Understanding the atomistic origin of the ultra-rapid crystallization and radiation hardness of the phase-change non-volatile memory material, Ge2Sb2Te5, via ab initio molecular-dynamics simulations

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Abstract

Non-volatile electronic computer memory has been provided up to now by Si CMOS floating-gate (FG) MOSFET 'flash' technology. However, its Moore's Law technology roadmap, driven by feature down-sizing, is shortly to come to an end due to the tunnelling of electrons, trapped on the FG, through ever-thinner layers of dielectric, resulting in memory volatility. Thus, there is a pressing need for a new technology to replace Si CMOS flash memory. One such potential non-volatile memory technology is 'phase-change random-access memory' (PCRAM), based on materials such as Ge2Sb2Te5 (GST), in which binary digital data are stored as a structural state of the material, viz. an electrically-resistive (semiconducting) amorphous/ glassy state and a conducting ('metallic') crystalline state. Reversible and ultra-rapid (_~ ns) transitions between these two phases can be induced by the application of appropriate voltage pulses which cause Joule heating of the material. In this paper, we will describe recent density-functional-theory-based *ab initio* molecular-dynamics (AIMD) simulations carried out on phase transitions in GST in which the atomistic origin of the ultra-rapid crystallization is clarified via a careful analysis of changes in the local atomic coordination characterized in terms of the actual chemical bonding. In addition, we have performed the first AIMD simulations of ion implantation in GST, which reveal the origin of the resilience of this memory material to radiation.

Keywords: ab initio molecular dynamics, phase, change memory, Ge, Sb, Te, radiation hardness, crystallization

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