MM 10: Invited talk Körmann

Time: Monday 15:00–15:30 Location: BAR 205

Invited Talk MM 10.1 Mon 15:00 BAR 205

High-Entropy Alloys: Materials design in high dimensional chemical space from ab initio thermodynamics — •Fritz Körmann — Max-Planck-Institut für Eisenforschung GmbH, D-40237 Düsseldorf, Germany — Materials Science and Engineering, Delft University of Technology, 2628 CD, Delft, The Netherlands

A well-targeted design of modern alloys such as high entropy alloys (HEAs) is extremely challenging due to their immense composition space. In this talk I will discuss recent advances in fully parameter-free ab initio calculations combining advanced statistical concepts and machine learning techniques. These novel techniques allow to computationally identify favorable composition islands in the high dimension chemical phase space solely on the computer. Using this approach, various mechanisms and concepts proposed in the literature have been tested: Besides lattice distortions, stacking-fault energies (SFEs) have been successfully used as a descriptor to link atomistic simulations to the macroscopic deformation mechanisms that are behind the superior mechanical performance. Interstitial alloying with C reveals, e.g., large fluctuations in solution energies depending on the specific local chemical environment and its impact on SFEs can be even qualitatively different depending on alloy composition. We also discuss BCC-HCP stability as promising descriptor to identify mechanically appealing refractory HEAs and the critical role of lattice distortions therefore. Based on these computationally highly expensive computations easy-to-use materials design rules will be derived and discussed for the various examples.