

Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Crystallization and glass formation in multi-component liquids¹ KAI ZHANG, MINGLEI WANG, STEFANOS PAPANIKOLAOU, JAN SCHROERS, COREY O'HERN, Yale University — When a liquid is cooled faster than the critical cooling rate, crystallization is avoided, and amorphous solids are formed. What sets the critical cooling rate? We perform molecular dynamics simulations of model metallic alloys—polydisperse spheres with hard-sphere and modified Lennard-Jones interactions—to study the critical cooling rate as a function of the particle size ratio, stoichiometry, and strength of the attractive interactions. We also characterize the structural properties of glassy and crystalline states that form at rapid and slow cooling/compression rates, respectively, using local order parameters, position correlation functions, and Voronoi and other tessellations.

¹NSF MRSEC DMR-1119826

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Date submitted: 08 Nov 2012

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