Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Electronic gap-driven amorphization mechanism: a new paradigm in phase-change materials R.A. NISTOR, D. SHAKHVOROSTOV, U. of Western Ontario, L. KRUSIN-ELBAUM, G.J. MARTYNA, C. CABRAL, IBM T. J. Watson Research Center, S. RAOUX, IBM Almaden Research Center, D.B. SHREKENHAMER, D.N. BASOV, UCSD, M.H. MUSER, U. of Western Ontario, D.M. NEWNS, IBM T. J. Watson Research Center — Phase change materials are materials that can be thermally interconverted between metallic (crystalline) and semiconducting (amorphous) phases. The interconversion process involves a change in local coordination number in some of the atomic constituents in these typically muticomponent materials. The electronic basis for the interconversion is still controversial. Here we report, in contrast to previous views, that the amorphization process is driven by an electronic reorganization in which lowering of the total energy by opening a Peierls-like gap drives the structural reorganization into the amorphous state, thereby explaining both the formation and semiconducting character of the amorphous phases. Our understanding of the process is based on phase transformation driven both thermally and by pressure, and in particular by analysis of long time *ab-initio* simulations of the amorphization process. We demonstrate the equivalence of thermal and pressure-driven interconversions in a system where vacancies are either at very low levels or enitrely absent. These discoveries open a new pressure-driven phase interconversion pathway.

Lia Krusin-Elbaum
IBM T.J. Watson Research Center

Date submitted: 15 Dec 2008 Electronic form version 1.4