Symposium N : Computational Materials and Artificial Intelligence

November 20 (Mon.), 2023

Session Title : Computational Materials and Artificial Intelligence 1
Time : 10:50 - 12:35, Nov. 20
Room # : 203, 2F
Session Chair : Katsuyuki MATSUNAGA, Nagoya University
Won-Seok Ko, Inha University

10:50 – 11:20 **Keynote** **K-N0824**

Material Discovery Using Machine-Learned Potentials

Seungwu Han, Seoul National University, Korea

11:20 – 11:40 **Invited** **I-N0428**

Role of triple junctions on slip localizations in polycrystalline Ni-based superalloys

Irene Beyerlein, University of California Santa Barbara, USA

11:40 – 12:00 **Invited** **I-N0427**

Crystal growth in Supercomputer: The cutting edge of large-scale molecular dynamics simulation of metallic materials

Yasushi SHIBUTA, The University of Tokyo, Japan

12:00 – 12:20 **Invited** **I-N1153**

The effect of atomic hydrogen on the behavior of a single dislocation of <111>{112} in bcc tungsten: atomistic study

Keonwook Kang, Yonsei University, Korea

12:20 – 12:35 **O-N0670**

Molecular dynamics analysis of interaction between screw dislocation motion and hydrogen diffusion in BCC iron

Shuhei Shinzato, Osaka University, Japan

Session Title : Computational Materials and Artificial Intelligence 2
Time : 14:00 - 15:30, Nov. 20
Room # : 203, 2F
Session Chair : Irene Beyerlein, University of California Santa Barbara
Keonwook Kang, Yonsei University

14:00 – 14:30 **Keynote** **K-N0166**

Electronic and atomic structures of glide dislocations in inorganic semiconductors relevant to their light-illumination dependent mechanical behavior

Katsuyuki MATSUNAGA, Nagoya University, Japan

14:30 – 14:50 **Invited** **I-N0216**

A generalizable and interpretable deep learning model to improve the prediction accuracy of strain fields in grid composites

Seunghwa Ryu, Korea Advanced Institute of Science and Technology, Korea

14:50 – 15:10 **Invited** **I-N0899**

Research and development in microforming technology of metallic composites

Zhengyi Jiang, University of Wollongong, Australia

15:10 – 15:30 **Invited** **I-N1159**

Sequential Decision-making for Compositional Design of Multicomponent Alloys using Reinforcement Learning

Dezhen Xue, Xi'an Jiaotong University, China

Session Title : Computational Materials and Artificial Intelligence 3

Time : 16:00 - 17:50, Nov. 20

Room # : 203, 2F

Session Chair : Dezhen Xue, Xi'an Jiaotong University

Seunghwa Ryu, Korea Advanced Institute of Science and Technology

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16:00 – 16:30 **Keynote** **K-N1099**

Constitutive modelling based on machine learning for anisotropic plasticity

Jeong Whan Yoon, KAIST/Deakin University, Korea

16:30 – 16:45 **O-N1147**

Application of Thermodynamic extremal principle to Phase Field Model for Non-equilibrium Interface Conditions

Yue Li, Northwestern Polytechnical University, China

16:50 – 17:05 **O-N0270**

Application of finite element simulations to nanosecond laser ablation process

Yutaka Tsumura, The University of Sydney, Australia

17:05 – 17:20 **O-N0175**

Finite element simulation of plastic flow in dealloyed heterogeneous materials

Sylvain Dancette, CNRS, Tohoku University, Japan

17:20 – 17:35 **O-N0126**

Crystal Plasticity Simulation Considering Microstructures of Metals on Mechanical Anisotropy Induced by Rolling

Nomun Gerel-Erdene, Tohoku University, Japan

17:35 – 17:50 **O-N0678**

A physics-constrained ANN model for material deformation modelling

Guowei Zhou, Shanghai Jiao Tong University, China

November 21 (Tue.), 2023

Session Title : Computational Materials and Artificial Intelligence 4
Time : 10:50 - 12:30, Nov. 21
Room # : 203, 2F
Session Chair : Lei Zhang, University of Science and Technology Beijing
Ki Sub Cho, Kookmin University

10:50 – 11:20 **Keynote** **K-N0540**

Deep learning-driven crystallography for inorganic materials

Keesun Sohn, Sejong University, Korea

11:20 – 11:40 **Invited** **I-N1044**

Learning Topological Data Representation and its Applications

Gang Li, Deakin University, Australia

11:40 – 12:00 **Invited** **I-N0252**

Artificial Intelligence for EELS/XAFS

Teruyasu MIZOGUCHI, The University of Tokyo, Japan

12:00 – 12:15 **O-N0486**

Using Unsupervised Learning to Cluster Fatigue Life Based on Small Crack Characteristics

Katelyn Jones, Carnegie Mellon University, USA

12:15 – 12:30 **O-N0323**

Prediction of Macroscopic Mechanical Properties of Heterogeneous Structured Metals Based on Neural Network

Masaki Nishimura, Tohoku University, Japan

Session Title : Computational Materials and Artificial Intelligence 5
Time : 14:00 - 15:30, Nov. 21
Room # : 203, 2F
Session Chair : Teruyasu MIZOGUCHI, The University of Tokyo
Seonghwan Kim, Sejong University

14:00 – 14:30 **Keynote** **K-N1016**

Design of low-dimensional materials using artificial intelligence algorithm

Jijun Zhao, Dalian University of Technology, China

14:30 – 14:50 **Invited** **I-N0397**

Exploring Optimal Water Splitting Bifunctional Alloy Catalyst by Pareto Active Learning

Yong Joo Kim, Kookmin University, Korea

14:50 – 15:10 **Invited** **I-N0952**

Cloud Platform based on the Materials Genome Engineering Database Architecture for Data Storage and online Modelling

Lei Zhang, University of Science and Technology Beijing, China

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Session Title : Computational Materials and Artificial Intelligence 6

Time : 16:00 - 17:55, Nov. 21

Room # : 203, 2F

Session Chair : Gang Li, Deakin University

Yong Joo Kim, Kookmin University

16:00 – 16:30 **Keynote** **K-N1031**

Generative AI to Accelerate Discovery of Materials

Truyen Tran, Deakin University, Australia

16:30 – 16:50 **Invited** **I-N0544**

High-Throughput Computational Screening and Machine Learning Modeling of Janus 2D III-VI van der Waals Heterostructures for Solar Energy Applications

Baisheng Sa, Fuzhou University, China

16:50 – 17:10 **Invited** **I-N**

Tiff Walsh, Deakin University, Australia

17:10 – 17:25 **O-N0369**

Effects of point defects on hydrogen diffusivity in B2-type PdCu alloys: A kinetic Monte Carlo study

Akihiro Mitsuhara, Nagoya University, Japan

17:25 – 17:40 **O-N1015**

Electrochemical stability map of bimetallic nanoparticles

Hongryol Jeon, Korean Institute of Science And Technology, Korea

November 22 (Wed.), 2023

Session Title : Computational Materials and Artificial Intelligence 7
Time : 10:50 - 12:30, Nov. 22
Room # : 203, 2F
Session Chair : Tomohito Tsuru, Japan Atomic Energy Agency
Kunok Chang, Kyung Hee University

10:50 – 11:20 **Keynote** **K-N0869**

Accelerating the Discovery and Design of Novel Materials by ALKEMIE

Zhimei Sun, Beihang University, China

11:20 – 11:40 **Invited** **I-N0238**

Precipitates in Al-Cu-Li alloys: First-principles and Experimental study

Kyoungdoc Kim, Pohang University of Science and Technology, Korea

11:40 – 12:00 **Invited** **I-N0179**

High-accuracy prediction of dendritic solidification microstructure through GPUs and AMR-accelerated computation

Shinji SAKANE, Kyoto Institute of Technology, Japan

12:00 – 12:20 **Invited** **I-N1018**

Augmented Phase-field Model with Finite Interface Dissipation

Lijun Zhang, Central South University, China

12:20 – 12:35 **O-N0830**

Super resolution of three-dimensional microstructural image of a steel using deep learning

Hoheok Kim, Korea Institute of Materials Science, Korea

Session Title : Computational Materials and Artificial Intelligence 8-1
Time : 14:00 - 15:30, Nov. 22
Room # : 203, 2F
Session Chair : Hyo-Sun Jang, Korea Institute of Materials Science

14:00 – 14:15 **O-N0275**

Molecular dynamics simulation of three-dimensional ferrite nucleation behavior during austenite-to-ferrite transformation in pure iron

Mizuki Serada, Tokyo University of Agriculture and Technology, Japan

14:15 – 14:30 **O-N0919**

Machine learning-based scale-bridging approach for the evolution of irradiation-induced defects in tungsten

Linyun Liang, Beihang University, China

14:30 – 14:45 **O-N0673**

Modeling defect sink mechanism of lath boundary dislocation network using anisotropic

linear elasticity method

Hadi Ghaffarian, KAIST, Korea

14:45 – 15:00 **O-N0274**

Development of continuous cluster-activation method and its application to various phenomena in materials science

Ryo Yamada, Hokkaido Univerisity, Japan

15:00 – 15:15 **O-N0525**

Molecular Dynamic Simulation of Primary Damage in High Entropy Alloys: Examining the Interplay of Alloying and Grain Boundary Effects for Superior Irradiation Resistance

Mosab Banisalman, Virtual Lab Inc, Korea

15:15 – 15:30 **O-N0546**

Nuclear quantum effects on hydrogen-isotope diffusion in vanadium and palladium: A path-integral molecular dynamics study

Hajime Kimizuka, Nagoya University, Japan

Session Title : Computational Materials and Artificial Intelligence 8-2

Time : 14:00 - 15:30, Nov. 22

Room # : 401, 4F

Session Chair : Kyoungdoc Kim, Pohang University of Science and Technology

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14:00 – 14:15 **O-N0130**

Data assimilation-integrated phase-field simulation of ternary alloy solidification in forced convection using local ensemble transform Kalman filter

Masahiro Kawasaki, Tokyo University of Agriculture and Technology

14:15 – 14:30 **O-N0707**

Phase field study of solid-state sintering process in Fe-Si alloys

Sandeep Sugathan, Kookmin University, Korea

14:30 – 14:45 **O-N0258**

Simulation of microstructural evolution during active metal brazing with Ag-Cu-Sn-Ti alloy by CALPHAD coupled phase-field method

Takumi Morino, Yokohama National University, Japan

14:45 – 15:00 **O-N0462**

Phase Field Modelling of Martensitic Phase Transformation by transient heat transfer

Dong-Wook Lee, Technology Innovation Institute, UAE

15:00 – 15:15 **O-N0141**

Modeling of Crystal Plasticity Predicting Microstructural Changes Caused by Twinning-Induced Plasticity

Haruki Ohashi, Tohoku University, Japan

15:15 – 15:30 **O-N0398**

Material parameter estimation for aluminum alloy sheet using non-sequential data assimilation

Michihiko Suda, Tokyo University Of Agriculture And Technology, Japan

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Session Title : Computational Materials and Artificial Intelligence 9-1

Time : 16:00 - 17:30, Nov. 22

Room # : 203, 2F

Session Chair : Minkyu Park, Virtual Lab. Inc.

16:00 – 16:15 **O-N0581**

Unraveling the electrochemical behavior of Mg based intermetallics: A first-principles study

Pragyandipta Mishra, Indian Institute Of Technology Madras, India

16:15 – 16:30 **O-N1017**

On-the-fly machine learning force field study of liquid-Al/α-Al_2O_3 interface

Tao Hu, Shanghai University, China

16:30 – 16:45 **O-N0387**

Application of Machine Learning to Optimize Electrodeposition Parameters for Ni-W Alloy Coatings with High Hardness

Sen Zhai, Hiroshima University, Japan

16:45 – 17:00 **O-N0044**

Material-Dlab, A digital research and development platform for metal materials

Weice Gao, China Iron & Steel Research Institute Group Co., Ltd, China

17:00 – 17:15 **O-N0674**

Synthesizability prediction for TiZrNb-Mo heterostructures using positive and unlabeled (PU) learning scheme

Aamir Malik, KAIST, Korea

17:15 – 17:30 **O-N0086**

Research and development of big data application platform for intelligent blast furnace intensive management and control

Jing Fei, Anshan Iron And Steel Co.,ltd., China

Session Title : Computational Materials and Artificial Intelligence 9-2

Time : 16:00 - 17:45, Nov. 22

Room # : 401, 4F

Session Chair : Hoheok Kim, Korea Institute of Materials Science

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16:00 – 16:15 **O-N0064**

Data mining of dislocation microstructures by deep learning

Yuqi Zhang, The Northeastern University, China

16:15 – 16:30 **O-N0724**

Development of Ultrahigh Strength Martensitic Steels with Improved Mechanical Properties via Artificial Intelligence-driven Material Design

YOONJUNG WON, Kookmin University, Korea

16:30 – 16:45 **O-N0911**

Studies on damage mechanisms of tungsten and molybdenum under ITER ELM-like heat load

Lisong Zhang, Dalian University of Technology, China

16:45 – 17:00 **O-N0400**

Structural analysis and interstitial site extraction in bcc Fe grain boundaries by persistent homology analysis

Bohao Zheng, Tohoku University, Japan

17:00 – 17:15 **O-N0445**

Gibbs Energy Estimation from Microstructure data by Combining Phase Field Simulation and Machine Learning Technique

Yusuke Matsuoka, Nagoya University, Japan

17:15 – 17:30 **O-N1023**

Simulation Model of Molten Salt Corrosion Using COMSOL

MaeHyun Cho, Kyung Hee University, Korea

17:30 – 17:45 **O-N0431**

Architecture of Materials data infrastructure and Its Application

Changchang Wang, Central Iron& Steel Research Institute, China