

Abstract Submitted
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Locally adaptive parallel temperature accelerated dynamics method¹ YUNSIC SHIM, JACQUES G. AMAR, University of Toledo — The recently-developed temperature-accelerated dynamics (TAD) method [M. Sørensen and A.F. Voter, J. Chem. Phys. **112**, 9599 (2000)] along with the more recently developed parallel TAD (parTAD) method [Y. Shim et al, Phys. Rev. B **76**, 205439 (2007)] allow one to carry out non-equilibrium simulations over extended time and length scales. The basic idea behind TAD is to speed up transitions by carrying out a high-temperature MD simulation and then use the resulting information to obtain event times at the desired low temperature. In a typical implementation, a fixed high temperature T_{high} is used. However, in general one expects that for each configuration there exists an optimal value of T_{high} which depends on the particular transition pathways and activation energies for that configuration. Here we present a locally adaptive high-temperature TAD method in which instead of using a fixed T_{high} the high temperature is dynamically adjusted in order to maximize simulation efficiency. Preliminary results of the performance obtained from parTAD simulations of Cu/Cu(100) growth using the locally adaptive T_{high} method will also be presented.

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