

Local Structural Order Of The Amorphous Phases Of Ge-Sb-Te Phase-Change-Memory Alloys

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The local structural order of the amorphous phases of Ge-Sb-Te phase-change-memory alloys has been the subject of considerable controversy. From extended x-ray absorption fine structure (EXAFS) experiments Kolobov et al. [1] first suggested that the local nearest neighbor coordination of Ge in $\text{Ge}_2\text{Sb}_2\text{Te}_5$ changed from six in both of the crystalline phases to four in the amorphous phase but that the Sb and Te coordinations remained essentially the same (six) in all phases. The conclusions regarding the Sb and Te coordination numbers in the amorphous form disagreed with the suggestions of a structural model [2], which is based on covalent bonding of s and p electrons to form closed shells for all elements (so-called *octet* or $8-N$ rules, where N is the elemental column number). In the simplest embodiment of this model the coordination numbers for Sb and Te should be 3 and 2, respectively. More recent EXAFS measurements of Baker et al. [3] and Jovari et al. [4] have largely confirmed these predictions, although the error bars on the average nearest-neighbor coordination numbers are significant. In addition these scattering techniques do not give any information concerning asymmetries in the local bonding configurations, and they only give information on the average site.

We have utilized nuclear magnetic resonance (NMR) of ^{121}Sb and ^{125}Te to confirm the EXAFS results and determine the coordination numbers more accurately for Sb and Te, and by inference for Ge, in the amorphous phase. Our results unequivocally establish the general applicability of the $8-N$ rule for the local structural order in the amorphous forms of Ge-Sb-Te alloys. In addition, we establish the existence of both 2-fold and 3-fold coordinated Te sites and track their relative fractions as a function of composition. Finally, we establish the existence of two Sb sites, both of which are essentially 3-fold coordinated with varying numbers of second nearest Te neighbors that are closer than normal. One Sb site is axial and well defined while the second site is non-axial with considerable distortions from site to site. By analogy with NMR results in crystalline Sb_2S_3 and Sb_2Se_3 we speculate that the local order surrounding Sb sites in the amorphous Ge-Sb-Te alloys resembles that which exists in these layered compounds rather than that which exists in Sb_2Te_3 . In total, these results provide detailed and essential structural data to guide any model interpretations of the phase-change process in these technologically important alloys.

1. A. Kolobov et al., *Nature Mater.* **3**, 703 (2004).
2. J. K. Olson, H. Li, and P. C. Taylor, *J. Ovonic Res.* **1**, 1 (2005).
3. D. A. Baker, M. A. Paesler, G. Lucovsky, S. C. Agarwal, and P.C. Taylor, *Phys. Rev. Lett.* **96**, 255501 (2006).
4. P. Jovari et al., *Phys. Rev.* **B77**, 035202 (2008).