Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

On the Molecular Structure of $Ge_xSb_xSe_{1-2x}$ glasses[1] K. GUNASEKERA, P. BOOLCHAND, University of Cincinnati, A. JACKSON, Central Michigan University — The $Ge_xSb_xSe_{100-2x}$ternary is isovalent to the phase-change material, $Ge_xSb_xTe_{100-2x}$, except the Selenides can be prepared as bulk alloy glasses while the Tellurides exist only as amorphous thin-films. Here we report on the Selenides synthesized over a wide composition range, $0 < x < 25\%$, and examined in modulated-DSC, Raman scattering and molar volume experiments. The enthalpy of relaxation at T_g shows the opening of a reversibility window or Intermediate Phase (IP) in the $13\% < x < 18\%$ range, or $2.40 < \boldsymbol{r} < 2.54$ mean coordination number range, where $\boldsymbol{r} = 2 + 3x$. FT- Raman studies reveal frequency of the CS mode of $GeSe_4$ tetrahedra to steadily blue-shift with increasing x as networks stiffen. New vibrational modes are observed near 150 cm^{-1} and near 220 cm^{-1} at $x > 18.18\%$, the chemical threshold, and are thought to result from homopolar bonds. Ab-initio cluster calculations place pyramidal $SbSe_3$ units and ethylene-like Sb_2Se_2 units to reveal Raman activity near 215 cm^{-1} and 228 cm^{-1} respectively. Evolution of glass structure with composition x will be discussed.

[1]Supported by NSF grant DMR- 08-53957

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Date submitted: 19 Nov 2009 Electronic form version 1.4