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Density functional/molecular dynamics simulations of phase-change materials: Characterizing disordered phases JAAKKO AKOLA, University of Jyvaskyla, Finland, R. O. JONES, IFF, FZ Juelich, Germany —
The technological importance of phase-change materials (PCM) is based on the rapid amorphous-to-crystalline transition and changes in optical (and electrical) properties. Our density functional (DF)/ MD simulations on $Ge_2Sb_2Te_5$ (GST-225) and Ge_xTe_{1-x} alloys showed that atoms can be classified as A (Ge,Sb) and B (Te). "ABAB squares" are essential structural units, many "tetrahedral" and "octahedral" Ge atoms coexist, and Sb and Te coordination numbers deviate from the "8-N rule". Small cavities provide space to allow rapid ordering of disordered ABAB squares. We describe simulations of tellurium, which has an unusual density maximum near the melting point, and of two PCM: $Ge_8Sb_2Te_{11}$ (melt-quench of 630 atoms over 400 ps) and liquid $Ag_{3.5}In_{3.8}Sb_{75.0}Te_{17.7}$ (AIST, 640 atoms at 850 K) alloys. The structures of amorphous GST-8,2,11 and GST-225 are similar. The structure factor and pair distribution function of liquid AIST agree well with HEXRD measurements, there is medium-range order, and Ag and In atoms prefer to be near Te atoms.

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