1st NOMATEN International Conference on Materials Informatics

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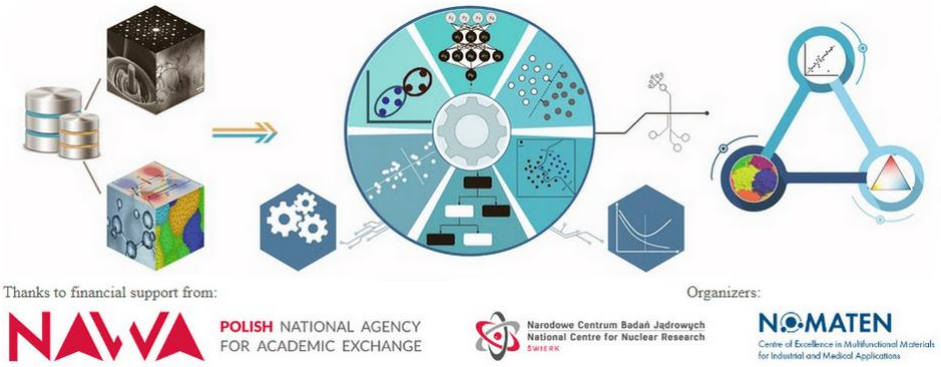

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Centre of Excellence in Multifunctional Materials for Industrial and Medical Applications

Book of Abstracts
with contribution type
(last updated: May 31, 2022)

TRACK: Materials Informatics (general track)

Communication

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2. Synergistic coupling in ab initio-machine learning simulations of dislocations
3. Structural features indicating local yielding in foams
4. Correlation between dislocation avalanches and the impact on the stress-strain curve
5. Atomic-scale modeling of chemically disordered compounds by means of generative models
6. Machine Learning Potential for Dislocations Near Free Surfaces
7. The Artificial Neural Network Model for the contamination source emergency localization system.
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2. Modelling of properties of Ta-Ti-V-W high-entropy alloys using DFT-based machine learning potentials
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11. Machine Learning for Atomistic Materials Science
12. Physics inspired Machine Learning (ML) Approaches for Materials Science: On the importance of representations, prior information and adaptive experimental design
13. From Ontologies and FAIR Data to Machine Learning-based High-Throughput Data Mining of In-Situ TEM Experiments on Dislocations in HEAs
14. Critical modelling and informatics need for materials in additive manufacturing
15. Selected legal aspects of AI/ML development and deployment
16. Sano Centre for Computational Medicine. Journey to transform healthcare.
17. Computational materials engineering with active learning

None

1. Ontological modelling of creep void analysis data to automate machine learning training process
2. Prediction of magnetic moment and formation energy per atom of Iron-based compounds using a data-driven machine learning approach

Other

1. A new AI/ML framework for materials innovation

Poster

1. Gamma irradiation assisted control of the structural, optical and electrical properties of PVP/NaAlg-Au NPs nanocomposite
2. Alloy informatics using charge profiles for energy and hydrogen storage applications
3. Configurational entropy and kinetic behavior of Co-Cr-Ni-Fe-Mn alloys: from solid solutions to metallic glasses
4. Ontologies in Material Informatics
5. Random Field Creep Model: Theoretical and Experimental Study
6. The role of short-range order and misfit components on deformation mechanism in fcc VCoNi concentrated solid solution alloys: A molecular dynamic simulation
7. Dynamics of stress propagation in crystals: comparing molecular dynamics simulations and analytical models.
8. AI-based modeling of crystal plasticity in concentrated solid solutions in extreme environments
9. Neural-network based atomistic modeling of plastic deformation mechanisms of crystalline molybdenum

Abstracts:

I)

Topic:

Gamma irradiation assisted control of the structural, optical and electrical properties of PVP/NaAlg-Au NPs nanocomposite

Author:

Mohammed Farea (1-Department of Physics, Faculty of Science, IBB University, Yemen. 2-Department of Physics, Faculty of Science, Mansoura University, Mansoura, 35516, Egypt)

Speaker:

Mohammed Farea

Abstract:

Using Chenopodium murale leaf, gold nanoparticles (Au NP's) were biosynthesized effectively in an amicable strategy. The casting process was used to create composite layers of sodium alginate and polyvinyl pyrrolidone. Gold nanoparticles were incorporated into the polyvinyl pyrrolidone (PVP)/ sodium alginate (NaAlg) polymer blend by casting technique. Before and after exposure to different doses of gamma irradiation (2, 4, 6 Mrad), thin films of synthesized nanocomposites were analyzed. XRD revealed the amorphous nature of polymer blends (PVP/ NaAlg), which decreased by both Au NP's embedding and consecutive doses of irradiation. FT-IR spectra revealed interactions and differences within the functional groups of their respective pristine components and dopant nano-fillers. The optical properties of PVP/NaAlg – Au NP thin films (refractive index n, energy gap Eg, Urbach energy Eu) were examined before and after the irradiation procedure. Transmission electron micrographs (TEM) demonstrated a decrease in the size of Au NP's and a narrow size distribution as the gamma irradiation dose was increased. Gamma irradiation was found to influence the electrical conductivity of synthesized composite films, as well as dielectric permittivity (ε') and dielectric losses (ε").

II)

Topic:

MARIA's reactor high-temperature irradiation capsules for advanced fusion and fission power technologies

Authors:
Maciej Lipka (National Centre for Nuclear Research)
Anna Talarowska (National Centre for Nuclear Research)
Marek Migdal (National Centre for Nuclear Research)
Grzegorz Wojtania (National Centre for Nuclear Research)
Rafał Prokopowicz (National Centre for Nuclear Research)
Piotr Mazerewicz (National Centre for Nuclear Research)

Speaker:
Maciej Lipka (National Centre for Nuclear Research)

Abstract:
Advanced nuclear power reactors prototypes (both fusion and fission) require testing under conditions that are as close to real-life as possible. Those include but not limited to: high temperature, specific atmosphere, and the high neutron flux with specific energy spectrum. The research reactor can provide the latter, but the previous two require appropriate thermostatic equipment. Thermostatic capsules that provide high-temperature up to 1000°C have been design and are operated in MARIA reactor. This paper presents the design of such capsules and revievs their capabilities in field of testing advanced nuclear power technologies. MARIA reactor and its unique research capabilities is also presented.

III)

Topic:

A new AI/ML framework for materials innovation

Author:
Surya Kalidindi

Speaker:
Surya Kalidindi

Abstract:
A novel information gain-driven Bayesian AI/ML (artificial intelligence/machine learning) framework is presented with the following main features: (i) explicit consideration of the physics parameters as inputs (i.e., regressors) in the formulation of process-structure-property (PSP) surrogate models needed to drive materials improvement workflows; (ii) information gain-driven autonomous workflows for training efficient AI/ML surrogates to otherwise computationally expensive physics-based simulations; (iii) versatile feature engineering for multiscale material internal structure using the formalism of n-point spatial correlations; (iv) amenable to a broad suite of surrogate model building approaches (including Gaussian Process regression (GPR), convolutional neural networks (CNN)); and (v) Markov chain Monte Carlo (MCMC)-based computation of posteriors for physics parameters using all available experimental observations (usually disparate and sparse). The benefits of this framework in supporting accelerated design and development of heterogeneous materials will be demonstrated using multiple case studies.

IV)

Topic:

Coarse-graining molecular systems with autoencoders and adaptive sampling

Authors:
Gabriel Stoltz (Ecole des Ponts and Inria Paris)
Paraskevi Gkeka (Sanofi)
Tony Lelièvre (Ecole des Ponts and Inria Paris)
Zineb Belkacemi (Sanofi)

Speaker:
Gabriel Stoltz (Ecole des Ponts and Inria Paris)

Abstract:
A coarse-grained description of atomistic systems in molecular dynamics is provided by reaction coordinates. These nonlinear functions of the atomic positions are a basic ingredient to compute more efficiently average properties of the system of interest, such as free energy profiles. However, reaction coordinates are often based on an intuitive understanding of the system, and one would like to complement this intuition or even replace it with automated tools. One appealing tool is autoencoders, for which the bottleneck layer provides a low dimensional representation of high dimensional atomistic systems. In order to have an efficient numerical method, autoencoders should be combined with importance sampling techniques based on adaptive biasing methods. The algorithm then iterates between an update of the reaction coordinate, and free energy biasing. I will discuss some mathematical foundations of this method, and present illustrative applications for biophysical systems, including alanine dipeptide and chignolin. Some on-going extensions to more demanding systems, namely HSP90, will also be hinted at. Depending on time, I will also mention current extensions aiming at sampling reactive paths.

V)

Topic:

Synergistic coupling in ab initio-machine learning simulations of dislocations

Authors:
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Thomas Swinburne (Aix-Marseille Universit ´e, CNRS, CINaM UMR 7325, Campus de Luminy, 13288 Marseille, France)

Speaker:
Petr Grigorev (Aix-Marseille Universit e, CNRS, CINaM UMR 7325, Campus de Luminy, 13288 Marseille, France)

Abstract:
Ab initio simulations of extended defects require system sizes at or beyond existing limits. Here, hybrid simulations coupling ab initio to linear machine learning potentials are used to overcome these limitations. Our method allows arbitrary sub-regions of large scale simulations to be treated with ab initio accuracy. Starting from a potential with correct elastic properties, we evaluate glide barriers edge and screw dislocations. The resulting ab initio forces are then targeted in a novel retraining procedure, which exploits the linear parametric form to precisely match core structures whilst preserving elastic and other properties. Coupling to this retrained potential allows dislocations to cross the quantum/classical boundary. Fully three dimensional studies of impurity segregation to edge and screw dislocations in tungsten show long-range relaxations qualitatively change impurity-induced core reconstructions compared to simulations using short periodic supercells. Our approach opens a vast range of mechanisms to ab initio investigation and provides new reference data to both validate and improve interatomic potentials.

VI)

Topic:

Modelling of properties of Ta-Ti-V-W high-entropy alloys using DFT-based machine learning potentials

Authors:
Jan Wróbel (Faculty of Materials Science and Engineering, Warsaw University of Technology)
Alexandra Goryaeva (Université Paris-Saclay, CEA, Service de Recherches de Métallurgie Physique)
Damian Sobieraj (Faculty of Materials Science and Engineering, Warsaw University of Technology)
Duc Nguyen-Manh (CCFE, United Kingdom Atomic Energy Authority)
Mihai-Cosmin Marinica (Université Paris-Saclay, CEA, Service de Recherches de Métallurgie Physique)

Speaker:
Jan Wróbel (Faculty of Materials Science and Engineering, Warsaw University of Technology)

Abstract:
High entropy alloys (HEAs) are the new class of materials incorporating four or more elements in similar concentrations. Due to their superior radiation resistance properties compared to pure elements and conventional alloys, HEAs are promising materials for applications in structural elements of future fusion and fission reactors [1].

In this work, we focus on the bcc-based HEAs Ta-Ti-V-W system, which has been shown from our combined DFT, cluster expansion and Monte-Carlo simulations to have the lowest solid solution temperature among five-component (Cr-Ta-Ti-V-W) HEAs [2]. The accurate and fast machine learning (ML) interatomic potentials has been developed based on thousands of DFT calculations for the representative structures of alloys obtained using DFT-based MC database for different alloy compositions, structures with different short-range orders and different classes of calculations. Different ML approaches, linear ML, quadratic noise ML and kernel models, and various types of atomic descriptors have been tested in order to achieve the good balance between accuracy, speed and predictive power [3]. The root-mean-square errors between the forces computed using DFT and ML potential are below 0.4 eV/A. The developed ML potentials have been applied in MD simulations to study the chosen properties of HEAs as a function of composition and temperature and the obtained results have been compared with the available DFT results.

[1] O. El-Atwani, N. Li, M. Li, A. Devaraj, J.K.S. Baldwin, M.M. Schneider, et al., Sci. Adv. 5 (2019) eaav2002.
[2] D. Sobieraj, J.S. Wróbel, T. Rygier, K.J. Kurzydłowski, O. El Atwani, A. Devaraj, et al., Phys. Chem. Chem. Phys. 22 (2020) 23929.
[3] A.M. Goryaeva, J. Dérès, C. Lapointe, P. Grigorev, T.D. Swinburne, J.R. Kermode, et al. Phys. Rev. Mater. 5 (2021) 103803.

VII)

Topic:

Structural features indicating local yielding in foams

Author:

Leevi Viitanen

Co-authors:

Oskar Tainio,
Jonatan Mac Intyre,
Mehmet Aydin,
Juha Koivisto,
Antti Puisto,
Mikko Alava

Speaker:

Leevi Viitanen

Abstract:

Recently, machine learning methods have proven a prominent tool for the predictions of local yielding in experiments and simulations of amorphous particulate systems. Similarly to shear transformation zones in amorphous solids, the plastic deformation in 2D foams occurs via subsequent rearrangements in the bubble configuration, known as T1 events. In the present study, we detect large amount of T1 events from a foam flow experiment in a Hele-Shaw cell and use the data set to train a neural network to predict T1 events from features describing the geometry of nodes joining liquid films. The tests show that the neural network can classify T1 events from the data with over 80 % accuracy. In addition, by restricting the available features, we apply the network to reveal the most important features that indicate yielding. This information allows constructing a model of nodes that are prominent to yield in T1 events adding a physical interpretation to the machine learning model.

VIII)

Topic:

Correlation between dislocation avalanches and the impact on the stress-strain curve

Author:
Henri Salmenjoki (Aalto University, Department of Applied Physics)

Co-authors:
Lasse Laurson,
Mikko Alava

Speaker:
Henri Salmenjoki (Aalto University, Department of Applied Physics)

Abstract:
Plastic deformation and eventual yielding of micron-scale crystals is dominated by collective dislocation avalanches. Due to the avalanches, response to external loading fluctuates drastically from sample to sample leading to a seemingly stochastic-like response. However, some predictability exists as recent results have shown that an adequate mapping between the initial dislocation structure and ensuing stress-strain curve can be obtained [1]. Although the forecast only recreates the overall shape of the response, individual avalanches still remain unpredictable. We present here results on observed correlations between subsequent avalanches in 2D and 3D discrete dislocation dynamics simulations [2]. The discovered correlations explain the previously encountered limits of predictions and reveal fundamental properties of the average response of dislocation ensembles.

1. H. Salmenjoki et al., Nat. Commun., 9, 5307 (2018)
2. H. Salmenjoki et al., Phys. Rev. Mat., 5(7), 073601 (2021)

IX)

Topic:

Ontological modelling of creep void analysis data to automate machine learning training process

Author:
Akhtar Zeb (VTT Technical Research Centre of Finland)

Co-author:
Teemu Mätäsniemi (VTT Technical Research Centre of Finland)

Speaker:
Akhtar Zeb (VTT Technical Research Centre of Finland)

Abstract:
This work focuses on the ontological representation of creep void analysis data to automate training of the machine learning (ML) model detecting creep voids in scanning electron microscope images. Metallic high-temperature structures are subject to creep that leads to rupture and component failure when prolonged. ML models can be deployed to detect and obtain information about the density and location of creep voids using images as input data. However, due to the irregularities in the size and shape of creep voids and the associated uncertainty in ML models, the materials engineer may need to inspect the detections and provide feedback on a regular basis. To facilitate close collaboration between the ML experts and materials engineers, domain ontologies providing common vocabularies can be utilized. We aligned the relevant concepts of EMMO ontology, ML-Schema, and PROV ontology to document creep void data for smooth information sharing and improving quality of the ML detection process, hence resulting in better analysis and higher productivity. The SPARQL queries are used to gain valuable insights, such as the condition of the metallic structure, accuracy of the detections, and the need for further training of the ML model.

X)

Topic:

Alloy informatics using charge profiles for energy and hydrogen storage applications

Authors:
Dario Massa (NCBJ, NOMATEN)
Stefanos Papanikolaou (NCBJ)

Speaker:
Dario Massa (NCBJ, NOMATEN)

BIOGRAPHY: Dario Massa has attained his Bachelor degree in Physics at the University of Roma La Sapienza, Italy and his M.Sc. in Physics at University of Padova, Italy. He has worked as a research fellow at University of Padova on the modelling of van der Waals interactions at the nanoscale. He is currently a PhD student at NOMATEN Center of Excellence in Warsaw, Poland, in the group of Prof. Stefanos Papanikolaou (Materials structure, informatics) where he is carrying on his project on material informatics applied to hydrogen storage.

Abstract:
Studies have confirmed the crucial role of solid-state based solutions in hydrogen storage, with respect to liquid or gas states which cannot ensure high amounts of storage per unit volume [1]. The empirical approach is not an option when it comes to the complexity of the quest for hydrogen storage materials, as well as to the strict urgency of a transition to clean and sustainable energy solutions. The compositional space to be explored is extremely vast, and still its vastness is not defined due to the on-going explorations, not only spanning the chemical compositions, but also the dimensionalities of the possible candidate systems [2]. Therefore, there is the need of finding a general predictive approach, possibly based on first-principles. Our approach is based on the ab-initio analysis of the charge profiles of hydrogen in bulk metallic single crystals of pure elements, as well as multiple ones (eg. hydrites). Electron charge profiles shall be illuminating for identifying and classifying local defect properties. We extract basic features of the profiles, such as radii and extremas, as well as consider the full profile properties, by performing unsupervised machine learning. We find distinctive features of the effects of hydrogen, that can be exploited to infer hydrogen mobility in the surrounding matrix. Preliminary tests have revealed well defined trends of the hydrogen mobility with the number of valence electrons of the system, which might pave the way to a new efficient material informatics method for the prediction of hydrogen storage behaviour. Our goal is to understand up to which extent such charge profiles method can be exploited to predict gravimetric capacities, diffusive, as well as the adsorption and desorption properties, overcoming the limited predictive capacity of empirical and thermodynamic based methods. Further interest will be upon the generalization of this method to the investigation of nanostructured materials for the same purposes.

[1] P. Jena, J. Phys. Chem. Lett., 2011, 2, 206–211.

[2] Xuebin Yu et al. Progress in Materials Science, 2017, 88, 1–48.

XI)

Topic:

Atomic-scale modeling of chemically disordered compounds by means of generative models

Authors:
Luca Messina (CEA Cadarache)
Maciej Karcz (CEA Cadarache)
Serenah Rajaonson (CEA Cadarache)
Didier Bathellier (CEA Cadarache)
Eiji Kawasaki (CEA Saclay)
Emeric Bourasseau (CEA Cadarache)

Speaker:
Luca Messina (CEA Cadarache)

Abstract:
The role of machine learning in computational material science is becoming more and more important to accelerate traditional atomic-scale calculation methods and facilitate the transfer of physical information across modeling scales. This is especially important for chemically disordered compounds, where the configuration space is so large that sampling it to compute the partition function becomes significantly challenging. This is the case for instance of MOX (uranium-plutonium mixed oxides) nuclear fuels, whose atomic-scale properties are strongly affected by chemical disorder. In addition, first-principles methods are computationally demanding due to the presence of strongly correlated f electrons.

We present in this work an approach to the exploration of the configuration space based on mixture density networks and applied to the study of defect concentration in MOX fuels. The approach relies on a dataset of interatomic-potential calculations to obtain the defect formation-energy distribution. This is achieved by exploring only a small fraction of the configuration space. We show as well how energy-based generative models may be used to optimize the exploration even further, in the aim of replacing interatomic-potential data by more accurate first-principles calculations.

XII)

Topic:

Predicting the failure of two-dimensional silica glasses.

Author:
Silvia Bonfanti (NOMATEN CoE, NCBJ, Poland)

Co-authors:
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Roberto Guerra (University of Milan)
Michael Zaiser (Friedrich-Alexander-University Erlangen-Nuremberg)
Stefano Zapperi (University of Milan)

Speaker:
Silvia Bonfanti (NOMATEN CoE, NCBJ, Poland)

Abstract:
Being able to predict the failure of materials based on structural information is a fundamental issue with enormous practical and industrial relevance for the monitoring of devices and components. Thanks to recent advances in deep learning, accurate failure predictions are becoming possible even for strongly disordered solids, but the sheer number of parameters used in the process renders a physical interpretation of the results impossible. Here we address this issue and use machine learning methods to predict the failure of simulated two dimensional silica glasses from their initial undeformed structure. We then exploit Gradient-weighted Class Activation Mapping (Grad-CAM) to build attention maps associated with the predictions, and we demonstrate that these maps are amenable to physical interpretation in terms of topological defects and local potential energies. We show that our predictions can be transferred to samples with different shape or size than those used in training, as well as to experimental images. Our strategy illustrates how artificial neural networks trained with numerical simulation results can provide interpretable predictions of the behavior of experimentally measured structures.

XIII)

Topic:

Configurational entropy and kinetic behavior of Co-Cr-Ni-Fe-Mn alloys: from solid solutions to metallic glasses

Authors:
RENE ALBERTO ALVAREZ DONADO (NCBJ)
Stefanos Papanikolaou (NCBJ)
Mikko Alava

Speaker:
RENE ALBERTO ALVAREZ DONADO (NCBJ)

Abstract:
We numerically determine the kinetic and thermodynamic behavior for several Co-Cr-Ni-Fe-Mn multi-principal element alloys in their crystalline and vitreous states. We first explore the glass forming ability during a heating/quenching process. The reversible scaling method is then used to estimate the temperature evolution of the entropy by means of free energy calculations in the antipodes crystal and glass states. We then compute the self-diffusion coefficient and study the validity of the Adams-Gibbs relation. Our results show that the relation is generally violated for these multi-principal element alloys suggesting that configurational entropy is not the only responsible for the critical slowing down in the supercooled regime.

XIV)

Topic:

Prediction of magnetic moment and formation energy per atom of Iron-based compounds using a data-driven machine learning approach

Author:
Yogesh Khatri (PhD Scholar, IIT Mandi)

Co-author:
Arti Kashyap (Associate Professor and Simons Associate ICTP Italy IIT Mandi, Mandi, H.P.)

Speaker:
Yogesh Khatri (PhD Scholar, IIT Mandi)

Abstract:
In this work, we have used various machine learning (ML) algorithms to predict the magnetic moment and formation energy per atom of Iron-based magnetic compounds. Data of 11545 Iron-based Magnetic compounds are collected from the Materials project repository. The structure of the materials is then converted into a 32*32 matrix known as a descriptor, using the orbital-field matrix (OFM) representation proposed by Pham et al., which is based on the distribution of the valence cell electrons. We applied various ML algorithms to our dataset and used grid search hyperparameter tuning technique to get the best parameters for all algorithms, and then we applied 5-fold cross-validation using the best parameters to get the merit matrix. Random Forest (RF) algorithm provides the best results for our dataset. The magnetic moment per atom of Ferromagnetic Iron-based compounds is predicted with a mean absolute error (MAE) of 0.14 µB /atom whereas MAE for formation energy per atom is 0.168. We also used SHAP interpretability analysis to understand the model

XV)

Topic:

Reduced order modeling to characterize the damage tolerance of metal/composite hybrid structure

Author:
Stephanie TerMaath (University of Tennessee)

Co-author:
Cody Crusenberry (University of Tennessee)

Speaker:
Stephanie TerMaath (University of Tennessee)

Abstract:
Layered fiber reinforced composite overlays (patches) co-cured to a metal substrate, called composite/metal hybrid structure, have been proven to effectively restore the load carrying capacity to fatigue-cracked or corrosion-damaged parts and reinforce under-designed regions. Application of the composite overlay has been demonstrated to reinforce or repair metallic structures in engineering fields such as aerospace, automotive, infrastructure, and marine. Even with the many advantages offered by composite/metal hybrids, a serious concern comes with the evaluation of their non-visible damage. Non-visible damage, occurring internally and potentially unidentifiable prior to complete failure, occurs within the composite overlay during designed loads or overloads such as from bending and low-velocity impact. This non-visible damage can progress as matrix cracking, fiber breakage (fracture or buckling), delamination within the composite, or disbond at the composite/metal interface. Previous studies have demonstrated that the damage within the composite patch can substantially reduce the performance of the repair or reinforcement. Therefore, it is necessary to capture multiple damage mechanisms and progressive failure to model and predict damage initiation and propagation in these hybrid structures.

A validated, high fidelity finite element model that includes the relevant damage mechanisms in the composite, interface, and metal has been developed to investigate the material parameter space and to address several challenges in the prediction and understanding of composite overlay performance with respect to damage tolerance. However, the computational time of running a single analysis compounded by the large number of model inputs encompassing material selection significantly increases the difficulty in identifying the most influential inputs on the damage tolerance, as generating the necessary amount of data needed for a surrogate model and performing sensitivity analysis becomes prohibitive for non-linear, highly dimensional parameter spaces, even with supercomputing. This challenge is compounded by the likelihood that, during preliminary design and evaluation, many of the parameters may be defined by sparse data, average values, or estimates based on the behavior of similar materials. The goal of this research was to evaluate several components that are essential to the formulation of a reduced order surrogate model using machine learning to enable rapid exploration of a large material property parameter space. The following topics will be presented: (1) evaluation of the effects of data quality on model accuracy, (2) investigation of sensitivity analysis methods for their computational efficiency on models of varying complexity and fidelity to focus surrogate model development on the most influential parameters, (3) exploration of a multi-scale, high-fidelity approach to capture material behavior, and (4) importance of 3D model validation of damage.

XVI)

Topic:
Ontologies in Material Informatics

Author:
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Co-authors:
Rene Alvarez (National Centre for Nuclear Research)
Francesco Javier Dominguez-Gutiérrez (National Centre for Nuclear Research)
Karol Frydrych (National Centre for Nuclear Research)
Kamran Karimi (National Centre for Nuclear Research)
Stefanos Papanikolaou (National Centre for Nuclear Research)
Fabrizio Rovaris (National Centre for Nuclear Research)

Speaker:
Michał Pecelerowicz (National Centre for Nuclear Research)

Abstract:
Digitalization is one of the main driving forces of technological and scientific progress, which leads to the creation of an enormous amount of heterogeneous data, originating from different methods and workflows, maintained by different communities. On the other hand, the abundance of incompatible data sources often causes reduced interoperability of the data, stored in different data repositories. In order to ensure that data is findable, accessible, interoperable, and reusable i.e. conforms to the FAIR principles, significant efforts were made toward creating a standardized representation of the domain knowledge, metadata standards, and sophisticated classification schemes called ontologies which are utilized to make complex data compatible, and efficiently searchable. In the presentation, I will discuss different aspects of materials information ontology relevant to the data-driven research of material deformation, as well as associated impacts, existing challenges, and prospects.

XVII)

Topic:

Machine Learning Potential for Dislocations Near Free Surfaces

Authors:
Daniele Lanzoni (University of Milano-Bicocca)
Fabrizio Rovaris (NOMATEN Centre of Excellence)
Francesco Montalenti (University of Milano-Bicocca)

Speaker:
Fabrizio Rovaris (NOMATEN Centre of Excellence)

Abstract:
We present a Machine Learning framework able to predict energies and forces for interacting dislocations near free surfaces within the assumptions of linear elasticity [1]. Our approach resembles the procedure widely exploited to develop Force Fields for Molecular Dynamics starting from data derived by ab-initio simulations, but at the continuum scale. In our work, high accuracy two-body Finite Element calculations are used to train a Neural Network model, exploiting Sobolev training for accurately reproduce both energies and forces. We apply the proposed methodology to heteroepitaxial semiconductor films, searching for the minimum-energy dislocation configurations by a Monte Carlo approach. We also introduced an interaction cutoff for the application of the method to systems of different sizes without repeating the training. Dislocation Dynamics simulations are also shown, enabled by the prediction of both force and energy contributions.

[1] D. Lanzoni et al., Sci Rep 12, 3760 (2022)

XVIII)

Topic:

The Artificial Neural Network Model for the contamination source emergency localization system.

Author:

Anna Wawrzynczak (National Centre for Nuclear Research)

Speaker:

Anna Wawrzynczak (National Centre for Nuclear Research)

Abstract:

Providing a real-time working system to localize the dangerous contaminant source is one of the main challenges for the city's emergency response groups. Unfortunately, all proposed frameworks capable of estimating the contamination source localization based on recorded by the sensors network the substance concentrations cannot work in real-time. The reason is the significant computational time required by the applied dispersion models. In such reconstruction systems, the parameters of the given dispersion model are sampled to fit the model output to the registrations; thus, the dispersion model is run tens of thousands of times.

The solution might be an application of the trained Artificial Neural Network (ANN) instead of the dispersion model in the reconstruction algorithm. To be used, the ANN must learn to simulate airborne contaminant transport. Training the ANN is computationally expensive, but once trained, the ANN would be a high-speed tool enabling the estimation of the contaminant concentration distribution. This paper presents the results of training the ANN to predict the time evolution of the dispersion of the airborne contaminant over a city domain. The measures discovering both time and spatial distribution are proposed to estimate the uncertainty of the ANN output distribution.

XIX)

Topic:

Random Field Creep Model: Theoretical and Experimental Study

Author:

Bakhtiyar Mammadli

Speaker:

Bakhtiyar Mammadli

Abstract:

In this work, theoretically we study the creep regime in the Ising model which is one of the simplest, and most useful systems in statistical mechanics. Its degrees of freedom are classical spins si which can take the values ±1 for each lattice site i of a d-dimensional lattice. The Ising model can often be difficult to evaluate numerically if there are many states in the system. Since every spin site has ±1 spin, there are different states that are possible. This motivates the reason for the Ising model to be simulated using Monte Carlo method. After numerically simulating our system we investigate the creep regime in 3-D Ising model with a quenched random field, as function of temperature, with variable being the strength of random field. Also, we consider the case without thermal fluctuations and analyze numericaly a moving magnetic moment in the random-field Ising model which is driven by a magnetic field, as function of random field, with variable being the strength of the RF disorder variance. For the experimental studies of creep behaviour of the materials, one of the paractical way can be Digital Image Correlation (DIC) which is an optical method employs tracking and image registration techniques for accurate 2D and 3D measurements of changes in images and the results of the DIC analysis gives us the ful-field strain map of the creep deformation.

XX)

Topic:

The role of short-range order and misfit components on deformation mechanism in fcc VCoNi concentrated solid solution alloys: A molecular dynamic simulation

Authors:

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Stefanos Papanikolaou (NCBJ)

Mikko Alava (Aalto University, Finland)

Speaker:

Amin Esfandiarpour (NOMATEN Centre of Excellence, National Centre for Nuclear Research, ul. A. Soltana 7, 05-400 Swierk/Otwock, Poland)

Abstract:

Single-phase, concentrated solid solution (CSS) CrCoNi medium-entropy alloys with face centre cubic (fcc) crystal structure, have been recently found to display excellent mechanical properties. In particular, equiatomic CrCoNi solid solutions show higher yield strengths than the famed Cantor CrMnFeCoNi high entropy alloy at cryogenic and room temperatures. The main explanation for the exceptional behavior of CrCoNisolid solutions, is based on the Labusch-Varvenne class of solid solution analytical models, which point to the larger atomistic mismatch that is induced by Cr atoms. To further investigate the extent of the validity of this theory, in this study, we numerically investigate equiatomic VCoNi fcc CSS alloys, given that vanadium has a larger atomic volume than chromium and produces a larger atomic mismatch. Using Molecular dynamics (MD) simulations, we calculate the depinning stress, dislocation roughness, and stacking fault width for edge dislocations for four fcc VCoNi CSS alloys including V0.33Co0.33Ni0.33, V0.35Co0.2Ni0.45 , V0.33Co0.17Ni0.5, and V0.17Co0.33Ni0.5. With a random distribution of atoms, we find that the alloy composition V0.35Co0.2Ni0.45 displays the larger atomic mismatch, and also exhibits the largest depinning stress at 300 K. Furthermore, we use the experimental structure motif of chemical short range order (CSRO) in VCoNi to model short-range order in the alloys. The causal effect of CSRO on the magnitude of depinning stress is discussed.

XXI)

Topic: **Characterizing discrete dislocation configurations with alignment tensors and correlations**

Authors: **Thomas Hochrainer (TU Graz), Benedikt Weger (TU Graz),**
Satyapriya Gupta (Indian Institute of Technology Dharwad)

Speaker: Thomas Hochrainer (TU Graz)

Abstract:
Crystal plasticity is the result of moving and interacting dislocations. However, line like nature of dislocations and their complex interactions via long range stress fields and short range reactions so far defy all attempts to directly connect the dislocation microstructure with macroscopic materials properties and their evolution; where the evolution should in principle follow from the evolution of the dislocation microstructure itself.

Machine learning techniques offer stunning perspectives for shedding light on the complex interplay between dislocation structures and mechanical properties of crystals as well as for establishing evolution laws for the salient characteristics of these structures. That is, machine learning may yield what is more classically sought as a statistical continuum theory of dislocations. And in that, machine learning is likely to benefit from concepts used in such statistical theories. One key to any statistical continuum theory of interacting particles is the consideration of spatial correlations. However, because dislocations are extended one-dimensional defects, the classical definition of correlations for point particles is not readily applicable to dislocation systems. The line-like nature of dislocations entails that already the dislocation state should be characterized by a hierarchy of socalled alignment tensors [1], and, consequently, a scalar pair correlation function does not suffice for characterizing spatial correlations and a hierarchy of two-point tensors is required in general [2]. The extended nature of dislocations as closed curves moreover leads to strong self-correlations along the dislocation line. In the current contribution, we provide an overview how dislocation alignment tensors and according curvature tensors may be routinely extracted from discrete dislocation data based on nodes and straight segments. We introduce the concept of pair correlations for general averaged dislocation systems and illustrate selfcorrelations as well as the content of low order correlation tensors using a simple model system. We furthermore detail how pair correlation information may be obtained from three-dimensional discrete dislocation simulations and provide a first analysis of correlations from such simulations. We moreover present a new algorithm for extracting time-averaged dislocation velocity information from consecutive snapshots of dislocation configurations, similar to the `sweep tracing algorithm' recently introduced in [3].

Finally, we discuss how the various tensorial measures and the pair correlation information may be employed to improve existing continuum dislocation theories and we consider contexts in which we expect these measure to help in utilizing machine learning methods for modeling and for improving experimental measurement techniques.

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XXII)

Topic:

Thermal gelation of cellulosic fiber methylcellulose mixtures: rheological phases using Bayesian optimization

Author:
Juha Koivisto (Aalto University)

Speaker:
Juha Koivisto (Aalto University)

Abstract:
A thorough understanding of a polymers' viscoelastic behavior is a prerequisite for its application beyond laboratory scale. Utilizing rheological characterization is a powerful tool to comprehend the complex nature and time-dependent properties of macromolecular materials. Nevertheless, it consumes time as rheometry involves iterating experiments under several conditions to visualize the non-linear behavior of materials under varying conditions. The work hereunder examines the rheology of cellulosic aqueous suspensions prepared using cellulose fibers as the dispersed phase (Refcell and Storacell) and methylcellulose (MC) as the polymeric matrix. Interfacial phenomena between MC and cellulose fibers arise in particle laden systems with supramolecular structures formed by non-covalent interactions. Therefore, this study elucidates the rheological evolution of these interactions as a function of temperature and fiber concentration. This study displays how researchers may reduce the number of rheological experiments and save time utilizing a novel method based on a Bayesian optimization with Gaussian processes.

XXIII)

Topic:

Strain-rate-dependent predictability of discrete dislocation plasticity

Authors:

Marcin Mińkowski (Tampere University)

David Kurunczi-Papp (Tampere University)

Lasse Laurson

Speaker:

Marcin Mińkowski (Tampere University)

Abstract:

Predictability of plastic deformation of individual small single crystals containing dislocations subject to external loading is studied by combining discrete dislocation dynamics with machine learning [1]. Statistical features and pixelized images of the initial relaxed dislocation configurations are used as the input for machine learning algorithms. As a result an intriguing strain rate dependence of deformation predictability is revealed. For small strains the predictability increases with the strain rate, while for larger strains that relation becomes non-monotonic. It is shown that the monotonic behaviour at low strains can be related to the complexity of the dislocation dynamics measured as the fraction of dislocations moving against the external stress. On the other hand, the non-monotonic predictability at high strains is explained by relating it to a transition from fluctuating to smooth plastic flow as the strain rate becomes very high.

[1] M. Mińkowski, D. Kurunczi-Papp, L. Laurson "Machine learning reveals strain-rate-dependent predictability of discrete dislocation plasticity", Phys. Rev. Materials 6, 023602 (2022)

XXIV)

Topic:

Dynamics of stress propagation in crystals: comparing molecular dynamics simulations and analytical models.

Author:

Zbigniew Kozioł (National Center for Nuclear Research)

Speaker:

Zbigniew Kozioł (National Center for Nuclear Research, Materials Research Laboratory;
Andrzeja Sołtana 7, 05-400 Otwock-Świerk, Poland;
E-mail: zbigniew.koziol@ncbj.gov.pl)

Abstract:

Simulations in molecular dynamics (MD) often are carried out in an applied pressure, as for instance in case of modeling the dynamics of dislocations in materials. In analysis of results a crucial role is played by the proper understanding of underlying process of pressure penetration itself, since this is a dynamic process occurring at the same time scales as the studied properties of material.

We use a combined approach to describe in details the phenomenon of pressure penetration: results of MD simulations are guiding our analytical analysis based on a simple mechanical model of crystallographic lattice planes as a chain of masses undergoing oscillations described by equations of damped harmonic waves.

When external pressure is exerted on material surface, it penetrates it's interior with the speed of sound, and, depending on used boundary conditions, that wave may be reflected from the opposite side and interfere with the incoming wave. In case of ideal materials where energy losses can be neglected, the process is easy for description in mathematical therms. In real situations, adding energy damping leads to less straightforward picture that although qualitatively understood has not been so far discussed in details.

We show how the frequency of oscillating waves and damping process depend on intrinsic material properties, on crystallographic direction of sound propagation, and how the amplitude of waves depends on details of MD simulation procedure itself (size and geometry of sample, time step used, etc).

The worked out description is helpful in case of analysis of any MD simulations under pressure, as well it offers a convenient alternative way to already existing methods deriving elastic properties of materials from MD simulations.

XXV)

Topic:

Machine learning based atomistic dislocation modeling of nanoindentation of irradiated crystalline materials

Authors:

Francisco Javier Dominguez Gutierrez (NOMATEN Centre of Excellence)

Amir Naghdi (NOMATEN CoE)

Wei Guanyin (University of Helsinki)

Byggmastar Jesper (University of Helsinki)

Djurabekova Flyura (University of Helsinki)

Stefanos Papanikolaou (NCBJ)

Mikko Alava (Aalto University, Finland)

Speaker:

Francisco Javier Dominguez Gutierrez (NOMATEN Centre of Excellence)

Abstract:

Modern industries in aerospace, chemical, and energy and the development of next-generation fission and fusion nuclear reactors require novel materials with improved physical and chemical properties. Materials that can withstand extreme operating conditions like irradiation doses, preserving their mechanical properties with low cost of maintenance. Thus, experiments design needs the support from computational modeling to save technological and financial resources that would be necessary for excessive trials. Using advanced modeling with machine learning (ML) capacities would help to overcome the bottlenecks due to the high costs of high temperature equipment and long cycles of experimental work [1, 2].

In this work, we present a ML-based atomistic modeling of high temperature nanoindentation of an irradiated material commonly used in fusion experiments: Molybdenum. For this, we perform Molecular Dynamics (MD) simulations to model and investigate the effects of irradiation on the mechanical properties and nanoscale plastic deformation of crystalline Mo under spherical nanoindentation at a constant-displacement rate. We analyze the dislocation nucleation mechanisms for samples at [100], [110], and [111] crystal orientations in room temperature and an irradiation dose range of 0.01 to 0.2 dpa. We utilize different interatomic potential that describe the dynamics of dislocation nucleation: 1) a traditional EAM [2]; 2) Tabulated Gaussian approximation potential framework [3]; and 3) Neural Network interatomic potentials framework [4]. Results point towards both qualitative and quantitative differences in the response of dislocation nucleation during irradiation and nanoindentation. We report results by tracking dislocation nucleation, shape and evolution during nanoindentation test, that are drastically influenced by increasing temperature and considering irradiated sample that can pinned dislocations nucleation during loading process. These results are aimed to better characterize and model plastic deformation of material in extreme operating conditions.

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XXVI)

Topic:

Crystal nucleation in metallic systems: Unsupervised topological learning approach.

Author:

Noel Jakse (Université Grenoble Alpes, CNRS, Grenoble INP, SIMAP, F-38000 Grenoble, France.)

Speaker:

Noel Jakse (Université Grenoble Alpes, CNRS, Grenoble INP, SIMAP, F-38000 Grenoble, France.)

Abstract:

Theoretical understanding of crystal nucleation is still a challenging issue as experimental confirmation remains out of reach for bulk materials. Large-scale atomic-level simulations are therefore a promising substitute for such experiments, and molecular dynamics (MD) of million to billion atoms may indeed lead to meaningful results [1]. Machine Learning (ML) tools propose powerful methods to analyse such a large amount of MD-generated big data. An unsupervised ML approach [2] based on topological descriptors using persistent homology concepts [3] is proposed to reveal the structural features of atomic arrangements without a priori knowledge on the studied system. This approach is applied to monatomic metals [4,5] and is extended here to aluminium-based alloys. Both translational and orientational orderings are thus evidenced together with nucleation pathways, whose revealed features are beyond the hypotheses of the Classical Nucleation Theory [1]. This promising methodology more generally opens the route to an autonomous and in-depth investigation of atomic level mechanisms in material science.

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XXVII)

Topic:

Inferring Microstructure-Property Relationships in Discrete Dislocation Plasticity: Deformation Predictability and Materials Design

Author: Lasse Laurson (Tampere University)
Speaker: Lasse Laurson (Tampere University)

Abstract:

Discovering relationships between materials' microstructures and mechanical properties is a key goal of materials science. In general, the problem is challenging due to the combination of high dimensionality of microstructural descriptors as well as non-linearities and statistical fluctuations in the material response to external stimuli. A consequence is that many conventional materials design strategies relying essentially on educated guesses and trial and error can be argued to be sub-optimal, calling for novel informatics approaches able to cope with the complexity of materials deformation.

Here, I will present an overview of our recent efforts to apply machine learning and related tools to establish relationships between microstructural features of crystalline samples and their response to applied stresses. I will first discuss the concept of deformation predictability of small crystals where the plastic response, modelled using discrete dislocation dynamics simulations, exhibits significant sample-to-sample fluctuations. Our aim is to predict the sample-dependent stress-strain curves using information about the system's initial state as input. As a practical measure of deformation predictability, we consider the maximal coefficient of determination machine learning algorithms can establish between various sample-specific microstructural features and the sample stress-strain curve. Due to collective dynamics of dislocations manifested as a sequence of strain bursts with critical-like, broad size distributions [1], deformation predictability is a rather subtle and non-trivial concept, and is shown to depend on, e.g., the system size, strain, and the imposed strain rate [2,3,4].

Next, I will describe our attempts to tackle essentially the inverse problem of the above, i.e., finding optimised material microstructures corresponding to desired mechanical properties. More specifically, we consider here the problem of optimising the size distribution of precipitate particles in alloys, acting as obstacles for dislocation motion, subject to the constraint of a fixed volume fraction of precipitates. To this end, we apply Bayesian optimisation to efficiently search the multidimensional space of different precipitate size distributions within a simple two-dimensional discrete dislocation dynamics model, with the specific aim of maximising the expectation value of the stress at a given strain. Considering different dislocation-precipitate interaction potentials, we demonstrate the convergence of the algorithm to the optimal solution as a proof-of-concept [5], and discuss its possible extensions to the more complex and realistic case of three-dimensional dislocation systems with precipitates [6].

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XXVIII)

Topic:

AI-based modeling of crystal plasticity in concentrated solid solutions in extreme environments

Authors:

Karol Frydrych (National Centre for Nuclear Research)

Stefanos Papanikolaou (NCBJ)

Speaker:

Karol Frydrych (National Centre for Nuclear Research)

Abstract:

This work presents our recent developments in crystal plasticity (CP) modelling, as well as a vision on combining various approaches into a unified tool that enables interpretation of experimental data. First, we present our progress in building a continuum model of complex solid-solution alloys (CSAs). Then, preliminary results on accounting for irradiation hardening and indentation size effects will be shown. Finally, starting from CP parameter optimization, we present our vision on applying artificial intelligence (AI) for materials classification. To this end, neural networks (NN) will be trained using CP simulations. Then, the experimental data coming from mechanical testing, digital image correlation, nanoindentation (load-penetration curves and surface topographies) or electron back-scattered diffraction will be used as input to trained NNs to obtain the material class and model parameters.

XXIX)

Topic:

Symmetry and uncertainty-aware machine learning models of atomic interactions and dynamics

Author:
Boris Kozinsky (Harvard University)

Speaker:
Boris Kozinsky (Harvard University)

Abstract:
I will describe our efforts in using machine learning regression to achieve quantum mechanical accuracy of atomic interactions in large scale molecular dynamics simulations, enabling the study of previously intractable realistic materials systems. To accelerate molecular dynamics calculations, we developed equivariant interatomic potential models (NequIP) based on symmetry-preserving layer architectures and used them to achieve state-of-the-art accuracy and training efficiency for simulating dynamics of molecules, liquids, heterogeneous catalysts, and ionic conductors. In order to enable autonomous selection of the training set for reactive systems, we developed the FLARE adaptive closed-loop algorithm that constructs accurate and uncertainty-aware Bayesian force fields on-the-fly from a molecular dynamics simulation, using Gaussian process regression. We demonstrate the performance of ML-accelerated MD simulations by studying dynamics of phase transformations and catalysis.

XXX)

Topic:

Machine Learning for Atomistic Materials Science

Authors:

Alexandra Goryaeva (Université Paris-Saclay, CEA, Service de Recherches de Métallurgie Physique)

Thomas Swinburne (Aix-Marseille Universiť e, CNRS, CINaM UMR 7325, Campus de Luminy, 13288 Marseille, France)

Mihai-Cosmin Marinica (Université Paris-Saclay, CEA, Service de Recherches de Métallurgie Physique)

Speaker:

Mihai-Cosmin Marinica (Université Paris-Saclay, CEA, Service de Recherches de Métallurgie Physique)

Abstract:

We will present recent advances in atomistic material simulations by means of machine learning and data-driven approaches. In previous years, we have used ML to advance the knowledge of materials related to energy applications. Using the recently developed package MiLaDy (Machine Learning Dynamics) [2]: (i) we redefine the concept of defects in materials science [1,3]; (ii) we provide reliable force fields for complex defects such as interstitial, dislocation loops, dislocations; (iii) we are able to explore the atomistic free energy landscape (including migration energies [nn, mm]) of point defects in metals with ab initio accuracy up to the melting temperature [4], and, finally, (iv) we are able to propose surrogate models that bypass the traditional approaches [5]. We exemplify and discuss in the framework of experimental findings the case of energetic landscape of defects in body centered and face centered cubic metals.

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XXXI)

Topic:

Physics inspired Machine Learning (ML) Approaches for Materials Science:
On the importance of representations, prior information and adaptive experimental design

Author:

Udo v. Toussaint (Max-Planck-Institute for Plasmaphysics (IPP) Boltzmannstrasse 2, 85748 Garching, Germany)

Speaker:

Udo v. Toussaint (Max-Planck-Institute for Plasmaphysics (IPP) Boltzmannstrasse 2, 85748 Garching, Germany)

Abstract:

In recent years the development of data-centered approaches has revolutionized several fields, such as image recognition. The ongoing growth of computing power together with the improvement in algorithms and the increasing availability of large datasets led to a tremendous interest in ML approaches which also displayed promising results in many areas and are likely to yield even more astonishing results in the future. However, the benefits of ML typically come at the cost of big data production which commonly scales exponentially with the number of parameters. Thus in the mid- and long-term further progress hinges on two pillars: a) The development and exploitation of adaptive experimental design approaches ('active learning') together with surrogate-based optimization to mitigate the combinatorial explosion of computational requirements and b) information compression, i.e. the extraction of physical understanding (e.g. using reduced-complexity models (RCMs)) from the findings of a derived ML model also taking into account available domain-knowledge.

In the presentation we outline strategies for the adaptive experimental design cycle, the development of RCMs and the opportunities and challenges in this growing field.

XXXII)

Topic:

From Ontologies and FAIR Data to Machine Learning-based High-Throughput Data Mining of In-Situ TEM Experiments on Dislocations in HEAs

Author:

Stefan Sandfeld (Forschungszentrum Jülich (FZJ or FZ Jülich, Germany))

Speaker:

Stefan Sandfeld (Forschungszentrum Jülich (FZJ or FZ Jülich, Germany))

Abstract:

This talk will give an overview over recent developments in the field of material informatics and materials data science. In particular current activities, problems and challenges around implementing the FAIR data principle are presented and some steps towards developing multiscale microstructure ontologies are explained where the focus is both on technical as well as on conceptual aspects. All of this is based on a concrete Use Case with strong materials science background that motivates many of the current materials informatics approaches.

Within the Use Case the goal is to understand some of the many open questions concerning the underlying structure-property relations in High Entropy Alloys (HEAs). Although in-situ Transmission Electron Microscopy (TEM) allows high-resolution studies of the structure and dynamics of moving dislocations and -- in a way -- makes the local obstacle/energy "landscape" directly visible through the geometry of dislocations; a truly three-dimensional analysis and high-throughput data-mining of the resulting images or movies is still not possible.

This presentation gives an overview over current, state-of-the-art machine learning and data-mining techniques in the context of TEM experiments. We then introduce a novel data-mining approach that we based on spatio-temporal coarse graining of TEM dislocation movies, making ensemble averaging of a large number of snapshots in time possible. Using dislocations as "probes" we investigate the effect of pinning points on the dislocation gliding behavior of CoCrFeMnNi alloy during in-situ TEM straining. Additionally, we use our Deep Learning-based dislocation extraction and 3D reconstruction to analyze the strain avalanche statistics of in-situ TEM recordings and discuss the dependency of the power law exponent based on 3D discrete dislocation dynamics simulations.

Finally, based on this Use Case as well as based on a number of other, extremely promising, recent developments in combining materials informatics and data science we will take a look into a crystal ball and speculate about the future of materials science.

XXXIII)

Topic:

Critical modelling and informatics need for materials in additive manufacturing

Author:

Wang Yinmin (Morris) (University of California, Los Angeles)

Speaker:

Wang Yinmin (Morris) (University of California, Los Angeles)

Abstract:

Materials made by additive manufacturing (also known as 3D printing) often have unique microstructures, leading to unexpected materials properties. For structural materials such as metals and alloys, the complex processes of laser-materials interactions tend to generate numerous flaws and crystalline defects that will dictate the mechanical properties of as-built materials. This presentation will first identify some key aspects of these unique microstructural features, and their correlations with the strength and ductility of 3D printed materials. Our overall view is that additively manufactured alloys (e.g., 316L stainless steel, Ti-6Al-4V) have hierarchical microstructures (including compositional inhomogeneity), with length scale spanning over six orders of magnitude. High residual stress is another signature of such materials. A variety of modelling approaches have subsequently been developed to address the needs to understand the influences of different length scale features on mechanical behavior. We will discuss some of these modeling results, including finite element crystal plasticity modeling, CALPHAD, and dislocation dynamics simulations. In the end, we will elaborate our ongoing machine learning framework to predict the mechanical properties of additively manufactured materials.

XXXIV)

Topic:

Selected legal aspects of AI/ML development and deployment

Authors:

Pawel Sobkowicz (Nomaten Centre of Excellence, National Centre for Nuclear Research)

Michal Pecelerowicz (Nomaten Centre of Excellence, National Centre for Nuclear Research)

Michal Wójtowicz (National Centre for Nuclear Research)

Speaker:

Pawel Sobkowicz (Nomaten Centre of Excellence, National Centre for Nuclear Research)

Abstract:

One of the conditions necessary for the successful application of Artificial Intelligence/Machine Learning tools is access to high-quality training data. Despite the growth of interest in AI in many domains, or perhaps due to the explosive nature of this growth, the legal issues connected with the access to such training data, the rights and obligations connected to its use in the training of the AI/ML, and, finally, the limitations on the further use of the trained models are seldom considered. The conflict of interests between the creators and "owners" of data and algorithms, protected by traditional IPR and copyright mechanisms, and proponents and developers of AI/ML solutions, requesting freedom to use existing data and loosening of the existing restrictions is quite tense. Based largely on "public good" arguments, various countries have recently tended to favor the latter group, but the situation is quite complex – a condition exacerbated by the differences in legal systems in major geographies (in particular between US, China and Europe).

In this paper, we review some of these issues, particularly in research activities, potential commercialization, and specific challenges related to materials science.

XXXV)

Topic: **Neural-network based atomistic modeling of plastic deformation mechanisms of crystalline molybdenum**

Author: Amirhossein Naghdi Dorabati (NOMATEN CoE, National Centre for Nuclear Research, ul. A. Soltana 7 05-400 Otwock, Poland)

Co-authors: Javier Dominguez-Gutierrez (NOMATEN CoE, National Centre for Nuclear Research, ul. A. Soltana 7 05-400 Otwock, Poland)
Mikko Alava (Aalto University, Finland)
Stefanos Papanikolaou (NCBJ)

Speaker: Amirhossein Naghdi Dorabati (NOMATEN CoE, National Centre for Nuclear Research, ul. A. Soltana 7 05-400 Otwock, Poland)

Abstract:
Numerical simulations of different mechanical testing procedures for metals and alloys are not feasible without availability of accurate interatomic potentials that can predict the energy and interatomic forces of those systems. Take the example of crystalline Molybdenum (Mo), which is a great candidate to be used in extreme environments such as fusion reactors for coating of tungsten plates (W) and protecting it from material degradation due to the interaction with hydrogen plasma [1]. Therefore, it is of high interested to compute the mechanical properties for these kind of materials by first principle and classical force fields methods [2]. Addressing this issue is nowadays possible by employing Neural Network interatomic potentials (NNIP) which are trained on data sets supplied by density functional theory (DFT) simulations [3]. By using NNIPs, one can perform molecular dynamics (MD) simulations of thousands atoms samples which leads to a better understanding of underlying mechanical and thermal properties, roughness, elastic moduli, heat capacity, material's hardness, and thermal conductivity considering extreme operating conditions. In this work, PANNA [3] software is used to create a NNIP for modeling nanoindentation testing of pure crystalline Mo to investigate mechanisms of dislocation nucleation and evolution in a temperature of 300 and 1000 K . Elastic constants, dislocation densities, strain maps and slip traces as a function of indentation depth of the system are compared with embedded atom method (EAM) potentials, by using LAMMPS to explore the advantages and limitations of NIPPs over traditional potentials. These results can improve the characterization and modelling of plasma facing components for applications in the design of next generation of fusion machines [4].

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XXXVI)

Topic:

Sano Centre for Computational Medicine. Journey to transform healthcare.

Author:

Arkadiusz Sitek (Sano Centre for Computational Medicine)

Speaker:

Arkadiusz Sitek (Sano Centre for Computational Medicine)

Abstract:

Healthcare systems around the world face many challenges. A low efficiency of healthcare delivery is the common denominator of many of those challenges. I introduce computational medicine and explain how, together with “big-data,” it will increase the efficiency and the precision of healthcare delivery and improve outcomes. I introduce Sano, a new computational medicine research institute in Krakow, created to carry on applied research in this area.

XXXVII)

Topic:

Computational materials engineering with active learning

Author:

Milica Todorovic (Department of Mechanical and Materials Engineering University of Turku, Finland)

Speaker:

Milica Todorovic (Department of Mechanical and Materials Engineering University of Turku, Finland)

BIOGRAPHY:

Milica Todorović is an Assistant Professor in Materials Engineering at the Department of Mechanical and Materials Engineering, University of Turku. She gained an MSci in Physics at University College London, followed by a DPhil in Materials Science from Merton College at the University of Oxford. She went on to specialise in development and high performance computing applications of large-scale first principles calculations at the National Institute for Materials Science, Japan, and scanning probe microscopy simulations at Universidad Autonoma de Madrid before settling in Finland. Her research focuses on interfacing artificial intelligence algorithms with first principles simulations of materials with the aim to optimise material functionality.

Abstract:

Data-driven materials science based on artificial intelligence (AI) algorithms has facilitated breakthroughs in materials optimization and design. Of particular interest are active learning algorithms, where datasets are collected on-the-fly in the search for optimal solutions. We encoded such a probabilistic algorithm into the Bayesian Optimization Structure Search (BOSS) Python tool for materials research. We utilized this versatile tool to study molecular surface adsorbates, thin film growth, solid-solid interfaces, molecular conformers and even optimise experimental outcomes. New algorithm developments will allow us to harness the power of exascale computing platforms for next-generation materials engineering.