MM 56: Topical Session (Symposium MM): Big Data in Materials Science - Managing and exploiting the raw material of the 21st century

Big Data III

Time: Thursday 11:45–13:15 Location: H 0107

Topical Talk MM 56.1 Thu 11:45 H 0107

On the need for a digital representation of materials data along scientific and industrial processes — •Christoph Schweizer, Eva Augenstein, Heiner Oesterlin, and Adham Hashibon — Fraunhofer Institute for Mechanics of Materials IWM, Freiburg, Germany

In the field mechanics of materials and material science and engineering in general, an ongoing challenge is to identify process-structure-property relationships. Due to the vast amount of manufacturing processes, mechanical properties as well as characterization and simulation methods on all scales, the resulting research data is extremely heterogeneous in nature. In this work, first steps are undertaken to set up an ontological knowledge base, which can be used to manage and analyze a large amount of material histories and provides the flexibility, which is needed to work on a scientific level. The ontology provides the structure and logical relations, which are needed to set up and later analyze the knowledge base. A small domain ontology is created based on the upper level Basic Formal Ontology (BFO) and the European Materials Modelling Ontology (EMMO), which are currently under development. The knowledge base which can be represented as a network graph is created and filled with research data from available public funded projects dealing with metallic high temperature materials, the underlying manufacturing processes, characterization methods, the microstructure and the mechanical properties. It is demonstrated, that the resulting network graph can be analyzed to identify process-structure-property relationships.

MM 56.2 Thu 12:15 H 0107

Probabilistic neural network design of an alloy for direct laser deposition — Bryce Conduit[1], Trevor Illston[2], Divya Vadgadde Duggappa[3], Scarlett Baker[1], Steve Harding[4], Howard Stone[5], and •Gareth Conduit[6] — [1]Rolls-Royce plc, PO Box 31, Derby, DE24 8BJ, United Kingdom — [2]Materials Solutions, Worcester, WR4 9GN, United Kingdom — [3]Rolls-Royce plc, Bangalore, India — [4]Rolls-Royce plc, PO Box 3, Bristol, BS34 7QE, United Kingdom — [5]Department of Materials Science & Metallurgy, University of Cambridge, 27 Charles Babbage Road, Cambridge, CB3 0FS, United Kingdom — [6]Cavendish Laboratory, University of Cambridge, J.J. Thomson Avenue, Cambridge, CB3 0HE, United Kingdom

A neural network tool was used to discover and characterize the new nickel-base alloy for direct laser deposition most likely to simultaneously satisfy targets of processibility, cost, density, phase stability, creep resistance, oxidation, and resistance to thermal stresses. Experimental testing confirms that the physical properties of the proposed alloy exceed those of other commercially available Ni-base alloys for combustor liner applications.

MM 56.3 Thu 12:30 H 0107

ab initio Phase Stability: From 0 K to Relevant Temperatures — •Moritz to Baben, Chandrahaasan Kattuputhur, and Klaus Hack — GTT-Technologies, Herzogenrath, Germany

Today, large repositories with ab initio calculation results for over a million compounds exist [1,2,3]. However, these contain only data from calculations at 0 K. Phase stability predictions on the other hand requires information on the Gibbs energy at elevated temperatures. Here, the current state of the art relies on CalPhaD (Calculation of Phase Diagrams) databases which have been derived mostly from experiments at high temperatures and contain only some thousands of compounds. In this contribution it will be discussed how ab initio phase stability data can be used at relevant temperatures -introducing the new aiMP database in FactSage [4]- and the veracity of the data is benchmarked. Systematic discrepancies between energy of formation from ab initio calculations and experiments e.g. for nitrates are discussed and the accuracy of high-throughput ab initio calculations for energy of formation of metallic systems is challenged. [1]: materialsproject.org [2]: aflowlib.org [3]: oqmd.org [4]: C.W. Bale et al., FactSage thermochemical software and databases, 2010-2016, CALPHAD 54 (2016) 35

MM 56.4 Thu 12:45 H 0107

Damage classification in DP steel using neural networks — •Tom Reclik[1], Carl F. Kusche[1], Ulrich Kerzel[2], and Sandra Korte-Kerzel[1] — [1]Institut für Metallkunde und Metallphysik, RWTH Aachen, Germany — [2]Lehrstuhl für Operations Research, RWTH Aachen, Germany

To this day, various methods are used in order to reveal the micromechanical mechanisms of damage in materials. Post-mortem analysis at different stages of stress reveals only snapshots of the material, while in-situ methods are spatially limited to observing the evolution of only a few damage events. A limiting factor in all those methods is the amount of work involved in controlling the microscope and the image analysis. In this work, we implement different structures and architectures of neural networks for the localization and classification of damages. As a sample material dual-phase steels are chosen, due to the different responses of the ductile ferrite matrix and the brittle martensite islands to stress, resulting in the formation of damage sites belonging to distinct classes at early stages of deformation. The developed algorithms can on the one hand be used in order to automate the statistical evaluation of post-mortem micrographs, while on the other hand enabling in-situ experiments to generate statistically relevant data. Due to the computational nature of this method, a high throughput of data is possible, enabling a more complete understanding of failure mechanisms in many materials.

MM 56.5 Thu 13:00 H 0107

A machine-learning approach for finding new hard-magnetic phases — Johannes J. Möller, Anna J. Lehner, Daniel F. Urban, and •Christian Elsässer — Fraunhofer IWM, Freiburg, Germany

Data-mining and machine-learning (ML) techniques play an increasingly important role in the discovery and development of new materials. In this contribution, we use kernel-based learning methods to predict optimal chemical compositions for new permanent magnets, which are key components in many green-energy technologies. The magnetic-property data used for training and testing the ML models were obtained by a combinatorial high-throughput screening (HTS) using density-functional theory calculations. For encoding the structural and chemical information of the HTS data in a machine-readable format, we use several existing and newly developed material descriptors and assess the predictive power of the ML models built with them. The accuracy of the ML models with an optimal choice of descriptor and model parameters enables the prediction of promising structure-composition combinations for substitutes of state-of-the-art magnetic materials like $Nd_2Fe_{14}B$ - with similar intrinsic hard-magnetic properties but no or less amounts of critical rare-earth elements.