Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Effects of interatomic potentials on mechanical deformation of glasses WEI-REN CHEN, Oak Ridge National Laboratory, TAKUYA IWASHITA, TAKESHI EGAMI, University of Tennessee — Apparently glasses behave like an elastic solid, which shows a linear relationship between stress and strain in mechanical deformation. However the understanding of the mechanical response of glasses remains elusive because of structural disorder. Mechanical deformation of monatomic model glasses was studied using athermal quasi-static shear (AQS) simulation and with three different potentials. As the interatomic potentials we employed the 12-6 Lennard-Jones (LJ) potential, modified Johnson (mJ) potential, and Dzugutov (Dz) potential, respectively. For mJ and Dz glasses the shear modulus keeps constant below a critical strain, below which it decreases rapidly or discontinuously with strain. Such changes in shear modulus were mostly related to the change in local topology of atomic connectivity or anelasticity. In contrast LJ glass shows a gradual decrease in shear modulus in a continuous manner. The results indicated that the difference arises from the nature of the potentials if the topology of atomic connectivity can be clearly defined.

Wei-Ren Chen
Oak Ridge National Laboratory

Date submitted: 28 Nov 2012 Electronic form version 1.4