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Parallel Temperature-Accelerated Dynamics Simulations of Epitaxial Growth[1] Y. SHIM, J. G. AMAR, University of Toledo, B. P. UBERUAGA, A. F. VOTER, Los Alamos National Laboratory — The temperature-accelerated dynamics (TAD) method is a powerful tool for carrying out non-equilibrium simulations of systems with infrequent events over extended timescales. However, since the computational time for a typical TAD simulation increases rapidly with the number of atoms N, TAD simulations have so far been limited to relatively small system sizes. By applying a recently proposed synchronous sublattice algorithm to parallel TAD simulations, we have been able to simulate the evolution of systems over much larger length- as well as time-scales. As a first test of our method, we have carried out simulations of the surface diffusion of Cu atoms on the Cu(100) surface. In contrast to serial TAD simulations for which the computational time scales as $N^{2.5} - N^3$, in our parallel TAD simulations the computational time scales as $log(N)$ and may even be independent of N for larger system sizes. In particular we find that for intermediate size systems our parallel TAD simulations are several orders of magnitude faster than the corresponding serial TAD simulations. Preliminary results for low-temperature multilayer Cu/Cu(100) growth obtained using parallel TAD simulations are also presented.

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