Abstract Submitted for the MAR09 Meeting of The American Physical Society

Atomistic origins of the phase transition mechanism in  $Ge_2Sb_2Te_5$ JUAREZ L. F. DA SILVA, ARON WALSH, SU-HUAI WEI, National Renewable Energy Laboratory, 1617 Cole Blvd., Golden, CO 80401, USA, HOSUN LEE, Dept. of Applied Physics, Kyung Hee University, Suwon 446-701, South Korea — The fast and reversible phase transition mechanism between crystalline and amorphous phases of  $Ge_2Sb_2Te_5$  has been in debate for several years. Through employing firstprinciples density functional theory calculations, we identify a direct structural link between the meta-stable crystalline and amorphous phases. The phase transition is driven by the displacement of Ge atoms along the rocksalt [111] direction from stable-octahedron to high-energy-unstable tetrahedron sites close to the intrinsic vacancy regions. Due to the instability of the tetrahedra, the Ge atoms shift away from those sites, giving rise to the formation of local-ordered 4-fold motifs coupled with long-range structural disorder. The high figures of merit of  $Ge_2Sb_2Te_5$  are achieved from the optimal combination of intrinsic vacancies provided by Sb2Te3 and the instability of the tetrahedron sites provided by GeTe.

> Juarez L. F. Da Silva National Renewable Energy Laboratory

Date submitted: 20 Nov 2008

Electronic form version 1.4