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Asymmetric crystallization upon heating and cooling in model glass-forming systems MINGLEI WANG, KAI ZHANG, YANHUI LIU, JAN SCHROERS, Yale Univ, MARK SHATTUCK, City College of New York, COREY O'HERN, Yale Univ — We perform molecular dynamics simulations of binary Lennard-Jones (LJ) and hard-sphere (HS) systems to understand the asymmetry in the critical cooling and heating rates for crystallization observed in experiments on bulk metallic glasses, where much faster heating rates are required to prevent crystallization. For the LJ systems, we cool the systems at different rates (above the critical cooling rate R_c) to temperatures below the glass transition, and subsequently begin heating the samples at different rates to measure the critical heating rate R_h below which the system crystallizes. We perform companion studies of HS systems, except we measure the asymmetry in the critical compression and dilation rates to enhance the asymmetry. We show that the asymmetry increases with the glass-formability of the binary mixtures and explain this result by characterizing the structural order of the systems.

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