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Cooling rates dependence of medium range order development in metallic glasses[1] C. Z. WANG, Y. ZHANG, F. ZHANG, M. I. MENDELEV, M. J. KRAMER, K. M. HO, Ames Laboratory, Iowa State University — Rapid cooling from metallic liquids is a widely used approach to synthesize novel alloys with desirable properties because such rapid cooling drives phase selection away from equilibrium phases resulting in new metastable phases and morphologies. However, molecular dynamics simulation of such rapid solidifications faces a well-known time-scale challenge that the cooling rate is several orders of magnitude faster than experiments. We propose an efficient cooling strategy in which most of the computer time is spent on a prolonged isothermal process slightly below the glass-transition temperature T_g. Such a sub-T_g annealing reduces the effective cooling rates in MD simulations to ~10^7 K/s. The effects of lowering cooling rates on the evolution of short-range and medium-range orders are investigated. The glassy samples prepared in this way demonstrate significant energetic stability, slow dynamics, and well-developed short-range and medium-range orders.

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