Copper nanocluster growth at experimental conditions using temperature accelerated dynamics C. S. DIAS, GCEP-Centro de Fisica da Universidade do Minho, 4710-057 Braga, Portugal, A. C. CADILHE, GCEP-Centro de Fisica da Universidade do Minho, Braga, Portugal. T-1 Group, MS B268, Los Alamos National Laboratory, Los Alamos, USA., A. F. VOTER, T-1 Group, MS B268, Los Alamos National Laboratory, Los Alamos, USA. — We study the dynamics of vapor phase cluster growth near experimental conditions of pressure at temperatures below 200K. To this end, we carried out temperature accelerated dynamics (TAD) simulations at different vapor pressures to characterize the morphology of the resulting nanoparticles, which leads to a range of values of the flux of impinging atoms at fixed vapor temperature. At typical experimental pressures of $10^{-3} - 10^{-4}$ bar TAD provides substantial boost over regular Molecular Dynamics (MD). TAD is also advantageous over MD, regarding the sampling of the network of visited states, which provides a deeper understanding of the evolution of the system. We characterize the growth of such clusters at different vapor pressures.

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