Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Ab Initio Simulation of Nickel-Palladium-Phosphorus Bulk Metallic Glasses RAYMOND ATTA-FYNN, Department of Physics, University of Texas at Arlington, PARTHAPRATIM BISWAS, Department of Physics and Astronomy, The University of Southern Mississippi — Using first principles molecular dynamics simulations, we model the structural and electronic properties of $Ni_{40}Pd_{40}P_{20}$ bulk metallic glasses. The calculations are carried out for large system sizes in order to probe structural features associated with the medium range order on the nanometer length scale. We discuss different approaches to modeling the glassy systems ranging from the cook-and-quench to the structural building block techniques. The nature of the medium range order on the nanometer length scale is examined using the theory of fluctuation electron microscopy. The localization nature of the electronic eigenstates and the dc conductivity (of the model configurations) will be discussed in relation to the real space atomic structure.

Raymond Atta-Fynn
Department of Physics, University of Texas at Arlington

Date submitted: 14 Nov 2014 Electronic form version 1.4