Mon. Oct 29, 2018

Poster Hall

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

[PO-A1] Poster Session 1

5:45 PM - 8:00 PM Poster Hall

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

[PO-C1] Poster Session 1

5:45 PM - 8:00 PM Poster Hall

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

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

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

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

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

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

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

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

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

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

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

unpinning dislocations with law of approach in residual magnetization

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

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

○Hideki MORI （College of Industrial Technology, Japan）

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

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

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

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

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

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

Poster Session | E. Deformation and Fracture Mechanism of Materials

[PO-E1] Poster Session 1

5:45 PM - 8:00 PM Poster Hall

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

[PO-F1] Poster Session 1

5:45 PM - 8:00 PM Poster Hall

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

○Duancheng Ma （Leichtmetallkompetenzzentrum Ranshofen GmbH, Austria）

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

[P1-52] Structural and dynamical properties of star block-copolymers in shear flow.

○Diego Felipe Jaramillo - Cano[1], Manuel Camargo[2], Christos N. Likos[1] (1.Faculty of Physics, University of Vienna, Austria, 2.CICBA, Universidad Antonio Nariño - Campus Farallones, Colombia)

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

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

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

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

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

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

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

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

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

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

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

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

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

○Kunok Chang (Kyung Hee Univ., Korea)

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

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

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

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

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

○Pan Li (Hebei Normal Univ., China)

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

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

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

○Ying-Jun Gao (Guangxi University, China)

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

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

Poster Session | J. Multiscale Modeling of Heterogeneous Layered Media

[PO-J1] Poster Session 1

5:45 PM - 8:00 PM Poster Hall

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

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

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

[PO-L1] Poster Session 1

5:45 PM - 8:00 PM Poster Hall

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

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

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

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

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

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

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

[PO-M1] Poster Session 1

5:45 PM - 8:00 PM Poster Hall

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

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

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

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

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

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

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

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

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

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

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

[PO-O1] Poster Session 1

5:45 PM - 8:00 PM Poster Hall

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

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

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

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

[P1-76] Atomistic modeling of polymer friction

○Robin Sam Vacher （SINTEF-NTNU, Norway）

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

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

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

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

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

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

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

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

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

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

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

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

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

[PO-A1] Poster Session 1

Symposium A

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

[PO-C1] Poster Session 1

Symposium C

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

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

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

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

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

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

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

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

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

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

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

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

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

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

○Hideki MORI （College of Industrial Technology, Japan）

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Acknowledgement

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

○Hideki MORI （College of Industrial Technology, Japan）

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Poster Session | E. Deformation and Fracture Mechanism of Materials

[PO-E1] Poster Session 1

Symposium E

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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[PO-F1] Poster Session 1

Symposium F

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

○Duancheng Ma （Leichtmetallkompetenzzentrum Ranshofen GmbH, Austria）

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

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

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

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

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

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

Germany）

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

in the γ'-Ni_3Al phase.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

○Duancheng Ma （Leichtmetallkompetenzzentrum Ranshofen GmbH, Austria）

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

[PO-H1] Poster Session 1

Symposium H

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

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

[P1-52] Structural and dynamical properties of star block-copolymers in shear flow.

○Diego Felipe Jaramillo - Cano[1], Manuel Camargo[2], Christos N. Likos[1] （1.Faculty of Physics, University of Vienna, Austria, 2.CICBA, Universidad Antonio Nariño - Campus Farallones, Colombia）

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

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

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

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

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

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

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

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

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

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

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

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

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

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[P1-52] Structural and dynamical properties of star block-copolymers in shear flow.

○Diego Felipe Jaramillo - Cano[1], Manuel Camargo[2], Christos N. Likos[1] (1.Faculty of Physics, University of Vienna, Austria, 2.CICBA, Universidad Antonio Nariño - Campus Farallones, Colombia)

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

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

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

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

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

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

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

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

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

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

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

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

This work was supported by the National Research Foundation of Korea (NRF) grants funded by the Korea government (Ministry of Science and ICT) (NRF-2016R1C1B2011098, NRF-2017M3D1A1039422, and NRF-2014M3A6B3063711).

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

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

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

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

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

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

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

ABSTRACT

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

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

[PO-I1] Poster Session 1

Symposium I

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

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

○Kunok Chang （Kyung Hee Univ., Korea）

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

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

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

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

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

○Pan Li （Hebei Normal Univ., China）

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

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

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

○Ying-Jun Gao （Guangxi University, China）

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

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

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

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

○Kunok Chang （Kyung Hee Univ., Korea）

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

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

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

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

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

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

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

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

○Pan Li （Hebei Normal Univ., China）

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

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

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

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

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

○Ying-Jun Gao （Guangxi University, China）

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

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

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

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

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

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

Poster Session | J. Multiscale Modeling of Heterogeneous Layered Media

[PO-J1] Poster Session 1

Symposium J

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

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

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

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

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

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

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

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

[PO-L1] Poster Session 1

Symposium L

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

[PO-M1] Poster Session 1

Symposium M

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

References

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

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

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

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

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

[PO-O1] Poster Session 1

Symposium O

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

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

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

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

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

[P1-76] Atomistic modeling of polymer friction

○Robin Sam Vacher （SINTEF-NTNU, Norway）

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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[P1-76] Atomistic modeling of polymer friction

○Robin Sam Vacher （SINTEF-NTNU, Norway）

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

Keywords : molecular dynamic, polymers, friction and wear

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

This study describes dynamics of viscosity index improver (VII) in bulk lubricants under shear flow. Small amount of polymer named VII is added in basis oil to control viscosity index (VI) which is a parameter to express temperature dependence of viscosity. Controlling VI is one of the commonly used methods to improve the fuel consumption of motor vehicles. Here we simulate the dynamics of polymer under shear flow in Bulk Solution. Polymer segment is modeled as sphere Brownian particle. The motion of the particle is tracked by the Langevin equation, whereas the Navier-Stokes equation governing the behavior of the base oil is analyzed by using the lattice Boltzmann method. The two equations are coupled through the friction between the particle and the fluid. The friction force is in proportion to the velocity of a particle relative to the host fluid, which is evaluated locally based on the velocity difference at the position of the point particle. The friction force acting on a particle is estimated by fitting the analytical solution or the flow around a

Stokes-let to the flow field obtained numerically. The reaction force acts on the position of the particle, which realizes two-way coupling between the particle and fluid motions. The lattice Boltzmann method is employed for the flow simulation, which is compatible with massive parallel computing, and is easy to apply various types of boundary conditions. In order to simulate the system, the computational domain has three-dimensions and Periodic boundary condition. External forces are introduced to form simple shear flow. The dynamics of polymer in shear flow is examined by using two computational methods.

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

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

Chemical mechanical polishing (CMP) is widely applied in the semiconductor industry to achieve ultra-high precision manufacturing of surfaces (such as Si and Cu), however, its mechanisms remain elusive because of interaction between chemical effects (such as the chemical reactions with the existence of H_2O_2 and glycine) and mechanical effects (such as the tribology process). By using molecular dynamics simulations based on the ReaxFF reactive force field, we have explored the CMP mechanisms at the atomic level and have revealed the importance of mechanochemistry induced atomic wear during the CMP processes.

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

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

Reducing the coefficient of boundary friction on steel surfaces is one of key technologies to improve the efficiency of machines such as automotive engines. It has been shown that the boundary friction on nanostructured steel surfaces in the sliding test using particular lubricant is smaller than the friction of normal steel surfaces [1]. This difference between the nanostructured and a normal surfaces lies in the density of the grain boundary as a surface defect. The surface defect can attract lubricant molecules and enhance lubricating film formation on metal surfaces. This can be one of the mechanism that induces the friction reduction on the nanosructured steel surface. In this work, using first principles calculations, the adsorptivity of a lubricant molecule, a fatty acid, on iron surfaces has been studied.The chemical adsorption of fatty acids is expected to be enhanced at the site near the crystal grain boundary which may have high chemical activity. Adsorption energy calculations were preformed for acetic acids as the simplest fatty acids. Adsorbability of a Fe (110) surface with symmetrical tilt Σ3 (111)grain boundarywas compared to clean Fe(100), (110) and (111) surfaces. As a result, we found that the molecule can adsorb on the particular site on grain boundary more strongly than that on Fe surfaces without grain boundary. [1]

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