Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Structure and shear dynamics in binary mixtures with tunable stiffness and composition GUO-JIE GAO, YUN-JIANG WANG, SHIGENOBU OGATA, Osaka University — We conduct 2D molecular dynamics (MD) simulations to study the structure and relaxation behavior of highly-dense (volume fraction = 0.793) binary mixtures at two temperatures, above (T = 2.0) or below (T = 0.2) the melting point. Particles in these mixtures interact via a pairwise n-6 Lennard-Jones (L-J) potential [Z. Shi et al. J. Chem. Phys. 135, 084513 (2011)], where n could be 8, 10 or 12 in this study. We also implement a polycrystal model where systematically increasing the number fraction of the large particle, the system changes over from crystal, polycrystal to glass [H. Shiba et al., Phys. Rev. E. 81, 051501 (2010)]. We find that lowering n increases the disorder parameter of the system at T = 2.0 significantly, while the same effect is not obvious at T = 0.2. Decreasing n increases the size of thermal fluctuations in both cases. Moreover, we compare the shear deformation of a polycrystal system containing either stiff grains of 10-6 L-J potential, or soft grains of 8-6 L-J potential, with that of another polycrystal system containing both kinds of grains, and address applying the results of our study to explain the enhanced ductility found in bimodal nanocrystalline copper.

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Date submitted: 13 Nov 2013 Electronic form version 1.4