

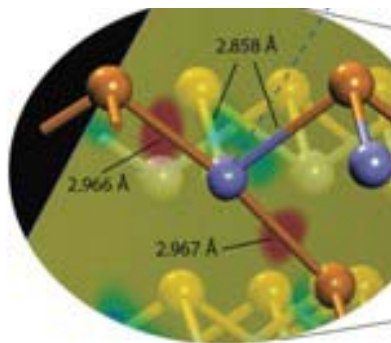
## Structure and bonding in phase-change materials

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When structures of the crystalline and/or amorphous phases are discussed, they are usually presented as ball-and-stick models. While this is acceptable at a certain point, proper understanding of the structure and properties requires knowledge of the nature of interactions between atoms, since a simple presence of a neighbor at a certain distance does not mean the existence of a covalent bond. In this work, we use charge density difference calculated from the first principles using the CASTEP code as a way to characterize bonding in phase-change alloys.

Using this approach we demonstrate pronounced difference between the crystal structures of binary GeTe and Ge-Sb-Te alloys. While the former is characterized by a strong bonding energy hierarchy [1], the latter is more cubic-like due to the formation of three-center four-electron bonds [2]. An example shown in Fig. 1 demonstrates that in Sb-doped GeTe the bond length difference between the shorter and longer bonds disappears.



**FIGURE:** Upon incorporation of Sb into GeTe, the difference between the shorter and longer bonds completely disappears.

Our results show that the defective octahedral Ge sites that are the dominant structural units of the amorphous phase pre-exist in the crystalline phase and the amorphization process consists in destruction of the three-center bonds and subsequent lattice relaxation that drastically modifies the electronic structure while preserving rather similar atomic structure [2].

We also demonstrate that despite an octahedral-like bonding angles suggesting pure p-type bonds, Ge atoms - at least in the amorphous state - are actually  $sp^3$ -hybridized [3]. Our results suggest some new insights into the structure and properties of phase-change alloys, e.g. the mechanism of phase-change and the resistance drift in the amorphous phase.

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2. A. V. Kolobov, P. Fons, J. Tominaga, and S. R. Ovshinsky, *Phys. Rev. B* 87, 165206 (2013)
3. A. V. Kolobov, P. Fons, and J. Tominaga, *Phys. Rev. B* 87, 155204 (2013)