Poster program

Poster session 1
Monday 29 October (17:45～20:00)

Symposium A

P1-01 **The coadsorption effect of Cl- and H_2O on the various defect Al_2O_3 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 $MABX_3$ perovskites (MA= $CH_3NH_3^+$; *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 Mg_2SiO_4 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

P1-11 **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

Symposium E

P1-21 **Large-scale molecular dynamics simulations: coupling with dislocation dynamics**
Pavel A. Pokatashkin, 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, Wuhan University, China

P1-23 **Study of solute effect on the yield strength of Fe-based dilute alloy using atomistically informed kinetic Monte Carlo method**
Shuhei Shinzato, Dept. of Mechanical Science and Bioengineering, Osaka Univ., Japan

P1-24 **Molecular dynamics simulations of low-cycle fatigue behavior in single layer molybdenum disulfide**
Yu-Cheng Su, National Chiao Tung University, Taiwan

P1-25 **Fracture behavior of multi-walled carbon nanotube under biaxial loading condition**
Masaomi Nishimura, Dept. of Mechanical Systems Engineering, Shinshu Univ., Japan

P1-26 **On the role of amorphous shells on mechanical properties of fcc Ni nanoparticles under compression**
Alexandra Goryaeva, DEN-Service de Recherches de Métallurgie Physique, CEA, Université Paris-Saclay, 91191 Gif-sur-Yvette, France

P1-27 **Molecular dynamics analysis of hydrogen diffusion behavior in alpha-Fe bi-crystal under stress gradient**
Ken-ichi Saitoh, Kansai Univ., Japan

P1-28 **Understanding interactions of dislocations with interfaces in nickle-based superalloys: insights from molecular dynamics simulations**
Jian Huang, Shanghai Institute of Ceramics Chinese Academy of Sciences, China

P1-29 **The influence of nano-sized Ti3Al particles on the mechanical properties of α-titanium alloys**
Yan He, IMR, CAS, China

P1-30 **The atomic study of tensile property for nickel nanowires with helium bubble**
Hengfeng Gong, CGN, China

P1-31 **Componets of fracture response of alkali-activated slag mortars with steel fibers**
Hana Simonova, 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, Mechanical and Electronical Engineering College, Lanzhou University of Technology, China

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 **Transition-metal alloying of γ'-Ni_3Al: effects on the ideal uniaxial compressive strength from first-principles calculations**
Minru Wen, Tsinghua University, China

P1-35 **The influence of deposition pattern on stress and mechanical properties in wire arc ddditive manufacturing**
Changmeng Liu, 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, 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 recrystallizazion 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 **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, Kyoto Institute of Technology, Japan

P1-60 **Density functional theory plus Hubbard U study of the segregation of Pt to the CeO_{2-x} grain boundary**
Zhixue Tian, 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, 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, University of La Rochelle, France

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 Tecnologico 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 Universite 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-Al_2O_3 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

P1-80 **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

Syposium 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

P2-13 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

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 **Dynamics of a solidification front made by invasion of fluid with a different temperature**
So Kitsunezaki, Nara Women's Univ., Japan

P2-35 **Strengthening through solid solution in W1-xTaxB system**
lijuan liu, Dept. of Applied Physics, University of Science and Technology Beijing, China

P2-36 **Desiccation crack patterns based on phase-field modeling and their statistical properties**
Shin-ichi Ito, The Univ. of Tokyo, Japan

P2-37 **Ce-terminated (111) surface of CeO_2**
YaNan Zhao, Dept. of Applied Physics, University of Science and Technology Beijing, China

P2-39 **Numerical analysis of elasto-plastic behavior of metallic architectured materials**
Filip Siska, Institute of Physics of Materials, Czech Academy of Sciences, Czech Republic

P2-40 **Automatic analysis and numerical prediction of flow stress curves for aluminium alloys**
Evgeniya Kabliman, Light Metals Technologies Ranshofen, Center fo Low-Emission Transport, Austrian Institute of Technology, Austria

P2-41 **Comparison of different alkali activated mortars with hemp fibres response during fracture test by acoustic emission method**
Hana Simonova, Brno University of Technology, Faculty of Civil Engineering, Czech Republic

Symposium F

P2-43 **Design of spontaneous formation- based 3D plasmonic optical structure, using multyphysics modeling**
Jihwan Song, Dept. of Mechanical Engineering, Hanbat National University, Korea

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 ZrO_2 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 Studying the kinetics of a self-propelled cruiser in 2D granular media under gravity
Guo-jie Jason Gao, Dept. of Mathematical and Systems Engineering, Shizuoka Univ., Japan

P2-59 A discrete tetris model showing two flow regimes for hard particles exiting a hopper with an adjustable obstacle
Tomoya Yasuno, 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 Durability analysis on the environmental aging of epoxy-based nanocomposite
Sunyong Kwon, Dept. of Energy Engineering, Chung-Ang Univ., Korea

Symposium I

P2-69 Topological evolution of the microstructures of thin films during grain growth
Ahu Oencue, Institute of Experimental Physics, Otto-von-Guericke University Magdeburg, Germany

P2-70 Molecular dynamics simulations of phase transformations in nanocrystalline NiTi shape-memory alloys
Won-Seok Ko, University of Ulsan, Korea

P2-71 An attempt to connect migration of grain boundaries to their atomic structures with help of molecular dynamics
Sylvain Queyreau, Universite Paris XIII, France

P2-72 Disconnection interaction in Cu grain boundaries
Christian Brandl, Karlsruhe Institute of Technology, Germany

P2-73 Phase-field approach to thermo-mechanical behavior of through-silicon vias
Jaekeun Yoon, Sogang Univ., Korea

P2-74 Grain-growth in nanocrystalline metals under ion irradiation: a thermal spike model
Djamel Kaoumi, North Carolina State University, United States of America

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