Abstract Submitted
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**Realistic simulations of low temperature Cu(100) growth: extending time and length scales by parallel temperature-accelerated dynamics**[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 dynamic 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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