Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

First principles modeling of structure and properties of multi-component amorphous steels VIATCHESLAV KAZIMIROV, DESPINA LOUCA, University of Virginia, MICHAEL WIDOM, Carnegie Mellon University, MICHAEL WIDOM COLLABORATION — Amorphous steels (iron based metallic glasses) exhibit unique physical properties that have opened the venue to new commercial applications as well as renewed the interest in this field. To provide a realistic description of the three dimensional structures and associate the coordinated environment of atoms to physical properties, first principles quantum mechanical molecular dynamics (MD) simulations along with the pair density function (PDF) analysis of neutron and X-ray diffraction data were used by way of considering chemical effects, ionic size ratio and concentration. Direct comparison of the simulated atomic structures obtained from MD with the local atomic structures determined experimentally show a very good agreement between the two, indicating that this theoretical approach can be applied towards simulating multi-component alloys. The atomic coordinates were used to develop the building blocks of cluster-like structures that give rise to the short-range order. The diffusion rates of different atom species were modeled at several temperatures that allowed us to describe the quenching process. In addition, the bulk moduli as a function of chemical composition were simulated and showed a very good agreement with the ones obtained experimentally.

Viatcheslav Kazimirov
University of Virginia

Date submitted: 05 Dec 2007 Electronic form version 1.4