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HOMOGENOUS NUCLEATION AND CRYSTAL GROWTH IN A MODEL LIQUID FROM DIRECT ENERGY LANDSCAPE SAMPLING SIMULATION NATHAN WALTER, YANG ZHANG, University of Illinois at Champaign-Urbana — Nucleation and crystal growth are understood to be activated processes involving the crossing of free-energy barriers. Attempts to capture the entire crystallization process over long timescales with molecular dynamic simulations have met major obstacles because of molecular dynamics' temporal constraints. Herein, we circumvent this temporal limitation by using a brutal-force, metadynamics-like, adaptive basin-climbing algorithm and directly sample the free-energy landscape of a model liquid Argon. The algorithm biases the system to evolve from an amorphous liquid like structure towards an FCC crystal through inherent structure, and then traces back the energy barriers. Consequently, the sampled timescale is macroscopically long. We observe that the formation of a crystal involves two processes, each with a unique temperature-dependent energy barrier. One barrier corresponds to the crystal nucleus formation; the other barrier corresponds to the crystal growth. We find the two processes dominate in different temperature regimes. Compared to other computation techniques, our method requires no assumptions about the shape or chemical potential of the critical crystal nucleus. The success of this method is encouraging for studying the crystallization of more complex

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