Experimental report

08/04/2016

Proposal: 6-05-966 **Council:** 4/2015

Title: The evolution of medium range order in GeAsSe glasses

Research area: Materials

This proposal is a new proposal

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Samples: Ge3As24Se73
Ge11.5As24Se64.5
Ge20As24Se56

Instrument	Requested days	Allocated days	From	To
D4	4	4	25/10/2015	29/10/2015

Abstract:

Understanding of the medium range order (MRO) is important in glass science since many physical properties are correlated with it. Unfortunately the number of experimental methods to characterize it is still limited. Here we propose a combined approach using neutron diffraction and reverse Monte Carlo in order to determine the MRO in Ge-As-Se glasses. We are planning to make measurements at D4 for Ge3As24Se73, Ge11.5As24Se64.5 and Ge20As24Se56. We aim at exploring how the MRO evolves with the temperature and chemical compositions. In parallel to the experiments we will employ Reverse Monte Carlo method to simulate the structural factors of these glasses in order to understand the atomic arrangements, and thus extract the information of medium range order.

Introduction

We report a neutron diffraction study on three ternary chalcogenides of composition $Ge_xAs_{24}Se_{76-x}$ with different Ge and Se contents x= 3, 11.5 and 20 at% at different temperatures. The object of this proposal was to understand the evolution of the medium range order with the sample composition and with the temperatures, keeping the As composition constant. The measurements have been performed with the two-axis diffractometer dedicated to structural studies of amorphous materials D4 at the ILL. We have derived the total structure factor S(Q) and the pair distribution function PDF(r) for each sample and each temperature.

Experiments

The experiments were carried out at a working wavelength of 0.5 Å. The measurements were performed for three different samples at temperatures ranging between ambiant and 300°C (see Table 1). The samples had been prepared in bulk form at the Australian National University. They were later grinded in coarse powder form and placed in a cylindrical sample holder made of Vanadium (about 4 cm high and with an outer diameter of 4 mm). The required ancillary measurements (empty cell, vanadium) were also carried out. Diffraction measurements were performed over a 1.7-140° angular range, giving a usable Q range of 0.37-23.6 $Å^{-1}$

Sample	**Density (g/cm^3)**	**Glass transition temperature (°C)**	**Temperatures (°C)**
$Ge_3As_{24}Se_{73}$	4.499	120	ambient, 80, 120, 140, 160
$Ge_{11.5}As_{24}Se_{64.5}$	4.489	200	100, 160, 180, 200, 220
$Ge_{20}As_{24}Se_{56}$	4.425	279	80, 180, 260, 280, 300

Table 1 Experimental conditions and characteristics of the different samples

First results

The data reduction was performed using routines and programmes written by the instrument scientists of D4 [1]. Figure 1 shows the evolution of the pair distribution function and of corrected total structure factor. All curves are very similar: the amplitudes of the peaks decrease with increasing temperatures. The main visible difference concerns the more intense first peak at about 1.05 $Å^{-1}$, which is more pronounced for the Ge-rich sample.

The analysis of these experiments is under way and will be complemented with numerical simulations and complementary investigations using Raman scattering and / or Extended X-Ray Absorption Fine Structure measurements.

References

[1] https://www.ill.eu/instruments-support/instruments-groups/instruments/d4/more/manual/

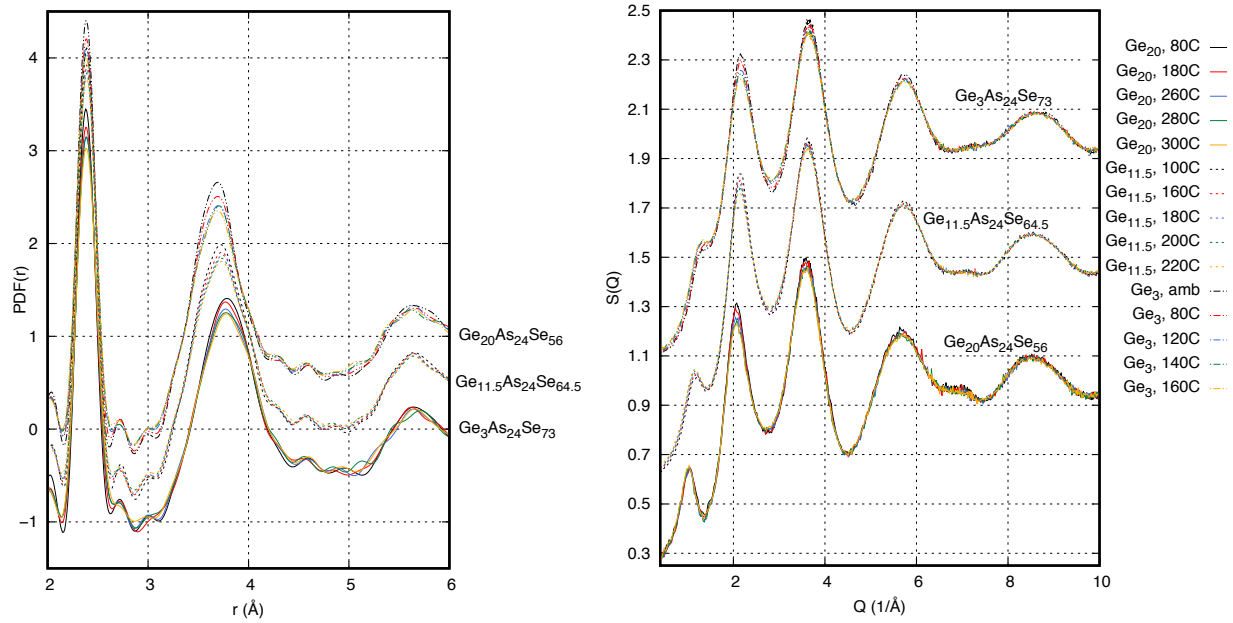

Figure 1 Measured pair distribution function PDF(r) and total structure factor S(Q) for the three samples at different temperatures. The data sets for the different samples have been offset vertically for clarity of presentation.