STUDIES OF THE STRUCTURE OF AMORPHOUS GeSbTe BY ELECTRON DIFFRACTION

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The amorphous state is important in controlling the properties of many materials. For example intergranular glassy films can control the toughness of ceramics, the rapid switching between the crystalline and amorphous state determines the usefulness of rapid phase change materials, and thin amorphous coatings can be used as hardened surfaces. The standard techniques for investigating the structure of amorphous materials are neutron and X-ray diffraction, but these are of no use for studying small volumes of material. Electron diffraction techniques have been developed for this purpose, and this paper will describe these techniques and their application to investigating the structure of the rapid phase change material Ge$_2$Sb$_2$Te$_5$.

Electron diffraction data can be used to give statistical information about the volume of material which scatters the electron beam. This statistical information is generally described in the form of the reduced density function (RDF), which for a monatomic material, shows the number of atoms at distance r from a general atom. The RDF can be obtained from the diffraction pattern I(q) by Fourier transformation.

In the case of alloys, the relationship of the Fourier transform of I(q) to the structure is not so straightforward, especially since, unlike for neutron and X-ray diffraction, partial structure factors cannot be obtained for electrons. Nevertheless model refinement can be carried out by comparison against the electron diffraction data.

In this way, we have investigated the structure of Ge$_2$Sb$_2$Te$_5$ (GST). This material has been the subject of intense study due to the importance of GST in phase change memory devices, and the fact that the structural changes during the phase change between the amorphous and crystalline phase are unclear. In our work [1] the energetics of the transition between the crystalline and the amorphous phase of Ge$_2$Sb$_2$Te$_5$ is explored using density functional theory (DFT) calculations, electron diffraction and reverse Monte Carlo model refinement. A model structure is proposed, made up from randomly oriented ring-shaped building blocks (figure 1) which derive from the Ge$_2$Sb$_2$Te$_5$ crystal structure (NaCl structure). The model structure is refined against the electron diffraction data (figure 2), and this structure is shown to agree with the experimental reduced density function determined from electron diffraction experiments and previously reported extended X-ray absorption fine structure measurements.

References:
Figure 1(a) shows the proposed ring structure obtained after relaxing the atoms around a vacancy without any surrounding environment (Ge - turquoise, Te – yellow, Sb – blue) and (b) shows a layer of the distorted ring model before (strong colours) and after (weak colours) refinement (from [1]).

Figure 2 shows the RDF acquired experimentally from a GST thin film (black line), of the unrefined distorted ring model (dashed line) and of the model after reverse Monte Carlo refinement (dotted line). The positions of the Ge-Te, Sb-Te and Te-Te nearest neighbour distances determined using EXAFS in Ref. 2 are shown (+), as well as the distances as they would be in a perfect NaCl type crystal with a=6.03 Å (vertical, dashed lines) (from 1).