Abstract Submitted
for the OSS13 Meeting of
The American Physical Society

Atomistic origin of doping-enhanced rapid crystallization in Ag-doped Ge-Sb-Te alloys: a joint experimental and theoretical study BINAY PRASAI, DAVID DRABOLD, GANG CHEN, Ohio University — We have applied extended X-ray absorption fine structure (EXAFS) analyses and *ab-initio* molecular dynamics (AIMD) simulations to study the atomic structure of Ag-doped (up to 42%) $Ge_1Sb_2Te_4$ alloys. Analysis of the models that are consistent with the EXAFS experiment reveals that the Ge environment is significantly modified by Ag doping whereas those of Sb and Te are barely affected (except for high Ag concentrations), and suggests that Ag prefers bonding with Te to Ge or Sb. Doping with Ag promotes the conversion of tetrahedral Ge sites to octahedral Ge sites and enhances the speed of crystallization of Ge-Sb-Te (GST) alloys as evidenced directly from the MD simulations. Our study shed light on the atomistic mechanism of rapid crystallization of GST alloys enhanced by Ag doping.

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Date submitted: 25 Feb 2013 Electronic form version 1.4