, SiO2 interfaces model with OH as end groups were conducted. At relaxation of the models, SiOH exists in the model. After relaxation, water molecules were put into the surfaces. However, changes of connection between SiO2 and H2O or SiO2 interfaces did not observed. Energetic or structural stability of SiOH surfaces were seemed to effect the result.
Distance of interfaces, conducting compressed SiO2 including OH as end groups models might be key to improve the ability of reaction between atoms.