MM 22: Data Driven Materials Science: Experimental Data Treatment and Machine Learning

Time: Wednesday 10:15–13:00 Location: H46

Topical Talk MM 22.1 Wed 10:15 H46

Ingredients for effective computer-augmented experimental materials science — •Christoph T. Koch, Markus Kühbach, Sherjeel Shabih, Benedikt Haas, and Sandor Bockhauser — Humboldt-Universität zu Berlin, Department of Physics & IRIS Adlershof, Berlin, Germany

Experimentally exploring the properties and uses of materials and improving them for particular purposes has been a major driving force for advancing the way people live over the last millennia. Experimental materials characterization techniques have now reached the level of detail that makes them converge with ab-initio computations based on fundamental building blocks: atoms and the electrons they share. During the last decades computers have surpassed the capacity of humans in the extraction of patterns in large amounts of data. It is thus a very natural consequence to involve their strengths also in further accelerating experimental materials science. In this talk we will use modern transmission electron microscopy as an example to illustrate current and future ways of how the process of linking the properties of materials to their fundamental structure can be supported computationally and by the availability of FAIR experimental and theoretical data sets. Along the way the contributions of the NFDI-project FAIRmat to this process will be highlighted, illustrating the importance of defining well-documented metadata catalogues, as well as providing community-specific online data processing capabilities.

MM 22.2 Wed 10:45 H46

A materials informatics framework to discover patterns in atom probe tomography data — •Alaukik Saxena, Nikita Polin, Baptiste Gault, Christoph Freysoldt, and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf 40237, Germany.

Atom probe tomography (APT) is a unique technique that provides 3D elemental distribution with near-atomic resolution for a given material. However, the large amount of data acquired during the experiment and the complexity of the 3D microstructures poses a challenge to fully quantify APT data. Here, taking APT measurements corresponding to a Fe-doped Sm-Co alloy as an example, we present an approach based on unsupervised machine learning to extract different phases in the data. On top of this method, we have built a PCA-based workflow to reduce secondary phase precipitates with complex morphology into simpler plate-like morphologies thus enabling the quantification of in-plane compositional and thickness fluctuations, and relative orientations of the precipitates. The labeled data acquired from the PCA-based approach is used to train a U-NET to perform the same task on different APT samples of the same material automatically. The composition and thickness-related insights are expected to help understand the contribution of the particles to the confinement of the magnetic domains of the dominant 2:17 bulk phase, providing further indications to guide the design of future permanent hard magnets.

MM 22.3 Wed 11:00 H46

Correcting density artifacts in Atom Probe reconstructions: A tip shape-corrected volume reconstruction approach — •Patrick Stender[1], Daniel Beinke[1], Felicitas Bürger[2], and Guido Schmitz[1] — [1]Institute for Materials Science, University of Stuttgart — [2]Fakultät für Mathematik, Universität Regensburg, D-93040 Regensburg, Germany

Atom Probe Tomography enables the chemical investigation of nanometric volumes with single atomic sensitivity in 3D. The tip shape sample is evaporated atom by atom. From the obtained data sequence, the respective volume is reconstructed.

Conventionally, this reconstruction is performed with the assumption of a hemispherical tip apex. This practice can lead to serious volume distortions (local-magnification effect). Instead of using in-situ correlative microscopy to discover the evolution of the tip shape during the measurement, we extract the emitter shape numerically from the event statistics on the 2D detector plane.

The method is based on the fundamental postulate that the detected density of events is linked to the local Gaussian curvature of the tip apex. Knowing the variation of this curvature, the surface profile is determined by a finite difference scheme. Except for convexity, no further restriction is imposed on the possible tip shapes.

Different simulated and experimental data sets of complex tip shapes will be discussed and compared. The method largely suppresses the local magnification effects appearing at interfaces between materials of contrasting evaporation thresholds.

MM 22.4 Wed 11:15 H46

Neural networks trained on synthetically generated crystals can classify space groups of ICSD powder X-ray diffractograms — •Henrik Schopmans[1,2], Patrick Reiser[1,2], and Pascal Friederich[1,2] — [1]Institute of Theoretical Informatics, KIT, Karlsruhe, Germany — [2]Institute of Nanotechnology, KIT, Eggenstein-Leopoldshafen, Germany

Machine learning techniques have successfully been used to extract structural information such as the crystal space group from powder X-ray diffraction (XRD) patterns. However, training directly on simulated patterns from databases like the ICSD is problematic due to its limited size, class-inhomogeneity, and bias toward certain structure prototypes. We propose an alternative approach of generating random crystals with random coordinates by using the symmetry operations of each space group. Based on this approach, we present a high-performance distributed python framework to simultaneously generate structures, simulate patterns, and perform online learning. This allows training on millions of unique patterns per hour. For our chosen task of space group classification, we achieve a test accuracy of 60.4% on new ICSD structure prototypes not included in the statistics dataset guiding the random generation. Instead of space group classification, the developed framework can also be used for other common tasks, e.g. augmentation and mixing of patterns for phase fraction determination. Our results demonstrate, using the domain of X-ray diffraction, how state-of-the-art models trained on large, fully synthetic datasets can be used to guide the analysis of physical experiments.

15 min. break

Topical Talk MM 22.5 Wed 11:45 H46

Physics guided machine learning tools in analytical transmission electron microscopy — •Cecile Hebert[1,3], Hui Chen[1], and Adrien Teurtrie[1,2] — [1]LSME - IPHYS Ecole Polytechnique Fédérale de Lausanne, Lausanne, Switzerland — [2]Unité Matériaux et Transformations, Université de Lille, France — [3]Institut de Matériaux, Ecole Polytechnique Fédérale de Lausanne, Lausanne, Switzerland

Modern transmission electron microscopes are capable of recording large datasets containing both structural and chemical information on a scale ranging from sub-micrometer to atomic resolution. Operated in scanning TEM mode, two kind of chemical information can be obtained: either via energy dispersive X-Ray spectroscopy of via electron energy loss spectroscopy. On modern instruments, both signals can be acquired at the same time. Turning this huge amount of information (datasets can weight up to several Gb) into segmented quantitative information representing the different phases of the specimen is a real challenge. Pure statistical analysis like principal component analysis generally fails because of two main reasons: artifacts linked to the detection chain and/or non uniqueness of a statistical decomposition. The task is generally complicated by the overlap of phases in the specimen thickness and the presence of the same elements in different phases

With the introduction of physical constraints, like a modelling of the spectrum based on prior knowledge, both on the specimen and on the physical process leading to the spectra, it is possible to obtain a physically meaningful spatial segmentation of the data and to proceed with chemical analysis.

MM 22.6 Wed 12:15 H46

Motif Extraction from Crystalline Images in Real Space — •Amel Shamseldeen Ali Alhassan and Benjamin Berkels — AICES Graduate School, RWTH Aachen University, Germany

Using modern transmission and scanning transmission electron microscopes ([S]TEM), atomic resolution images are readily available. In particular, the amount of data produced is so large that automatic analysis tools are needed.

During the last decade, automatic data analysis methods concerning different aspects of crystal analysis have been developed, for example, unsupervised primitive unit cell extraction and automated crystal dis-

tortion and defects detection. However, an automatic, dedicated motif extraction method is still called for by experimentalists. While previous works on motif extraction did good work in, for example, finding the plane symmetries and restoring smeared out features or finding positions in atomic columns, they were either not automated enough, not applicable to atomic scale images, or required special calibration.

Here, we propose and demonstrate a novel method for automatic direct motif extraction from crystalline images based on variational methods. Given an atomic resolution crystalline image, our method employs unit cell extraction to find the atomic structure then solves a minimization problem involving the unit cell projection operator to find the motif. The method was tested on various synthetic and experimental data sets. The results are a representation of the motif in form of an image, primitive unit cell vectors and a denoised reconstruction of the input image.

MM 22.7 Wed 12:30 H46

Analysis of acoustic emission spectra for structural health monitoring — •Klaus Lutter, Viktor Fairuschin, and Thorsten Uphues — Institute for Sensor and Actuator Technology, Coburg, Germany

Today, the analysis of vibration and acoustic emission spectra is routinely used for health monitoring of gears in industrial production. Recent developments of extended IIoT networks provide even fleet comparison and optimization of required field service.

Here, we present an extended approach to utilize acoustic emission spectra to monitor the structural health of machining tools like mills or drills to extract degradation and lifetime information from the acoustic emission. A successful application of a spectral analysis will provide a huge impact on production quality as well as tool quality according to different production parameters which are transferred into related spectral properties. Furthermore we follow an experimental approach using contact microphones. Our diagnostic approach is a detailed analysis of the corresponding frequency spectra and in particular the existing harmonic frequencies during milling processes.

We demonstrate the classification of different process parameter sets according to different dominant frequencies via classification algorithms. The retrieved classes of spectra are used for a classical regression model assisted by neural networks to analyse characteristics changes over time. From an industrial perspective this type of analysis is a non-invasive and versatile approach and easily implementable, even in existing production machinery.

MM 22.8 Wed 12:45 H46

Optimizing laser powder bed fusion by machine learning methods — •Dmitry Chernyavsky — IFW Dresden, Germany

Additive manufacturing (AM) is a revolutionary manufacturing technique, providing design freedom and environmental advantages. Each newly AM processed material usually requires the identification of the optimal parameter set, a cost and time-consuming process, mostly conducted by trial and error. Here we discuss a machine learning approach for AM process parameter optimization on an example of a Zr-based alloy.