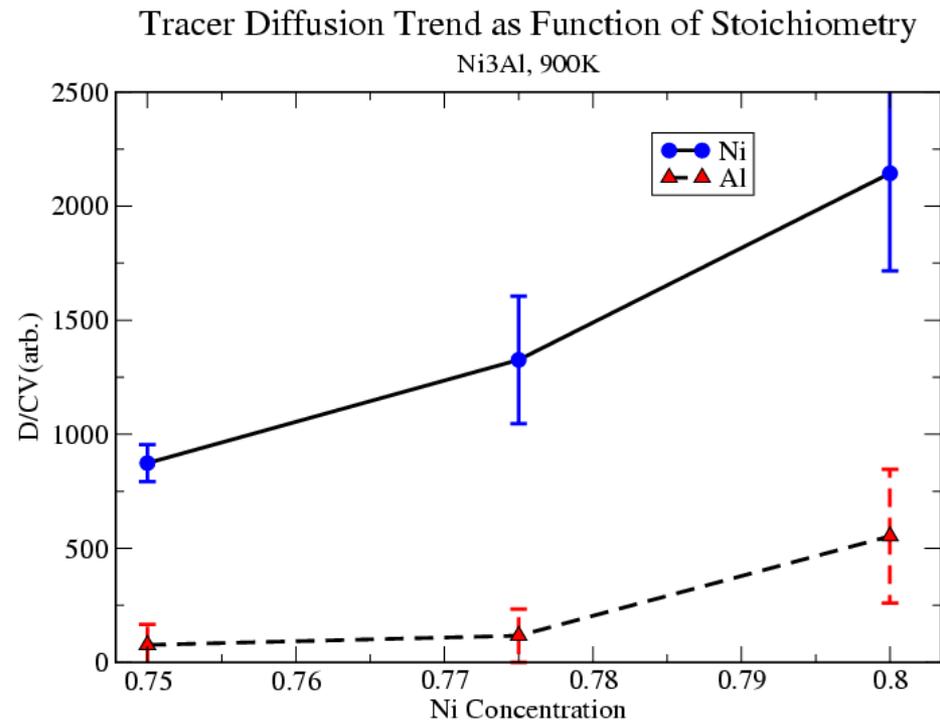


Atomic-Scale Simulation of Diffusion in Alloys

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Mass-transport in metals occurs by motion of vacancies. Ordinary Molecular Dynamics is much too slow to simulate diffusion. Using **Accelerated MD**, we are able to calculate diffusion rates even in ordered metal alloys.



According to our simulations, Ni diffuses much more quickly than Al in the alloy Ni₃Al.