Abstract for an Invited Paper
for the MAR05 Meeting of
The American Physical Society

Novel methods for first principles modeling of glasses[1]

DAVID DRABOLD[2], Ohio University

Recently, we have explored new methods to form models of binary glasses that offer significant computational advantage and enable inclusion of *a priori* information about structure from experiments or other considerations. For glassy SiO_2 and some other IV-VI binary glasses, we find that placement of column VI atoms at bond centers in a good quality tetrahedral amorphous network followed by rescaling and relaxation leads to a highly realistic and large (648 atom) *ab initio* model of silica and other glasses. The problem of "freezing in" too much disorder from the liquid state, familiar from quench from melt simulations, appears to be ameliorated. Next, we show that Reverse Monte Carlo (RMC) may be used to produce chemically and topologically realistic models *if* appropriate constraints are employed in addition to forcing models to agree with diffraction measurements. The method has a high degree of flexibility that enables us to include information from Fluctuation Electron Microscopy (FEM) experiments, which have recently shown that some samples of a-Si:H exhibit medium range order. We have successfully fit diffraction and FEM data and thus formed models reproducing the experimental MRO. It seems unlikely that melt quench or continuous random network models would reproduce such complex ordering. By adopting an information theoretic viewpoint, we have merged RMC with first principles simulation to build models which simultaneously reproduce experimental data *and* are a minimum energy configuration of a density functional prescription for interatomic interactions. The method is applied to a 648 atom model of g-$GeSe_2$ and produces an essentially perfect neutron static structure factor (including first sharp diffraction peak), electronic density of states and vibrational spectrum.

[1]Work undertaken in collaboration with P. Biswas, D. Tafen and R. Atta-Fynn

[2]Supported by the National Science Foundation