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ABSTRACT:

Grain Boundary Segregation Beyond the Dilute Limit Combining Calphad and Ab-Initio Modeling

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Ab-initio calculations are frequently used to compute grain boundary (GB) segregation energies and to investigate the segregation behavior of alloying elements in metals. In particular, the spectrum of segregation energies arising from the GB crystallography can be explored conveniently. In most cases, however, segregation spectra have been provided in simple host crystal structures, i.e. either the fcc, hcp or bcc phase, for binary alloys and in the dilute limit. Going beyond such conditions can be non-trivial and requires a consistent thermodynamic framework to guide the ab-initio calculations.
In this talk we show how the compound energy formalism, that is often applied in CALPHAD simulations, can be used to establish a clear link between DFT energies, the GB energy and the GB excess for general solid solution phases [1,2]. An example of a concentrated binary solution is presented with the W-Ti system where we demonstrate how ab-initio calculations provide the relevant endmember energies and how a moment tensor potential is trained and used to completely describe the grain boundary surface of reference of the symmetrical Σ3[1-10](111) GB. Our results reveal that the segregation of Ti changes from anti-segregation to segregation behavior with increasing Ti content as a result of the treatment beyond the dilute limit. Further, no thermodynamic stabilization of nanocrystalline W-Ti is expected. As a second example we move to a ternary system and discuss the segregation behavior of B in Ti(B,N) PVD layers that are used in hard coating applications.

[1] T. Spitaler, D. Scheiber, C. Dösinger, M. Hodapp, L. Romaner Acta Materialia 286, 120725 (2025).
[2] A. Reichmann, C. Kainz, N. Schalk, T. Spitaler, M. Burtscher, L.Romaner Materials & Design 260, 114912 (2025).