AI/ML for Scientific Discovery
Room Central Hall - Session AIML-ThP
AI/ML for Scientific Discovery Poster Session

AIML-ThP-1 High-Throughput Ab Initio Screening of MAB Phases: Phase Stability and Mechanical Property Relationships*, Nikola Koutna,* TU Wien, Austria*; L. Hultman,* Linköping Univ., IFM, Thin Film Physics Div., Sweden*; P. Mayrhofer,* TU Wien, Austria*; D. Sangiovanni,* Linköping Univ., IFM, Thin Film Physics Div., Sweden

MAB phases (MABs)—alternating atomically-thin ceramic and metallic-like layers—offer an interesting combination of mechanical, magnetocaloric, and catalytic properties, high-temperature oxidation resistance as well as damage tolerance, and have conquered a prominent role in the development of 2D materials. Despite their vast chemical and phase space, relatively few MABs have been achieved experimentally. In this poster I will present high-throughput ab initio screening of MABs that combine group 4–7 transition metals (M); Al, Si, Ga, Ge, or In (A); and boron (B). I will aim on revealing and understanding their phase stability trends and mechanical properties derived from elastic-constants-based descriptors. Considering the 1:1:1, 2:1:1, 2:1:2, 3:1:2, 3:1:3, and 3:1:4 M:A:B ratios and 10 competing phase prototypes for each elemental combination, the corresponding formation energy spectra of dynamically stable phases will be used to estimate the synthesisability of a single-phase MAB. Furthermore, the volumetric proximity of energetically-close MABs will allow identifying systems with possible transformation toughening abilities. The analysis of directional Cauchy pressures and Young's moduli will allow to analyze mechanical response parallel and normal to M–B/A layers. The poster will also suggest the most promising MAB candidates, including Nb_3AlB_4, Cr_2SiB_2, Mn_2SiB_2 or the already synthesised MoAlB.

AIML-ThP-2 Leak Detection Algorithm Through 2D Image Transformation of Multi-Wavelength Data from SPOES and Application of CNN*, Youngjun Yuk,* *k. Kim, H. Kim,* Tech University of Korea, Korea (Democratic People's Republic of)

In semiconductor processing, vacuum chambers are utilized for contamination prevention, plasma generation and so on. External air can enter through cracks in the chamber, which is referred to as a "leak." Leak can lead to a reduction in semiconductor yield. Therefore, it is essential to detect leaks in real-time. SPOES(Self-Plasma Optical Emission Spectroscopy) can analyze the gas composition inside the chamber in real-time through spectroscopic analysis and detect changes in gas composition instantaneously.

During the process of detecting leaks using SPOES, the DC offset can change due to various chamber conditions or noises such as thermal noise. If the offset changes, it becomes difficult to determine whether the increase in signal is due to a leak or a change in offset when only a single peak is used for leak detection. As a result, this can lead to the misclassification of leaks, thereby reducing the reliability of the system.

In this paper, to improve the misclassification problem, we propose a leak detection system with high reliability by using CNN classification algorithm with using 2D image transformation to monitor multi-wavelengths.

The most significant characteristics of the leak and offset change appear in the wavelengths where the signal changes. A leak signal affects only within specific wavelengths, whereas an offset change affects all wavelengths. A 2D image transform was applied to emphasize these characteristics, and by adding color changes, it became possible to simultaneously represent three dimensions of data: time, intensity, and wavelength. By utilizing this characteristic and monitoring both the wavelengths where leaks are detected and where leaks are not detected, we were able to collect SPOES data corresponding to leak, offset, and normal conditions, and clearly to identify the distinguishing features of each.

When CNN was applied to multi-wavelength data, higher accurate leak detect was achieved compared to applying machine learning to single-wavelength data. In an environment with 2.5 Torr N2 gas flow and no offset variation, a leak of approximately 0.4 ppm was detected with a maximum validation accuracy of 97.46% when three types of filters and machine learning algorithms were applied to the single-wavelength data. In contrast, when CNN was applied for classification, the leak was detected with a validation accuracy of 99.5%.

Acknowledgement: This paper was funded by the MOTIE (1415181071) and KSRC (Korea Semiconductor Research Consortium) (20019500) support program for the development of future semiconductor devices.

AIML-ThP-4 Neo: An Artificial Intelligence-Based Framework to Address Reproducibility Challenges in Materials Characterization*, Min Long,* *M. Lau,* Boise State University*; A. Burleigh, J. Terry,* Illinois Institute of Technology

We address the reproducibility challenges of improper analysis of the large and growing materials characterization data from modern and next-generation instruments by developing an open-source, artificial intelligence (AI) based framework: Neo that can reliably, more efficiently, and automatically analyze the data from various types of measurements. The datasets are usually complex and often require significant human effort to interpret and extract meaningful physicochemical insights. AI techniques have the potential to improve the efficiency and accuracy of surface analysis by automating data analysis and interpretation. Thus, we adopted intelligent methods like genetic algorithms, differential evolution, and neuroevolution algorithms to efficiently find the physical and chemical properties of materials that lead to high-quality fits of the experimental spectra. A human analyst suggests a set of initial parameters potentially present in the sample, used as theoretical standards and passes it to the framework. The framework then searches the large multidimensional space of combinations of these materials to determine the set of structural paths using the theoretical standards that best reproduce the experimental data. Our AI-based framework integrates with knowledge by not only finding the best mathematical description of the data but also the most physical and chemically meaningful results to improve the interpretability of models. The framework has been applied to various spectroscopy measurements and created sub-packages, such as EXAFS-Neo for extended X-ray absorption fine structure (EXAFS) measurements, Nano-Neo for nanoindentation load-displacement curve analysis, XES-Neo for X-ray emission spectroscopy (XES) analysis. We are also planning to extend this frame to other measurements like X-ray photoelectron spectroscopy (XPS). Our published results show that the method can successfully provide refined structures in simple molecules, bulk crystals, and from an operando lithium-ion battery with much less human intervention in comparison with conventional methods.

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