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ABSTRACT:

Ab Initio Thermodynamics of Defect Phases in Metals

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Thermodynamic bulk phase diagrams have become the roadmap used by researchers to identify alloy compositions and process conditions that result in novel materials with tailored microstructures. On the other hand, recent progress in experimental atomic-scale characterization techniques allows one to study the local chemical composition at individual defects such as interfaces, grain boundaries, dislocations and surfaces. They show that changes in the alloy composition can drive not only transitions in the bulk phases present in a material, but also in the concentration and type of defects they contain. Defect phase diagrams, using chemical potentials as thermodynamics variables, provide a natural route to study these chemically driven defects [1]. Our results show, however, that the direct application of thermodynamic approaches can fail to reproduce the experimentally observed defect formation.
Therefore, we extend the concept to metastable defect phase diagrams to account for kinetic limitations that prevent the system from reaching equilibrium [2]. We use ab initio calculations based on density functional theory to quantify the extension of regions where defect formation is expected. We successfully applied this concept to explain the formation of large concentrations of planar defects in supersaturated Fe2Nb Laves phases. In addition, we identify in a joint study with experiments conditions and structures in Mg-Al-Ca alloys for defect phase occurrence. The concept offers new avenues for designing materials with tailored defect structures.

[1] S. Korte-Kerzel, T. Hickel, L.Huber, D. Raabe, S. Sandlöbes-Haut, M. Todorova, J. Neugebauer, Int. Mat. Rev. 67, 89-117 (2021).
[2] A. Tehranchi, S. Zhang, A. Zendegani, C. Scheu, T. Hickel, J. Neugebauer, arXiv:2303.07504 [cond-mat.mtrl-sci] (2023).