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Simulation studies of GST phase change alloys GLENN MARTYNA, IBM Research — In order to help drive post-Moore's Law technology development, switching processes involving novel materials, in particular, GeSbTe (GST) alloys are being investigated for use in memory and eFuse applications. An anneal/quench thermal process crystallizes/amorphosizes a GST alloy which then has a low/high resistance and thereby forms a readable/writeable bit; for example, a "one" might be the low resistance, conducting crystalline state and a "zero" might be the high resistance, glassy state. There are many open questions about the precise nature of the structural transitions and the coupling to electronic structure changes. Computational and experimental studies of the effect of pressure on the GST materials were initiated in order to probe the physics behind the thermal switching process. A new pathway to reversible phase change involving pressure-induced structural metal insulator transitions was discovered. In a binary GS system, a room-temperature, direct, pressure-induced transformation from the high resistance amorphous phase to the low resistance crystalline phase was observed experimentally while the reverse process under tensile load was demonstrated via ab initio MD simulations performed on IBM's Blue Gene/L enabled by massively parallel software. Pressure induced transformations of the ternary material GST-225 (Ge2Sb2Te5) were, also, examined In the talk, the behavior of the two systems will be compared and insight into the nature of the phase change given.

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