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Composition fluctuation, local clustering, and crystallization in multi-component systems MINGLEI WANG, KAI ZHANG, STEFANOS PAPANIKOLAOU, JAN SCHROERS, COREY S. O'HERN, Yale University — We perform molecular dynamics simulations of model multi-component metallic liquids to study mechanisms for non-polymorphic crystallization. We measure local concentration fluctuations, nucleation rates, and clustering as a function of the cooling rate for different size ratios, stoichiometries, and attraction strengths. In preliminary studies, we find that over a wide range of particle size ratios and cooling rates, small particles cluster in the interstices of contact networks formed by the large particles. These studies are important for understanding which systems are prone to crystallization and which are good glass-formers.

Minglei Wang
Yale University

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