

Poster session 1

Monday 29 October(17:45~20:00)

Symposium A

- P1-01 The Coadsorption Effect of Cl⁻ and H₂O on the Various Defect Al₂O₃ Film Surface**
Chuan-Hui Zhang, University of Science and Technology Beijing, China
- P1-02 Incorporation of double cross-slip in continuum dislocation dynamics**
Xingjian Zhou, 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, 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, Graduate School of Engineering, Osaka 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, Guilin University of Electronic Technology, China
- P1-07 First-principles Study on Electronic Properties of Hybrid MABX₃ perovskites (MA= CH₃NH₃⁺; B= Pb, Sn, Ge; X= I, Br, Cl)**
Narasak Pandech, School of Physics and NANOTEC-SUT Center of Excellence on Advanced Functional Nanomaterials, Suranaree University of Technology, Thailand

Symposium C

- P1-08 Pressure effects on dislocation core structures in Mg₂SiO₄ olivine: insights from atomic-scale modeling**
Philippe Carrez, 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, Magnesium Research Center/POIE, Kumamoto Univ., Japan
- P1-10 Atomistic modeling of thermally activated plasticity in UO₂**
Jean-Paul Crocombette, CEA Saclay, SRMP, France
- P1-11 Dislocation transmission behaviors of bi-crystal BCC Tantalum with high and low angle symmetric tilt grain boundaries: Multiscale simulation study**
Moon Sunil, Dept. of Mechanical Engineering, Yonsei Univ., Korea
- P1-12 Ab Initio Dislocation Core Calculations using a Cluster Model**
Jonas Frafjord, Dept. of Physics, 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, 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**
Dan Mordehai, Mechanical Engineering, Technion - Israel Institute of Technology, Haifa, Israel, Israel
- P1-18 Machine learning interatomic potentials for molecular dynamics simulations of dislocations**
Eyal Oren, Dept. of Materials Engineering, Ben-Gurion University of the Negev, Israel
- P1-19 First-principles Calculations of Deformation Twins in Hexagonal Titanium Alloys**
Daisuke Matsunaka, Dept. of Mechanical Engineering, Shinshu Univ., Japan
- P1-20 The effect of dislocation character on dislocation line tension in bcc tungsten and its impact on kink-pair enthalpy**
David Cereceda, Dept. of Mechanical Engineering, Villanova University, United States of America

Symposium E (P1-21 – P1-32)

Symposium F

- 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, Research Centre REZ, Czech Republic
- P1-34 Phase-field model for microstructure change in L10 type ordering with lattice distortion**
Ryuichiro Oguma, Fukuoka Univ., Japan
- P1-35 Delamination cracks in wire-drawn fully pearlitic steels**
Masaki Tanaka, Kyushu Univ., Japan
- 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 α -iron and its decohesion effect in martensitic steel**
Wen-Tong Geng, Department of Mechanical Science and Bioengineering, Osaka University, Japan

- P1-38 Size Scale Effect on Energy Absorption Property of Aluminum Foam**
Zengyou Liang, North University of China, China
- P1-39 Development of charge-transfer type interatomic potential for SiC oxidation**
So Takamoto, The Univ. of Tokyo, 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, Kyoto Institute of Technology, Japan
- P1-42 Simulation of Extrusion Process of TiAl alloy prepared by Triple VAR**
Fan Gao, AECC BEIJING INSTITUTE OF AERONAUTICAL MATERIALS, China
- P1-43 Experimental-Computational Analysis of Primary Static Recrystallization in DC04 Steel**
Martin Diehl, Max-Planck-Institut fuer Eisenforschung GmbH, Germany
- P1-44 Combining 4D experiments and phase-field modeling to determine reduced grain boundary mobilities**
Jin Zhang, Northwestern University, United States of America
- P1-45 Fiber-intersectant microstructure of fish scale and biomimetic research**
Bin Chen, College of Aerospace Engineering, Chongqing University, China
- P1-46 Microstructures of turtle shell and biomimetic fabrication**
Bin Chen, College of Aerospace Engineering, Chongqing University, China
- P1-47 Phase-field Simulation of Solidification Process in Welding Pool of Fe-C Binary Alloy**
Lan Zhan, Jiamusi Univ., China
- P1-48 Phase field simulation of the phase separation in the TiC-ZrC-WC system**
Zelin Luo, State Key Lab of Powder Metallurgy, Central South University, China
- P1-49 Switching of coordinate transformations of a repetitive bar-and-joint framework under uniaxial compression**
Hiro Tanaka, Dept. of Mechanical Engineering, Osaka Univ., Japan
- P1-50 Understanding the effect of Residual Stresses in 3D Printed Metals**
Alankar Alankar, IIT Bombay, India

Symposium H

- P1-51 Multi-scale modeling of DNA-dendrimers in electrolyte solutions**
Natasa Adzic, Faculty of Physics, University of Vienna, Austria
- P1-52 Structural and dynamical properties of star block-copolymers in shear flow**
Diego Felipe Jaramillo - Cano, Faculty of Physics, University of Vienna, Austria
- P1-53 Multiscale simulation of polymeric solids for fracture processes**
Takahiro Murashima, Dept. of Physics, Tohoku Univ., Japan
- P1-54 Quantification and validation of the mechanical properties of DNA nicks**
Jae Young Lee, 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, Dept. of Mechanical and Aerospace Engineering, Seoul National Univ., Korea
- P1-56 FTMP-based Modeling and Simulations of Glassy Polymers.**
Soushi Miyamoto, 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

Symposium I (P1-58 – P1-64)

Symposium J

- P1-65 Multiscale Model for Interlayer Defects in Heterogeneous Bilayer Material**
Shuyang Dai, Wuhan University, China

Symposium L

- P1-66 Molecular dynamics study on temperature and loading rate dependence of nano-indentation pop-in load**
Yuji Sato, Department of Mechanical Science and Bioengineering, Osaka University, Japan
- P1-67 Geometry of curved surface and energetics of in graphene with defects**
Ako Kihara, Dept. of Mechanical Engineering, Univ. of Fukui, 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

Symposium M

- P1-69 FORMATION OF PHYSICAL GELS BY ARRESTED SPINODAL DECOMPOSITION IN CHARGED COLLOIDS**
Jose Manuel Olais-Govea, Instituto Tecnológico y de Estudios Superiores de Monterrey, Mexico
- P1-70 How to improve the ductility of CuZr BMGs based on cyclic pre-straining: MD simulations and mechanical testing**
Jonathan Amodeo, MATEIS, Univ. Lyon 1, France
- P1-71 Modeling plastic deformation of amorphous solids from atomic scale mechanisms**
Francesca Boioli, LEM, CNRS-ONERA, Chatillon, France
- P1-72 Thermally Activated Creep and Constant Shear Rate Deformation in Amorphous Materials**
Samy Merabia, CNRS and Université Lyon 1, France
- P1-73 Numerical analysis of shrinkage process based on the experimental data**
Barbara Kucharczykova, Brno University of Technology, Faculty of Civil Engineering, Institute of Building Testing, Czech Republic

Symposium O

- P1-74 Designing Lubricant Additives for Titanium Carbide Surface: First-principles and Molecular Dynamics Investigations**
Tasuku Onodera, Research & Development Group, Hitachi, Ltd., Japan
- P1-75 Crystal Growth Molecular Dynamics Simulation of alpha-Al₂O₃ Cutting Tools for Realizing Their Best Tribological Properties**
Shandan Bai, KYOCERA Cop., 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, Department of Physics, Stockholm University, Sweden
- P1-78 Analysis of Friction Characteristics of Steel Powders using Parallelized Discrete Element Method**
Naoki Yashiro, Graduate School of Simulation Studies, University of Hyogo, Japan
- P1-79 Molecular Simulation of adsorption process of anti-corrosion additives**
Kohei Nishikawa, University of Hyogo, Japan
- P1-80 Dynamics of Polymer Under Shear in Confinement Geometry**
Taiki Kawate, Univ. of Hyogo, Japan
- P1-81 Dynamics of a Polymer in Bulk Solution under Shear Flow**
Soma Usui, Univ. of Hyogo, Japan
- P1-82 Mechanochemistry induced atomic wear in chemical mechanical polishing processes**
Jialin Wen, Dept. of Mechanical Engineering, Tsinghua Univ., China
- P1-83 Adsorption property of a fatty acid on iron surface with grain boundary**
Yuki Uchiyama, Toyota Technological Institute, Japan

Poster session 2

Wednesday 31 October (17:45~20:00)

Symposium A

- P2-01 Multiscale model of solid state amorphization during processing of pharmaceutical materials**
Alejandro Strachan, Purdue University, United States of America
- P2-02 FTMP-based Modeling and Simulations of HCP Mg Single Crystal**
Takahiro Kitano, Dept. of Mechanical Engineering, Kobe Univ., Japan
- P2-03 Nonlinear elasticity on Riemannian manifold and its application to general surface development**
Yuto Horikawa, Dept. of Mechanical Engineering, Osaka Univ., Japan
- P2-04 The challenge of achieving quantitative phase field models for microstructure evolution in irradiated solids - the case of voids**
Anter El-Azab, Purdue University, United States of America
- P2-05 A Molecular-Dynamics Study of Surface Tension: From Alloy Droplets to Bubbles in Molten Alloy**
Xiangming Ma, East China Normal University, China

Symposium B

- P2-06 Effects of rhenium on the mechanical behavior of irradiated tungsten: a molecular dynamics study using neural-network potential**
Ryo Kobayashi, Nagoya Institute of Technology (NITech), Japan
- P2-07 Diffusion behavior and temperature dependence of hydrogen in tungsten and molybdenum under isotropic strain state**
QuanFu Han, Beihang University, China
- P2-08 Diffusion of Point Defects on Tungsten Surface**
Shuo Jin, School of Physics and Nuclear Energy Engineering, Beihang University, China
- P2-09 Influence of anisotropic strain and temperature on hydrogen dissolution in tungsten**
Ying Zhang, Beihang University, China
- P2-10 Screw dislocation-interstitial solute coevolution in W-O alloys using atomistically-informed kinetic Monte Carlo simulations**
Yue Zhao, Dept. of Materials Science and Engineering, University of California, Los Angeles, United States of America
- P2-11 Kinetic Monte-Carlo Simulations of Radiation Damage in W(Re,Os) Alloys**
Matthew James Lloyd, Department of Materials, University of Oxford, UK
- P2-12 Defect production in cascade overlap with defect clusters in iron and tungsten**
Jesper Byggmatar, Department of Physics, University of Helsinki, Finland

- P2-13 Dynamics of Magnetism in Neutron Irradiated Iron-Chromium Steels**
Jacob B. J. Chapman, Culham Centre for Fusion Energy (CCFE), UK
- P2-14 Atomistic insights into the grain boundaries interaction with radiation-induced point defects in bcc Fe-Cr alloys**
Marcin Roland Zemla, Faculty of Materials Science and Engineering, Warsaw University of Technology, Woloska 141, 02-507 Warsaw, Poland
- P2-15 Production and Process of Cascade Development in Irradiated Pure α -Zr from Molecular Dynamics Simulations**
Rongjian Pan, The First Sub-Institute, Nuclear Power Institute of China, China
- P2-16 Microstructure evolution of cascade annealing in irradiated pure α -Zr from molecular dynamics simulations**
Bang Wen, The First Sub-Institute, Nuclear Power Institute of China, China
- P2-17 Linking Polycrystal and Reduced Order models for efficient simulation of irradiation creep and growth of Zr cladding**
Carlos Tome, Materials Science Division, Los Alamos National Laboratory, United States of America

Symposium C

- P2-18 Prediction of Biaxial Tensile Deformation Behavior of Aluminum Alloy Sheets using Crystal Plasticity Finite Element Method and Machine Learning**
Kota Koenuma, Tokyo University of Agriculture and Technology, Japan
- P2-19 MobiDiC: A 3-D Dislocation Dynamics Simulation**
Ronan Madec, CEA, DAM, DIF, France
- P2-20 Temperature dependence of fatigue crack growth in Ti-6Al-4V**
Bhargavi Rani Anne, Dept. of Materials Science and Engineering, Kyushu University, Japan
- P2-21 Parametric model of discrete dislocation dynamics based on mathematical theory of moving curves**
Miroslav Kolar, Czech Technical University in Prague, Czech Republic
- P2-22 On Visualization of Multiscale Information Transfer/Exchange Processes via FTMP-based Duality Diagram Representation Scheme**
Takuya Takagi, Dept. of Mechanical Engineering, Kobe Univ., Japan
- P2-23 Rotational Field Evolutions based on Field Theory of Multiscale Plasticity (FTMP)**
Tadashi Hasebe, Kobe Univ., Japan
- P2-24 A 2D MESOSCALE STUDY OF DISLOCATIONS, CRACKS AND MARTENSITIC PHASE TRANSFORMATIONS**
Rachel Derby, TU Bergakademie Freiberg, Germany
- P2-25 Effects of Stress Distribution on the Plastic Deformation of Metallic Glasses under Different Geometries**
Chih-Jen Yeh, National Cheng Kung University(Taiwan), 2.Chung Yuan Christian University, Taiwan

Symposium D

- P2-26 Generalized nano-thermodynamic model for predicting size-dependent surface segregation in multi-metal alloy nanoparticles from smaller particles**
Abhijit Chatterjee, Dept. of Chemical Engg., Indian Institute of Technology Bombay, India
- P2-27 Development of thermodynamic database of Nd-Fe-B-based permanent magnet alloys**
Jiang Wang, School of Material Science and Engineering, Guilin University of Electronic Technology, China
- P2-28 Design of proteins and biopolymers: role of directional interactions and of water.**
Valentino Bianco, University of Vienna, Austria
- P2-29 Aquatic pollutant removal by adsorption in zeolite structures: An experimental and molecular simulation study**
Mate Erdos, Process & Energy Department, Faculty of Mechanical, Maritime and Materials Engineering, Delft University of Technology, Netherlands
- P2-30 Optimizing elastic moduli of the silicate glasses through high-throughput atomistic modeling and machine learning techniques**
Liang Qi, Dept. of Materials Science and Engineering, University of Michigan, United States of America
- P2-31 High pressure phase transition and structural stability of transition metal compounds**
Fanyan Meng, Dept. of Physics, University of Science and Technology Beijing, China
- P2-32 Development of artificial neural network model for prediction of electronic density of states in atomistic systems**
Atsushi Kubo, Institute of Industrial Science, the University of Tokyo, Japan
- P2-33 Development of First-principles Platform Technology for Energy Research**
Kanghoon Yim, R&D Platform Center, Korea Institute of Energy Research, Korea

Symposium E (P2-34 – P2-41)

Symposium F

- P2-42 Impact of local symmetry breaking on the physical properties of tetrahedral liquids**
Rui Shi, University of Tokyo, Japan
- P2-43 Mechanics of Cilia Beating – A Relationship Between Metachronal Wavelength and Fluid Flow Rate**
Jon Hall, The University of Sheffield, UK
- P2-44 Characterization of $K_xNa_{1-x}NbO_3$ powders and ceramics prepared by hydrothermal synthesis**
Jing Yang, Dept. of Materials Science and Engineering, Xi An Univ. of Science and Technology, China
- P2-45 Numerical and experimental investigation of liquid metal dealloying of Cu-Ni alloy in liquid silver.**
Pierre-Antoine Geslin, INSA Lyon/CNRS, France
- P2-46 Application of DLVO theory to predict dispersion stability of ZrO₂ submicron particles in electrolyte solutions**
Ming-Hong Chiueh, Industrial Technology Research Institute, Taiwan

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

Shinji Sakane, Kyoto Institute of Technology, Japan

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

Hiroki Sakakima, The Univ. of Tokyo, Japan

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

Vahidullah Tac, Middle East Technical University, Turkey

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

Shih Kuang Lee, National Chiao Tung University, Taiwan

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

Xianqi Xu, East China Normal University, China

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

Wenliang Lu, EAST CHINA NORMAL UNIVERSITY, China

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

Byung-Hyun Kim, R&D Platform Center, Korea Institute of Energy Research, Korea

Symposium G

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

Yuta Amano, Dept. of Mechanical Engineering, Kobe Univ., Japan

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

Se-Yun Kim, Dept. of Civil and Environmental Engineering, Yonsei Univ., Korea

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

Ji-Su Kim, Yonsei Univ., Korea

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

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

Symposium H

P2-58 A Tetris model showing a universal enhanced flow rate for hard discs exiting a hopper with an adjustable obstacle

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

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

Tomoya Yasuno, Dept. of Mathematical and Systems Engineering, Shizuoka Univ., Japan

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

Isamu Riku, Osaka Prefecture Univ., Japan

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

Stefano Poggio, School of Physics, University College Dublin, Ireland

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

Kosuke Ohata, JSOL Corporation, Japan

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

Yoshihiro Takai, Graduate school of Science and Engineering, Kansai Univ., Japan

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

Kentaro Takada, Graduate School of Science and Engineering, Kansai Univ., Japan

P2-65 Bubble dynamics of foam flow around an obstacle

Antti Puisto, Aalto University, Department of Applied Physics, Finland

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

Wei-Chun Lin, Department of Civil Engineering, National Cheng Kung University, Taiwan

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

Jeong-ha Lee, Dept. of Energy Engineering, Chung-Ang Univ., Korea

P2-68 Multiscale analysis on the hygroelastic behavior of epoxy-based nanocomposite

Sunyong Kwon, Dept. of Energy Engineering, Chung-Ang Univ., Korea

Symposium I (P2-69 – P2-74)

Symposium N

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

Dan Wei, University of Chinese Academy of Sciences, China

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

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

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

Haris Rudianto, Gunadarma University, Indonesia

Symposium O

- P2-78 Adsorption of Volatile Organic Compounds (VOCs) on Silicene by Density Functional Theory Calculations**
Thi Viet Bac Phung, Nanotechnology Program, Vietnam Japan University – Vietnam National University, Viet Nam
- P2-79 Atomistic insights into defect formation mechanism in single crystal SiC based on molecular dynamics simulation**
Kenji Nishimura, AIST, Japan
- P2-80 Potential cathode material Na_xVOPO_4 for rechargeable Sodium – ion batteries: DFT investigation**
Duc Huu Luong, Nano Technology Program, Vietnam Japan University, Viet Nam
- P2-81 Two-dimensional Na_xSiS as a promising anode material for rechargeable Sodium-based batteries: Ab initio material design.**
Van An Dinh, Nanotechnology Program, Vietnam Japan University, Viet Nam
- P2-82 Modelling and analysis of SiO_2 interfaces of non-firing solids**
Tomohiro Sato, Dept. of Mechanical Engineering, Kansai Univ., Japan