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Continuous random network models of Cu–As–Te glasses

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Abstract

Reverse Monte Carlo simulations using neutron data show that the structure of $Cu_xAs_{0.45-x}Te_{0.55}$ chalcogenide glasses ($0.10 \leqslant x \leqslant 0.20$) is well described by the continuous network model. Cu substitutes randomly for As and the rigidity of the network increases with increasing Cu concentration.

Keywords: Glasses; Diffraction; Monte Carlo simulations

Among binary chalcogenide glasses, As–Te glasses show the highest electric conductivity [1]. Addition of monovalent metals like Cu and Ag increases further their conductivity and thermal stability [1,2]. The structure of Cu–As–Te glasses was studied by X-ray [3] and neutron diffraction [4]. Structural models have been reported for the $Cu_{0.20}As_{0.25}Te_{0.55}$ composition using combined X-ray and neutron diffraction data [5]. In the present paper, we present reverse Monte Carlo (RMC) simulations of three $Cu_xAs_{0.45-x}Te_{0.55}$ glasses ($x = 0.10$, 0.15 and 0.20) using neutron diffraction data and discuss the changes in the short-range order and network topology with composition.

The Cu–As–Te glass samples were prepared by melt quenching. The neutron diffraction experiments for $x = 0.15$ and 0.20 were performed on the LAD time-of-flight diffractometer at the neutron spallation source ISIS, UK and for the $x = 0.05$ and 0.10 compositions on the E2 diffractometer at BENSC, Berlin. Detailed description of the experiments and the data reduction is given elsewhere [4]. The RMC simulations were made with the RMCA program [6]. Models with 3000 atoms in a cubic box with periodic boundary conditions were used for all compositions. RMC fits were made to the corresponding total pair correlation functions $g(r)$ with the standard deviation parameter σ equal 0.005. All cut-off constrains were equal to 2.0 Å, except the minimum Te–Te distance which was set equal to 2.75 Å.

Previous EXAFS and AWAXS experiments on binary As_xTe_{100-x} glasses [7] as well as comparison of the bond lengths in crystalline Cu–Te, As–Te and Cu–As compounds, indicate that random bonding rather than chemical short-range ordering better describes the structure of Cu–As–Te glasses. That is why we have allowed for the presence of homopolar As–As, Te–Te and Cu–Cu bonds and have not used any coordination constraints. The final RMC fits reproduce well the experimentally measured $g(r)$ functions for all samples (Fig. 1). The very small concentration of non-bonded Cu atoms indicates that the samples are regular ternary glasses. The variation of the partial coordination numbers (PCN), calculated from the RMC models, is shown in Fig. 2. Compared with the data for the binary $As_{0.45}Te_{0.55}$ composition [7], the decrease of the As–As and Te–As PCN at the expense of the Cu–Cu, Cu–Te and Te–Cu PCN in conjunction with the constant Te–Te coordination for $x \leqslant 0.10$ indicates that Cu substitutes randomly for As forming $CuTe_3$ pyramidal and $CuTe_4$ tetrahedral structural units as well as short Te–Cu–Te chains. The

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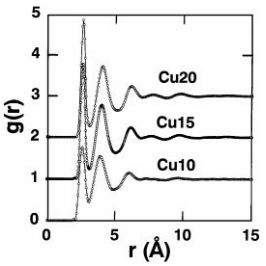

Fig. 1. Experimental (◦) and RMC (—) pair correlation functions $g(r)$.

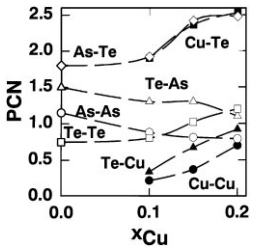

Fig. 2. Dependence of the partial coordination numbers on the Cu content. The dashed lines are only a guide for the eye.

increase of the copper leads, however, to changes in the network topology as well. The As–Te coordination number increases with x and additional Te–Te bonds are formed for $x > 0.10$. As a result the total coordination number of Cu and As increases from 3 to 4 and the continuous random network becomes more and more overconstrained.

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