

Supplementary Materials

An Effective Approach to Acquire the Impurity Diffusion Coefficients in Binary Alloys with Quantified Uncertainties

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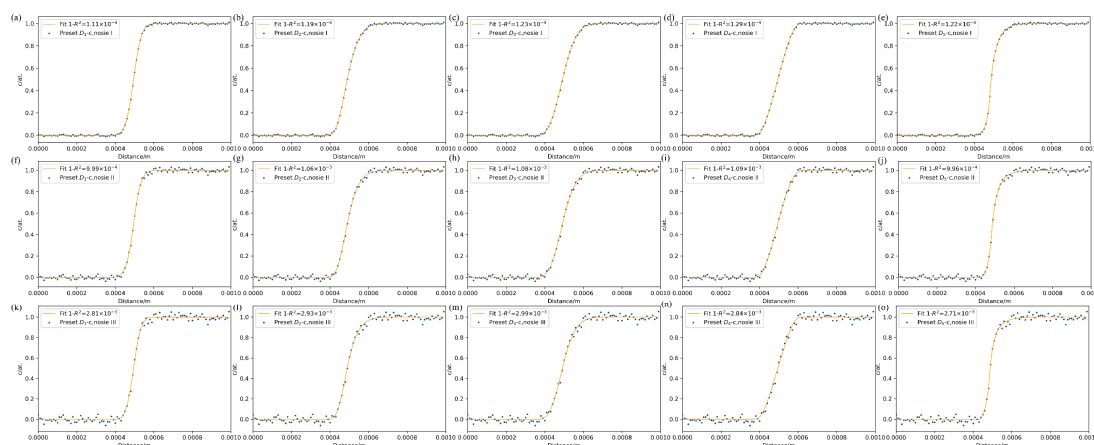


Figure S1. Composition profiles fitted by distribution functions compared with the $c-x$ data due to the pre-set D_1 , D_2 , D_3 , D_4 , D_5 with different noise levels. (a–e) noise level I; (f–j) noise level II; (k–o) noise level III.

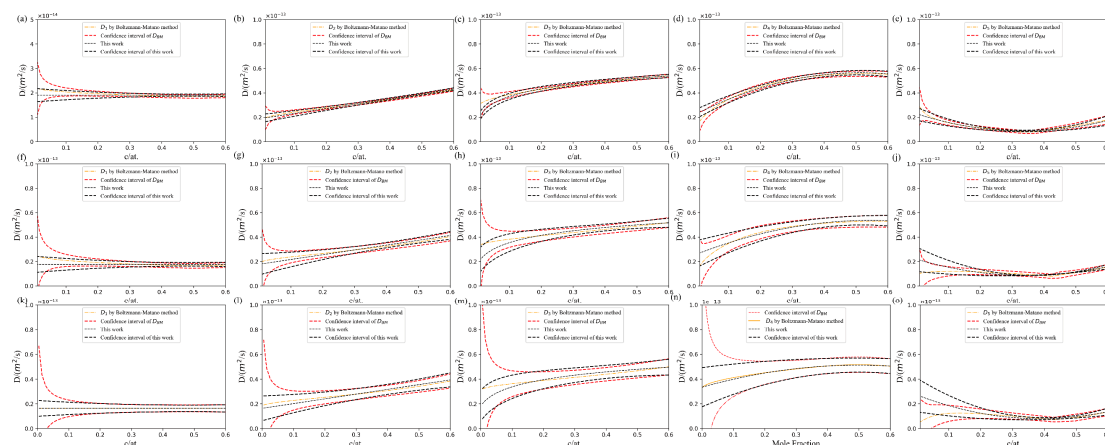


Figure S2. Fitted interdiffusion coefficients together with uncertainties compared with the interdiffusion coefficient evaluated using the Boltzmann–Matano method from the $c-x$ data due to the pre-set D_1 , D_2 , D_3 , D_4 , D_5 with noise and uncertainties evaluated using the uncertainty quantification approach. (a–e) noise level I; (f–j) noise level II; (k–o) noise level III.

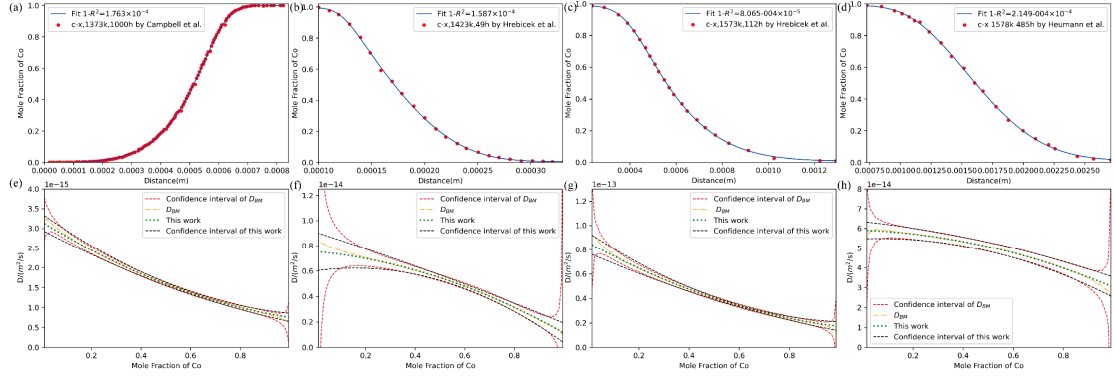


Figure S3. (a–d) Composition profiles fitted by distribution functions compared with the experimental data of the Co/Ni diffusion couples annealed at different temperatures [1–4]; (e–h) presently fitted interdiffusion coefficients and uncertainties compared with the interdiffusion coefficients evaluated using the Boltzmann–Matano method and the uncertainties quantified using the uncertainty quantification approach.

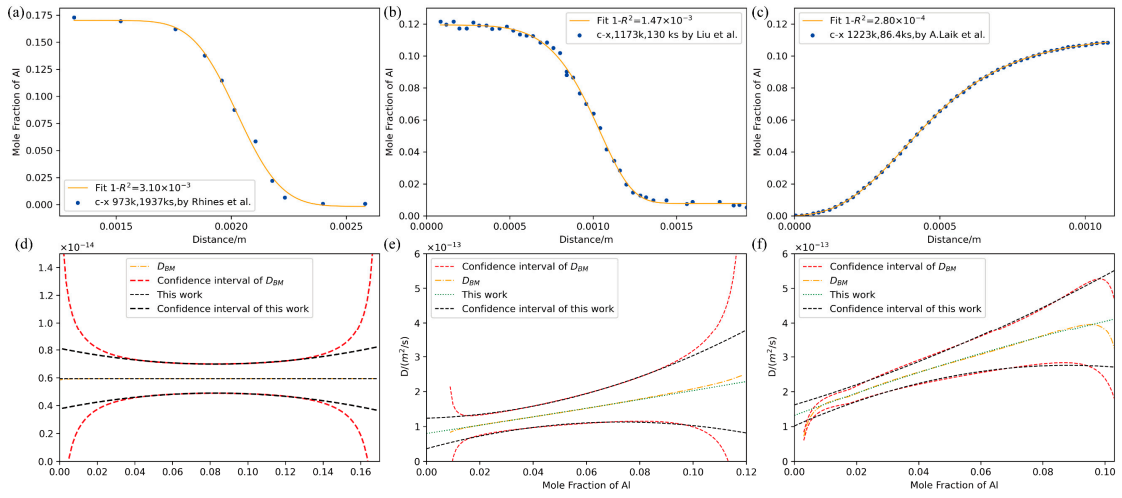


Figure S4. (a–c) Composition profiles fitted by distribution functions compared with the experimental data of the Al - Cu/Cu diffusion couples annealed at different temperatures [5–7]; (d–f) presently fitted interdiffusion coefficients and uncertainties compared with the interdiffusion coefficients evaluated using the Boltzmann–Matano method and the uncertainties quantified using the uncertainty quantification approach.

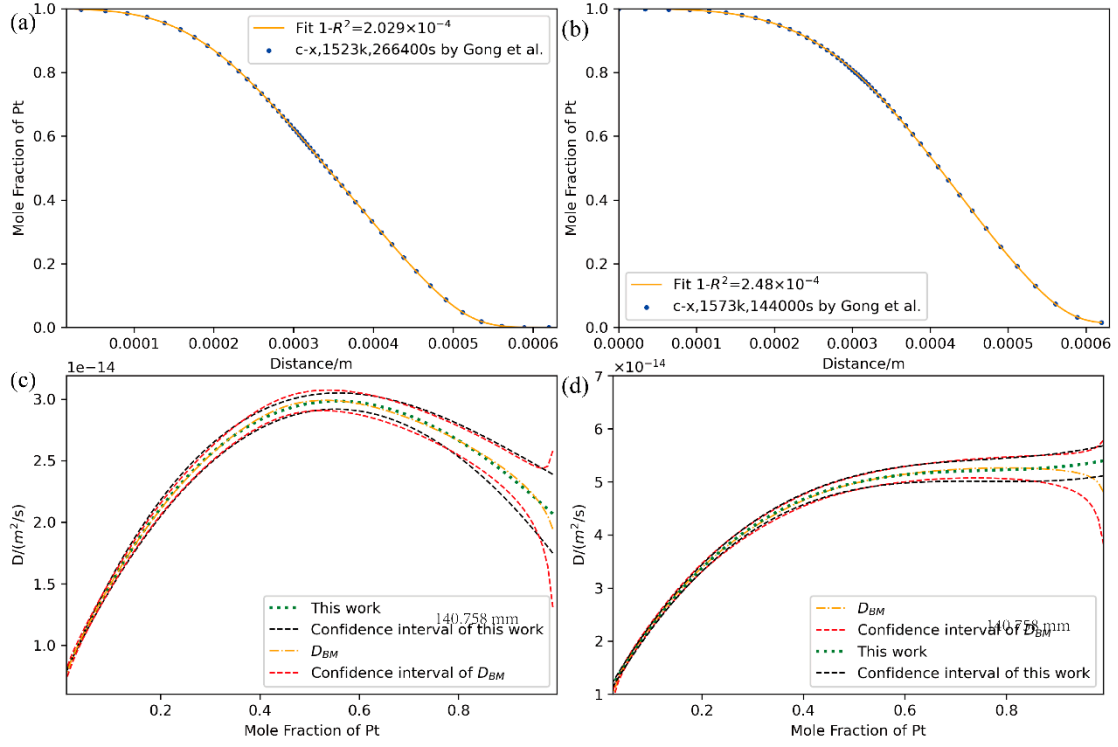


Figure S5. (a–b) Composition profiles fitted by distribution functions compared with the experimental data of the Ni/Pt diffusion couples annealed at different temperatures [8]; (c–d) presently fitted interdiffusion coefficients and uncertainties compared with the interdiffusion coefficients evaluated using the Boltzmann–Matano method and the uncertainties quantified using the uncertainty quantification approach.

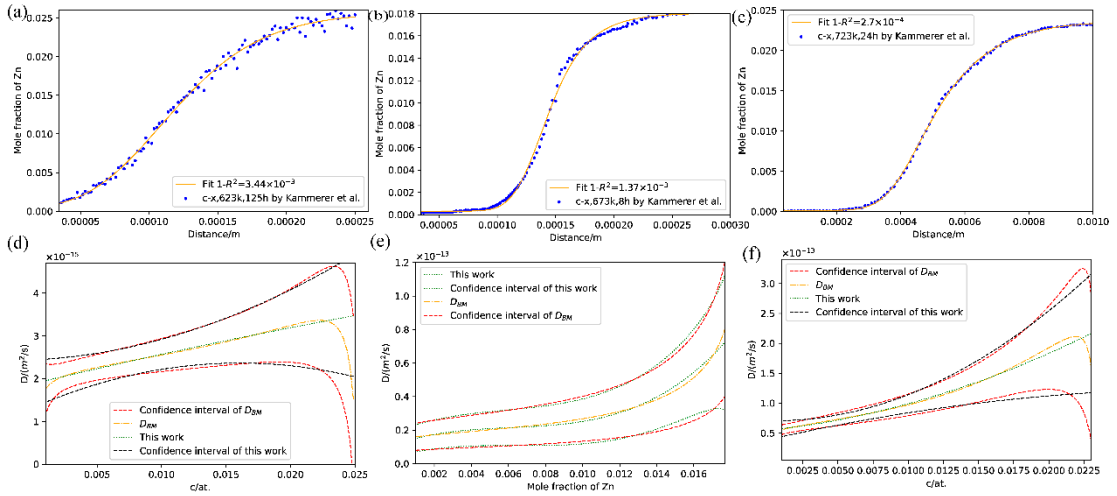


Figure S6. (a,b) Composition profiles fitted by distribution functions compared with the experimental data of the hcp Mg/Zn diffusion couples annealed at different temperatures [9]; (c,d) presently fitted interdiffusion coefficients and uncertainties compared with the interdiffusion coefficients evaluated using the Boltzmann–Matano method and the uncertainties quantified using the uncertainty quantification approach.

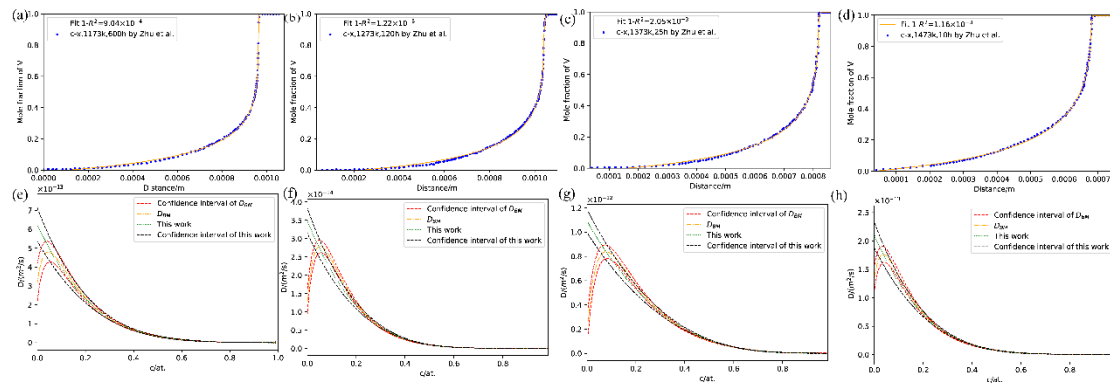


Figure S7. (a–b) Composition profiles fitted by distribution functions compared with the experimental data of the bcc Ti/V diffusion couples annealed at different temperatures [10]; (c, d) presently fitted interdiffusion coefficients and uncertainties compared with the interdiffusion coefficients evaluated using the Boltzmann–Matano method and the uncertainties quantified using the uncertainty quantification approach.

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