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-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）

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

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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.

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[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.

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[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)

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

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(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[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.

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[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）

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.

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[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）

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.

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[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.

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(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[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）

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.

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(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[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.

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[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

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）

[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.

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[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.

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(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[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.

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[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.

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[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.

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[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).

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[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.

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[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.
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(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.

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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.

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(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.

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[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.

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(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[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.

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(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.

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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.

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[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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(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.

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(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

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）

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.

(Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall)

[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.

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[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.

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[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.

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[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.

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[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

Wed. Oct 31, 2018 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)

(Wed. Oct 31, 2018 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)

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.

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[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)

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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[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)

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.

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[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)

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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[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)

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.