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Molecular Dynamics Simulations of Substitutional Diffusion

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ABSTRACT

In atomistic simulations, diffusion energy barriers are usually calculated for each atomic jump path using a nudged elastic band method. Practical materials often involve thousands of distinct atomic jump paths that are not known a priori. Hence, it is often preferred to determine an overall diffusion energy barrier and an overall pre-exponential factor from the Arrhenius equation constructed through molecular dynamics simulations of mean square displacement of the diffusion species at different temperatures. This approach has been well established for interstitial diffusion, but not for substitutional diffusion at the same confidence. Using $In_{0.1}Ga_{0.9}N$ as an example, we have identified conditions where molecular dynamics simulations can be used to calculate highly converged Arrhenius plots for substitutional alloys. This may enable many complex diffusion problems to be easily and reliably studied in the future using molecular dynamics, provided that moderate computing resources are available.

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