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ABSTRACT:

A Multiobjective Optimization-Based Numerical Inverse Method for Determination of Diffusion Coefficients in Multicomponent Alloys from Pseudo-Binary and Pseudo-Ternary Diffusion Couples

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Numerical inverse methods are developed to estimate the composition-dependent interdiffusion coefficients from the measured concentration profiles in binary or ternary diffusion couples. The aim of such an inverse method is to minimize the difference between the numerically computed profiles and the experimental profiles. Problems with such techniques are non-uniqueness of solutions and mathematical ill-posedness leading to divergence of the estimated interdiffusion coefficients. These problems can be avoided or reduced if multiple diffusion couples are used instead of a single one. However, for multicomponent diffusion couples, the problem of uniqueness of solution remains. This is because of the rapid increase in the number of unknown parameters to be determined when the number of components increase beyond three. To keep a check on the number of unknown parameters, one needs to use either experimental estimates of diffusion coefficients or measured interdiffusion flux as constraints in addition to inequality conditions on interdiffusivity matrix arising due to positive definiteness of the matrix of Onsager coefficients. Since measured interdiffusion coefficients can be non-unique in nature as they strongly depend on the experimentally developed concentration profiles, experimentally measured tracer or intrinsic diffusion coefficients are much more fundamental and reliable constraints.

Here we present a numerical inverse method based on a novel PDE-constrained multiobjective optimization technique for analysis of diffusion profiles where we utilize experimentally estimated tracer and intrinsic diffusion coefficients as well as measured interdiffusion fluxes as constraints and pseudo-binary (PB) and pseudo-ternary (PT) diffusion profiles as design targets for the prediction of reliable composition-dependent mobility data. Since experimental PB and PT methods produce accurate analytical estimates of tracer/intrinsic diffusion coefficients at the intersections of diffusion paths in multicomponent alloy systems, these constraints have enabled reliable estimation of mobility data across the composition range of PB and PT diffusion profiles. We will discuss how different methods such as evolutionary optimization algorithms or physics-informed neural

networks (PINN) can be used for multiobjective optimization to reliably estimate diffusion coefficients in multicomponent systems. We will also discuss the robustness of our method and ways to further improve it.