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

Moderator: Davide G. Sangiovanni, Linköping University, Sweden

10:00am **CM4-1-MoM-1 Crystal Symmetry Determination in Electron Diffraction Using Machine Learning**, ***Kevin Kaufmann [kevin.kaufmann@oerlikon.com]***, 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.

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 [david.holec@unileoben.ac.at]***, 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 Machine Learning Prediction of Work Functions for No, No_2, Co, Co_2, and H_2S Gas Molecules Adsorbed on $Znga_2O_4$(111) Surfaces**, ***Po-Liang Liu [pliu@dragon.nchu.edu.tw]***, *Hsiang-Yu Hsieh, Chao-Cheng Shen,* National Chung Hsing University, Taiwan

Zinc gallium oxide is a metal oxide gas sensing layer with exceptional thermal and chemical stability, capable of detecting gases such as NO, NO_2, CO, CO_2, and H_2S. The work function of Zinc gallium oxide can be assessed through first-principles calculations based on Density Functional Theory, which allows for the prediction of the sensor's sensitivity. Although Density Functional Theory provides accurate computational results, its high computational cost and time requirements limit its applicability for large-scale surface screening. This study used a database based on a density functional theory-based zinc gallium oxide sensor model. We developed an automated workflow using Python programming to extract crystal structure features as input for the machine learning model. The processed and filtered input features were employed to predict the work function of the sensor model, achieving a mean absolute percentage error below 6% in the prediction results. This study presents a trained machine-learning model interface that allows users to input crystal structure files for the rapid and accurate evaluation of the work function of Zinc gallium oxide sensors.

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