Ab initio modelling of radiation damage in amorphous phase-change memory materials: The case of Ge2Sb2Te5

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Abstract

Radiation-hard non-volatile memories with large capacity and low production cost are in high demand by the space community for implementation in solid-state data recorders. In phase-change memories, binary data are represented as a structural phase rather than by stored electrical charge; thus, these devices are supposed to be tolerant to ionising radiation effects. Radiation effects on phase-change memories have been investigated by several experimental studies, while radiation-hard memories of relatively small size are already available by BAE systems. In this work, we present the first *ab initio* calculations of radiation-damage in amorphous phase-change materials by carrying out a thermal-spike simulation in order examine the effect of the ionizing radiation on the short- and medium-range order of the amorphous network and shed light on its atomistic structure. The local environments of irradiated amorphous Ge2Sb2Te5 have been investigated by employing a mixed Born-Oppenheimer and generalised Langevin molecular-dynamics approach in order to model the radiation-damage cascade, dissipate the heat from the irradiated area and probe the structural evolution of the amorphous network. Density-functional theory calculations, with hybrid-functionals, have been used to characterise the electronic structure of the irradiated glass and identify the effect of the ionising radiation on the electronic properties of the glass. The most significant damage of the amorphous network occurs at approximately 300 fs after the detonation of the thermal-spike, since a considerable loss of the quasi-binary chemical order and substantial modifications of the medium-range order were quantified at that time. The equilibrated glass shows a recovery from the damage imposed during ion irradiation, as it manages to maintain its amorphous network. Specific structural rearrangements inside the glass were observed in the modelled glass systems. The total electronic density of states exhibits negligible differences in the electronic structure of the glass before and after irradiation, while the absolute value of the band gap also was not significantly affected. Our simulations manifest the remarkable ability of Ge2Sb2Te5 phase-change random-access memory material to be radiation-tolerant, and hence indicating its potential applications in future space and other radiation-present environments.

Keywords: phase change memory, radiation hardness, molecular dynamics simulations, atomistic structure

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