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Diffusion Limited Processes Using Accelerated Molecular Dynamics[1] ERDI BLEDA, XING GAO, MURRAY DAW, Department of Physics and Astronomy / Clemson University — We present a systematic microscopic approach to diffusion-limited processes for intermetallic alloys using Accelerated Molecular Dynamics. On-the-fly kinetic Monte Carlo is combined with the Dimer Method to find the saddlepoints exiting a valley, based on energetics from the Embedded Atom Method. With this technique, we compute the tracer diffusivities as a function of composition and temperature for strongly ordered (Cu_3Au), weakly ordered (Ag-Au) and weakly clustered (Cu-Ni) alloys.

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