CPP 14: Topical Session: Data Driven Materials Science - Materials Design I (joint session MM/CPP)

Time: Monday 10:15–11:30 Location: BAR 205

Topical Talk CPP 14.1 Mon 10:15 BAR 205

Data-Mining Strategies for Understanding Strength and Failure of Materials — •Stefan Sandfeld — TU Bergakademie Freiberg, Lampadiusstr. 4, 09599 Freiberg

Experimental observations and simulation data should – in principle – help to shed light on the 'inner workings' of a physical system, say, a material or specimen. There, the 'inner workings' would be the interaction of microstructural features among themselves, with the surfaces of the specimen, with defects, or with phase boundaries, to name but a few. Both experiment and simulation, however, suffer from particular problems which in many situations makes it difficult to directly compare them or to use results from one as input or support for the other.

In this presentation, we will start by giving an overview over current attempts for integrating experiment and simulation. We will then demonstrate, on the one hand, how data science approaches might be used to access data from experiments that would be otherwise inaccessible and, on the other hand, how data science also might help to reduce the high level of abstraction inherent to most simulations. With those methods, experiment and simulation might get a little closer to each, thereby helping to understand relevant mechanisms in strength and failure from a new point of view.

CPP 14.2 Mon 10:45 BAR 205

Stabilities of novel Mg-based light metal high entropy alloys — •Wernfried Mayr-Schmölzer[1], Johannes Kirschner[2], Clemens Simson[4], Christoph Eisenmenger-Sittner[2], Johannes Bernardi[3], Stefan Müller[1], and Gregor Vonbun-Feldbauer[1] — [1]Institute of Advanced Ceramics, Hamburg University of Technology — [2]Institute of Solid State Physics, TU Vienna — [3]USTEM, TU Vienna — [4]LKR, Austrian Institute of Technology GmbH

Compositionally Complex Alloys (CCAs) consist of four or more elements alloyed in approximately equal fractions and often crystallize in a simple crystal lattice. In many cases, their mechanical properties like structural stability or ductility exceed that of common modern alloys. Usually, they contain heavy d-Orbital metals, but investigations into low density light metal CCAs have been rare up to now due to the complex binding modes of their constituents.

We use both a Cluster Expansion approach, augmented by stochastic prescreening steps, and neural network based pair potentials to scan the large configuration space of the Mg-Al-Cu-Zn system for stable phases. The training data was generated using density functional theory calculations implemented in the VASP code. In conjunction with experiments, we find that while the introduction of Al into the brittle $MgZn_2$ hexagonal Laves phase leads to phase separation and does not improve the mechanical properties of the alloy, the addition of Cu inhibits this process and leads to the formation of a highly stable cubic phase.

CPP 14.3 Mon 11:00 BAR 205

Automatic design of reversible shape changing metamaterials — Silvia Bonfanti, Francesc Font Clos, Roberto Guerra, and •Stefano Zapperi — University of Milan, Milan, Italy

We have developed a computational method to design metamaterials that perform pre-determined input/output mechanical operations. Our numerical scheme to design metamaterials combines a reinforced dynamic Monte Carlo method with finite element simulations. We performed 3D printing of selected metamaterial configurations, showing that the machine-generated solutions present effciencies far exceeding those of man-designed ones. Finally, we show that machine learning algorithms can be trained to identify efficient solutions without performing simulations. The designed metamaterial units can be exploited as the building blocks of generic metamaterial machines or other actuators with higher complexity.

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CPP 14.4 Mon 11:15 BAR 205

Towards Building New Zeolites with Machine Learning — •Benjamin A. Helfrecht[1], Rocio Semino[1,2], Giovanni Pireddu[1,3], Scott M. Auerbach[4], and Michele Ceriotti[1] — [1]École Polytechnique Fédérale de Lausanne, Lausanne, Switzerland — [2]Université de Montpellier, Montpellier, France — [3]Università degli Studi di Sassari, Sassari, Italy — [4]University of Massachusetts Amherst, Amherst, Massachusetts USA

Synthesizing new zeolites, which are useful for applications like gas separation and catalysis, with specific properties is an ongoing challenge in the zeolite community. Ideally, one would like to select a handful of compatible "building blocks" from which a new zeolite with desired properties can be synthesized. In this work, we make progress toward this goal by constructing an "atlas" of local atomic environments comprising several thousand all-silica zeolites from the Deem SLC PCOD database [1] using machine learning techniques. We evaluate the utility of this atlas by examining correlations between the locations of the atomic environments in the atlas and their energy and volume contributions to their parent frameworks.

[1] R. Pophale, P. A. Cheeseman, M. W. Deem, A database of new zeolite-like materials, Phys. Chem. Chem. Phys 13(27):12407-12412, 2011.