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Structure of Cu–As–Te glasses – Neutron diffraction and reverse Monte Carlo simulations

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Abstract

Reverse Monte Carlo simulations of the structure of $Cu_{0.20}As_{0.25}Te_{0.55}$ chalcogenide glass using combined neutron and X-ray diffraction data indicate that the first sharp diffraction peak arises mainly from Cu–Cu and Cu–As correlations.

Keywords: Glasses; Diffraction; Reverse Monte Carlo simulations

1. Introduction

Recently, the first neutron diffraction measurements on $Cu_xAs_{0.45-x}Te_{0.55}$ ($x = 0.20, 0.15, 0.10, 0.05$) glasses [1, 2] have shown that a weak but well-defined first sharp diffraction peak (FSDP) is observed in the distinct scattering curves at about $Q = 0.98\,\text{Å}^{-1}$ ($Q = 4\pi\sin(\Theta)/\lambda$) for $x = 0.20$ and 0.15 which disappears for $x \leqslant 0.10$. The FSDP has often been taken as a signature of the medium-range order (MRO) in network glasses [3]. That is why in the present contribution we investigate the MRO in the $Cu_{0.20}As_{0.25}Te_{0.55}$ composition using the reverse Monte Carlo (RMC) method [4] and combined neutron and X-ray diffraction refinements in order to reduce the range of possible structural models taking advantage of the different scattering lengths for neutrons and X-rays.

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2. Experimental

The $Cu_{0.20}As_{0.25}Te_{0.55}$ sample was prepared by melt-quenching from 900°C in ice water. The neutron diffraction experiments were performed at the neutron spallation source ISIS, UK on the LAD time-of-flight diffractometer and the data were analysed with the ATLAS suite of programs [5]. Further experimental details are given elsewhere [1, 2]. The X-ray diffraction measurements were performed on a Siemens D500 automatic powder diffractometer using Mo Kα radiation.

The RMC simulations were made with the RMCA program [6]. Random distribution of 3000 atoms in a cubic box (box edge = 43.4 Å, corresponding to atom number density $\rho_0 = 0.0758\,\text{atoms/Å}^3$) with periodic boundary conditions was used as initial configuration. Comparison of the first nearest-neighbour distances in compositionally related crystalline compounds indicated that models with random bonding rather than with chemical

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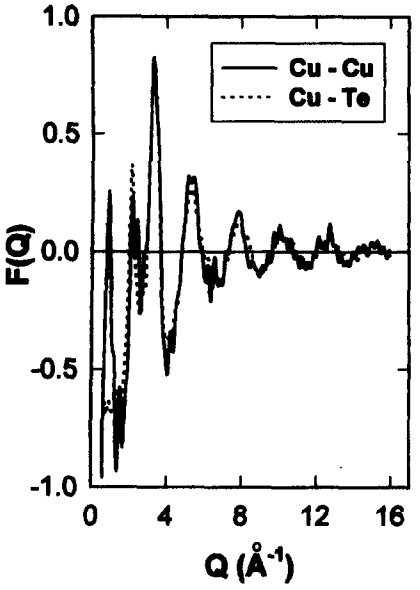

Fig. 1. Cu–Cu (full line) and Cu–Te (dashed line) partial structure factors for the $Cu_{0.20}$ $As_{0.25}Te_{0.55}$ chalcogenide glass.

short-range ordering would better describe the structure of the Cu–As–Te glasses. That is why no coordination number constraints were applied.

3. Results and discussion

The final RMC fits reproduce very well all features of the total structure factors (TSF) (goodness-of-fit factors $\chi_N = 8.6$, $\chi_{X\text{-ray}} = 1.5$). The difference in the intensity of the FSDP measured by neutrons and X-rays indicates that more than one type of atoms contribute to the FSDP. Since the TSF represents a linear sum of all partial structure factors (PSF), the PSF obtained from the RMC simulations were considered. The Cu–Cu and Cu–Te PSF are shown in Fig. 1. The variation of the Cu–Te, as well as the As–Te and Te–Te PSF (not shown in the figure), in the range of the FSDP (0.6–1.4 Å^{-1}) is within the statistical errors. At the same time the Cu–Cu PSF (as well as the As–As and Cu–As PSF) exhibits a strong peak at about 0.9 Å^{-1}. Taking into account the magnitude of the weighting coefficients of the different PSF it may be concluded that the FSDP in the investigated chalcogenide glass arises mainly from the Cu–Cu correlations. The contributions from the As–As and Cu–As PSF lead to broadening and shift of the Cu–Cu FSDP to slightly higher Q values. It has been shown that cation–cation correlations are responsible for the FSDP in other chalcogenide glasses as well [7]. A detailed topological analysis to show how the FSDP arises from the Cu–Cu correlations will be the subject of future studies using larger structural models.

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