Advanced Characterization, Modelling and Data Science for Coatings and Thin Films
Room Town & Country C - Session CM4-1-MoM

Simulations, Machine Learning and Data Science for Materials Design and Discovery I

Moderators: Ferenc Tasnadi, Linköping University, Sweden, **Davide G. Sangiovanni**, Linköping University, Sweden

10:00am **CM4-1-MoM-1 Crystal Symmetry Determination in Electron Diffraction Using Machine Learning**, ***Kevin Kaufmann,*** Oerlikon Metco, USA **INVITED**

The recent adoption by the general public of artificial intelligence (AI) tools such as ChatGPT has reinvigorated research into AI applied to material science.Deep learning, a subset of AI, allows computer systems to autonomously learn patterns in data and construct efficient decision rules for tasks including classification, regression, or segmentation.In material analysis, these tools have primarily been applied to techniques requiring analysis of data collected in the form of images. Electron backscatter diffraction (EBSD) is one such technique benefitting from these recent efforts to improve material analysis by leveraging deep neural networks.Within the last decade, advancements in EBSD equipment have enabled the capture of high-definition diffraction patterns at rates exceeding 3,000 Hz.This creates significant opportunities for increasing the amount of information that can be ascertained from a sample, as well as opens the door for training data intensive deep neural networks.

Deep neural network-based classification of the diffraction patterns is motivated by Hough-based EBSD's susceptibility to structural misclassification; a failure mode that modern EBSD can encounter even when the researcher has complete knowledge of the sample prior to beginning analysis.While several methods to improve phase-differentiation have been proposed, each still requires pre-selection of phases and additional data (e.g. chemistry or simulated diffraction patterns) to be available.In contrast, deep neural network-based methods have demonstrated effective phase differentiation and identification of phases to the space group level without the need for further information.The deep learning approach to EBSD diffraction pattern analysis is capable of these more advanced analyses because it uses all information in the image when assessing a diffraction pattern, whereas traditional Hough-based EBSD pattern analysis discards a significant amount of information.

To promote adoption of AI tools, it must be determined if and when it is prone to error.To test the ideal operating conditions, the deep neural network model is trained using diffraction patterns captured with a fixed geometry and SEM settings, and a parametric study is performed to develop an understanding of model performance as several of the most common EBSD operating conditions are varied. Each time one parameter is varied, the diffraction patterns are re-collected, and the CNN used to reassess the space group identification.Ultimately, the model is found to retain a high classification accuracy even with significant changes to the diffraction conditions.

10:40am **CM4-1-MoM-3 Perturbation Analysis and Solutions to the One-Dimensional Cahn-Hilliard Equation in Thin Films**, ***Rahul Basu,*** 71 Nagavarpalyam, India

This paper presents an analytical investigation of phase separation dynamics in thin films using the one-dimensional Cahn-Hilliard equation. The main focus is on the development of perturbation solutions for Greens functions under various boundary conditions, specifically periodic, Neumann, and Dirichlet. The derived solutions provide insight into the behavior of concentration profiles, essential for understanding the phase separation process in technologically relevant thin film materials.

Thin films are widely used in various technological applications, including microelectronics and energy storage. The phase separation within these films is critical to their performance and properties. The one-dimensional Cahn-Hilliard equation serves as a fundamental model for studying the evolution of concentration profiles during phase separation. This paper aims to explore the dynamics of phase separation under different boundary conditions by deriving similarity transform and perturbation solutions to the Cahn-Hilliard equation.

Starting with the 1D Cahn Hilliard equations, Perturbation expansions are applied to the Green function solution and then evaluated for various boundary conditions. Alloys evaluated were Cu-Ni and Pd-Si.

Results showed differences for the different Boundary conditions and material parameters involved. The small perturbation parameter is chosen to be k the interface parameter. in the CH equation.

The results are hoped to be useful in designing surface thin films, using inputs like thermal diffusivity M and the interface parameter appearing in the CH equation.

11:00am **CM4-1-MoM-4 Predicting Segregation Behaviour in Polycrystalline Materials: A Case Study of P in Fe**, *Amin Reiners-Sakic, Christoph Dösinger, Alexander Reichmann, Ronald Schnitzer, Lorenz Romaner,* ***David Holec,*** Montanuniversität Leoben, Austria

The segregation of solutes to grain boundaries has a significant impact on material behaviour, particularly with regard to its mechanical properties and microstructural evolution. Computational tools have previously been employed to investigate this phenomenon, although the majority of studies are limited to coincidence site lattice (CSL) symmetrical boundaries. A methodology incorporating geometries associated with general grain boundaries, as observed in polycrystals, has recently been employed to investigate the substitutional segregation of phosphorus in iron. In this study, we further develop this approach to include interstitial sites. The model of polycrystalline bcc Fe comprises approximately $7x10^5$ atoms distributed across 12 grains of ~8 nm^3 total volume. Of these, approximately $1x10^5$ are substitutional segregation sites. In addition, approximately 1.2 million interstitial sites have been identified. The full segregation spectra for all of the aforementioned sites have been investigated using interatomic potentials in conjunction with state-of-the-art machine-learning techniques. The results demonstrate that phosphorus segregates to both site types, with a lower mean segregation energy for substitutional sites in comparison to interstitial sites. However, due to the higher number of interstitial sites, the total number of sites with comparable segregation energies to substitutional sites is significantly greater. By incorporating both segregation distributions, we can accurately predict P enrichment at different concentrations and temperatures, in agreement with experimental data. To validate this approach, we applied it also to Ni and H, showing that Ni segregates, albeit moderately, only to substitutional sites, while H segregates exclusively to interstitial sites, in line with existing literature.

11:20am **CM4-1-MoM-5 Tunable Interface Stress in Cu/W Nanomultilayers**, ***Yang Hu,*** *Giacomo Lorenzin, Jeyun Yeom,* Empa, Swiss Federal Laboratories for Materials Science and Technology, Switzerland*; Manura Liyanage, William A. Curtin,* EPFL, Switzerland*; Lars P.H. Jeurgens, Jolanta Janczak-Rusch, Claudia Cancellieri, Vladyslav Turlo,* Empa, Swiss Federal Laboratories for Materials Science and Technology, Switzerland

Controlling the intrinsic stresses developed during the growth of nanomultilayers (NMLs) is critical for their performance and applications. In Cu/W NMLs, a transition from positive to negative interface stresses has been observed under varying film deposition conditions, yet the underlying mechanisms driving this transition remain unresolved. The sign of experimentally measured interface stress has long been debated, highlighting the complexity of interface phenomena in NMLs.To address this, we employed atomistic simulations using a state-of-the-art neural network potential to uncover the strong influence of intermixing and metastable phase formation at Cu/W interfaces on interface stress. These simulations provide a direct link between interface chemistry and stress, a connection that is challenging to establish experimentally due to the difficulty of characterizing interfacial structures and compositions at atomic resolution for the Cu/W system.The insights gained from this work offer a deeper understanding of the interplay between interface structure, stress, and deposition conditions, paving the way for the rational design of NML coatings with tunable stress states. This approach enables the optimization of the thermomechanical stability and multifunctional properties of NMLs, advancing their applications in fields such as flexible electronics, energy storage, and protective coatings. Our findings also underscore the power of advanced computational methods in guiding materials design and addressing long-standing challenges in interface engineering.

11:40am **CM4-1-MoM-6 Understanding the Effects of Underlayer Materials on Electron Beam Resists Through the Use of Monte Carlo Simulations and the Development of a New Simulation Tool**, ***David Castillo Lozada,*** *Toby Thomassen, Scott Lewis, Axel Scherer, Guy De Rose,* California Institute of Technology, USA*; Luisa Bozano, Kevin Gu,* Applied Materials, USA

The ability to write structures at the nanoscale using lithography underpins all modern society. The electronic devices we take for granted contain integrated circuits, the key component being the field-effect transistors

(FETs). They have reduced in size by a factor of two every two years for over fifty years, following “Moore’s Law”. This size reduction is dependent on the continuous development of materials and techniques that produce better line resolution. The technical program aimed to apply a simulation tool called Excalibur to materials and processing problems critical to Applied Materials Inc. The Excalibur simulation suite can model the behavior of electrons and ions in the range of 100 keV to 3.6 eV. This software allows rapid prototyping of the next-generation resists for electron beam lithography (EBL) and ion beam lithography (IBL) for the semiconductor industry. Although Excalibur currently does not simulate extreme ultraviolet (EUV) radiation, we propose that it can provide a first-order analysis and prediction of EUV based on e-beam behavior. This project provides evidence that such prediction can be well modeled using the Excalibur tool. We also provide an alternative simulation, which we call Merlin, that aims to be more accurate and faster than its predecessor.

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