Realistic simulations of low temperature Cu(100) growth: extending time and length scales by parallel temperature-accelerated dynamics
dynamics\textsuperscript{1} Y. SHIM, J.G. AMAR, University of Toledo, A.F. VOTER, B.P. UBERUAGA, 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 time-scales. However, due to the
serial nature of the method the computation time scales as $N^2 - N^3$, where $N$
is the number of atoms. As a result, TAD simulations have been limited to relatively
small system sizes. By combining temperature-accelerated dynamics with a recently
proposed parallel synchronous sublattice algorithm, we are able to simulate the dy-
namic evolution of systems over much larger length as well as longer time scales.
In particular, we find that the computational time using our parallel accelerated
dynamics method scales as $\log(N)$ or better. Preliminary results for the growing
film morphology in low-temperature Cu(100) growth will also be presented. These
include the observation of a wide variety of defect configurations.

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