Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

The electronic structures and structural properties of the amorphous $Ge_2Sb_2Te_5$, a phase change memory material EUNAE CHO, Department of Physics, Ewha Womans University, JINO IM, JISOON IHM, Department of Physics and Astronomy, Seoul National University, SEUNGWU HAN, Department of Physics, Ewha Womans University — Ge-Sb-Te compound is one of the most promising materials for phase change random access memory. Recently, $Ge_2Sb_2Te_5$ has been under intensive researches. However, there exists a critical discrepancy between experimental and theoretical observations. In experiment, the ideal glass following 8-N rule has been observed. There are deviations from 8-N rule for melt-quench structures obtained by molecular dynamics calculations. In this presentation, we compare the melt-quench structure with ideal glass. We theoretically obtained the ideal glass using Si-As-Se compounds with a higher covalency The amorphous structure of $Si_2As_2Se_5$ is obtained by the melt-quench process and the elements are replaced by Ge-Sb-Te. It is found that the resulting $Ge_2Sb_2Te_5$ structures satisfy the 8-N rule and all Ge atoms are tetrahedrally coordinated. The total energy of the ideal glass is higher than that of the melt-quench structure, explaining why the ideal glass has not been observed in the MD simulations. The electronic structures are also compared between ideal glass, melt-quench structure, and crystalline phase. It is concluded that the electronic character of the melt-quench structure lies in between those of ideal glass and crystalline phase.

Eunae Cho
Department of Physics, Ewha Womans University

Date submitted: 25 Nov 2008 Electronic form version 1.4