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ABSTRACT:

Ideal and Non-ideal Pseudo-binary Diffusion Profiles for Estimation of Diffusion Coefficients in Multicomponent Systems

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The concept of the pseudo-binary diffusion couple method was one of the first experimental methods proposed for the estimation of meaningful diffusion coefficients in a multicomponent system [1]. This is a straightforward and most versatile method if used intelligently. Two issues can be witnessed for the practice of this method. The elements, which are expected to remain constant, may have a different composition in the end members of a pseudo-binary diffusion couple. This can be solved by remelting the alloys. Moreover, one or more elements may produce a diffusion profile instead of remaining constant. It can be ignored if the non-ideality is negligible or minor. This is explained in detail with experimental and simulated profiles. Ideal pseudo-binary diffusion profiles can be utilised to estimate tracer and intrinsic diffusion coefficients at the Kirkendall marker plane [2, 3]. This is otherwise impossible to achieve following the Kirkendall marker experiment in a multicomponent diffusion profile. Even non-ideal pseudo-binary diffusion couples are helpful to constrain the diffusion paths intelligently for intersecting or passing the diffusion paths with negligible distance for estimation of diffusion coefficients of all the elements from only two diffusion paths. This is explained in NiCoFeCrAl high entropy alloys [4]. We have further shown that the discussion of relative mobilities with estimated interdiffusion coefficients of the elements may be vague or misleading in a multicomponent system unless the tracer diffusion coefficients are estimated. Moreover, we have shown that the contribution of the vacancy wind effect must be addressed, which may have a very significant role in a multicomponent system.

[1] A. Paul, A pseudo binary approach to study interdiffusion and the Kirkendall effect in multicomponent systems, Philosophical Magazine, 93 (2013) 2297-2315
[2] A. Dash, N. Esakkiraja and A Paul, Solving the issues of multicomponent diffusion in an equiatomic NiCoFeCr medium entropy alloy, Acta Materialia 193 (2020) 163-171

[3] H Kumar, A Dash, A Paul, S Bhattacharyya, A physics-informed neural network-based numerical inverse method for optimization of diffusion coefficients in NiCoFeCr multi principal element alloy, Scripta Materialia 214 (2022) 114639
[4] A. Dash, S. Bhattacharyya and A. Paul, under review, 2023.