Phase Change Materials: The Importance of Resonant Bonding

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Abstract

Phase change media are among the most promising materials in information technology. There are already employed in rewriteable optical data storage, where the pronounced difference of optical and electrical properties between the amorphous and crystalline state is used for data storage. This unconventional class of materials is also the basis of a storage concept to replace flash memory. Among the various demands materials have to meet in order to enable phase change memory applications, the most obvious one is a sufficient property contrast between the amorphous and crystalline state. This contrast is attributed to a pronounced change in bonding between the two phases. While the amorphous phase exhibits coordination and properties expected for 'ordinary' covalent systems, we have recently shown that the crystalline state of phase change materials is characterized by the occurrence of resonant bonding, a particular flavour of covalent bonding [1]. The concept of resonant bonding leads to an intuitive understanding of the observed material properties, e.g. the approximately octahedral coordination and the polarizability enhancement in the crystalline state, and the impact of stoichiometry variations. In order to quantify resonance bonding and to identify trends, both infrared spectroscopy experiments, i.e. a combination of FTIR-reflectometry and ellipsometry, and density functional theory calculations have been performed. Here, the results of these investigations will be presented. It will be shown that a map can be developed [2] which shows phase change behaviour for a selected range of chalcogenides with a well defined structure and unique bonding properties. The consequences of resonance bonding for the material properties will be discussed and demonstrated for different compounds.

[1] K. Shportko et al., Nature Materials 7, 653 (2008)

[2] D. Lencer et al., Nature Materials 7, 972 (2008)