ABSTRACT

Prediction of Multicomponent Diffusion Coefficients from Unary and Binary Data

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This talk employs ample examples to illustrate the process and outcomes of predicting diffusion coefficients of multicomponent solid solutions using unary and binary diffusion coefficient data. The unary data include self-diffusion and impurity-diffusion coefficients of pure elements. The general methodology is based upon the Andersson-Ågren treatment of atomic mobilities [1] under the CALPHAD framework. The required thermodynamic factor is directly computed from CALPHAD assessments of the pertinent binary and multicomponent systems. The 1-parameter Z-Z-Z model [2] allows both tracer, intrinsic and inter-diffusion coefficients to be reliably computed for any composition at any temperature after the sole constant is evaluated from the diffusion data. A simple combination of the Z-Z-Z binary model parameters without any additional fitting parameters already provides impressive predictions of the ternary diffusion coefficients when the 3 cross-binary parameters are set to be the 3 corresponding binary Z-Z-Z model interaction parameters, leading to a robust Z-Z-ternary diffusion model [3]. When ternary diffusion coefficients are available for a ternary system from experimental measurements, 3 cross-binary parameters can be directed fitted and employed to yield more accurate predictions of ternary diffusion coefficients using the binary and cross-binary parameters only (BCBPO) model [3]. Further extrapolation into multicomponent solutions is very straightforward via the Andersson-Ågren treatment. Examples will be given to show the reliability of such predictions of diffusion coefficients in ternary and multicomponent systems, including high-entropy alloy compositions. The overall methodology will significantly accelerate the establishment of diffusion coefficient databases for simulation of kinetic processes in materials, especially multicomponent alloys where experimental data are scarce.

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[3] W. Zhong and J.-C. Zhao, Scripta Mater., 207, 114227 (2022).