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Modeling amorphous thin films: Kinetically limited minimization
PAWEL ZAWADZKI, JOHN PERKINS, STEPHAN LANY, National Renewable Energy Laboratory — Amorphous materials become increasingly attractive components of thin film devices such as thin film displays or solar cells. They are typically prepared using physical vapor deposition (PVD) techniques at temperatures well below the melting point of deposited material ($< 0.2T_m$). Computational models of amorphous structures, however, are almost elusively constructed from a high temperature equilibrated crystal melt using simulated annealing (SA) protocol. While such procedure imitates the quench form melt preparation of bulk glasses, its applicability to modeling low temperature synthesized amorphous thin films is unclear. To account for low T growth conditions we propose a new method. The method, kinetically limited minimization (KLM), starts from a randomly initialized structure and minimizes the total energy in a number of local structural perturbation-relaxation events. We compare KLM and SA with quench rates ranging from 64 K/ps to 2500 K/ps using two prototypical ionic and covalent materials: In2O3 and Si, respectively. While both methods provide qualitatively similar structures, we find that, compared to KLM, slow quench SA provides stronger medium range order in a-In2O3 and fast quench SA provides weaker short range order in a-Si.

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