

STRUCTURAL STUDY OF AMORPHOUS $P_{0.5}Se_{0.5}$ BY X-RAY DIFFRACTION

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Experimental intensity and radial distribution function for the amorphous $P_{0.5}Se_{0.5}$ were obtained by X-ray diffraction. Theoretical intensity and radial distribution function were computed and found to be in agreement with those derived from experiment. The bond distances present in the calculations show a reasonable fit with the experimental data.

Key Words: Amorphous $P_{0.5}Se_{0.5}$; X-ray Diffraction; Theoretical Intensity; Radio Distribution Functions

Introduction

Electrical and optical properties of amorphous alloys with some of the chalcogenide element present a strong dependence^{1,2} on the content of their elements. The properties of amorphous alloys depend strongly on their composition. The knowledge of short-range structure gives partial information since it comes limited by the monodimensional character of a radial distribution function (RDF) analysis.

The aim of this work is to present and discuss the results of the X-ray diffraction investigation for amorphous $P_{0.5}Se_{0.5}$ and analysed its radial distribution function.

Experimental

The X-ray measurements were made using reflection geometry and monochromatic CuK_{α} radiation ($\lambda = 1.54 \text{ \AA}$). The diffractometer used is a Philips 1840 equipped with a solid state silicon counter and standard electronics. The observable range of scattering angle was $4^{\circ} \geq 2\theta \geq 100^{\circ}$, corresponding to the interval $0.285 \text{ \AA}^{-1} \geq s \geq 6.251 \text{ \AA}^{-1}$ in which the variable $s = (4\pi/\lambda)\sin\theta$, where θ is half the scattering angle.

Three series of data were collected. The measured intensities, at the same angle agreed reasonably and the intensity of each observation point was the mean value of those measured at that point.

The mean intensities were corrected for background, polarization, absorption in sample and incoherent scattering. The absolute scale was established by normalizing the intensity by the method of Kroph Moe³.

Results and Discussion

The reduced intensity $i(s)$ represents the structurally sensitive part of the total coherent intensity $I(s)$ in electron units. It is computed from the equation

$$i(s) = I(s) - \sum_i f_i^2(s), \quad \dots (1)$$

where $\sum f_i^2(s)$ is the part of scattering ascribable to independent atoms, and the sum is over the stoichiometric unit (one PSe molecule). A radial distribution function $D(r)$ is obtained by Fourier inversion of (1) according to

$$D(r) = 4\pi r^2 \rho_0 + (2r/\pi) \int_0^{\infty} s i(s) M(s) \sin(sr) ds, \quad \dots (2)$$

where ρ_0 is the average number density of molecules, and $M(s)$ is a modification function included to sharpen the features of the radial distribution function (RDF).

The modification function used in this study is

$$M(s) = \left\{ \sum_i f_i(s) \right\}^{-2}, \quad \dots (3)$$

where f_i refers to the coherent scattering amplitudes of phosphorus and selenium, and summation is again over the stoichiometric unit. This modification function removes the average breadth of the distribution of electron density in the atom. It also changes the scale so that if $i(s)$ is in electron units, $i(s)M(s)$ and $D(r)$ are in units characteristic of one molecule. The physical meaning of the function $D(r)$ has been discussed in detail elsewhere⁴.

It is convenient to introduce a normalized radial distribution function:

$$G(r) = D(r)/4\pi r^2 \rho_0, \quad \dots (4)$$

which approaches unity for large values of r .

The experimental reduced intensity function of amorphous $P_{0.5}Se_{0.5}$ is shown in Fig. 1 (dotted). Fig. 2 (dotted) shows the corresponding radial distribution function $G(r)$ to distances of 10 Å. The experimental reduced intensity curve shows two maxima at $s=2.11 \text{ \AA}^{-1}$ and $s=3.70 \text{ \AA}^{-1}$ while the RDF curve shows two maxima around 2.20 and 3.40 Å. The peak around 2.20 Å is

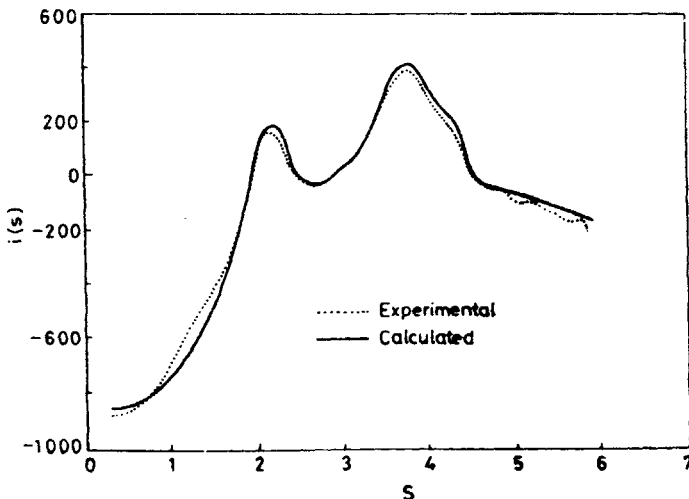


Fig 1 The experimental and calculated reduced intensity for amorphous $P_{0.5}Se_{0.5}$

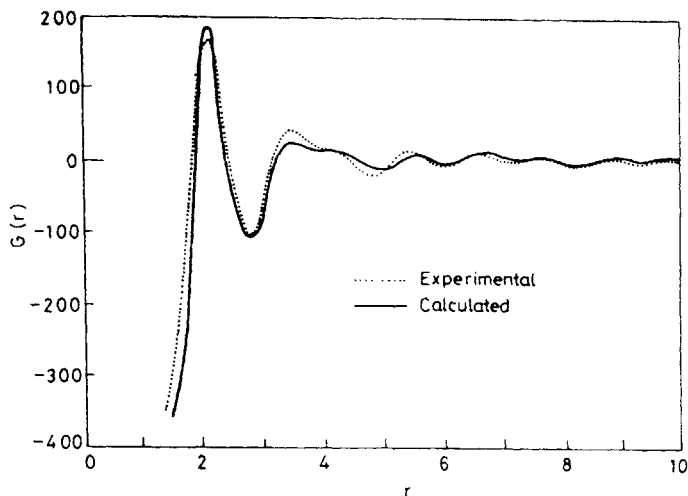


Fig 2 The experimental and calculated radial distribution function for $P_{0.5}Se_{0.5}$

mainly due to the intramolecular distances with the PSe molecule, while the peak around 3.4 Å in the RDF curve is due to the intermolecular distances between the PSe molecules.

Analysis of the Radial Distribution Function (RDF)

Reduced intensity function can be computed from the equation

$$i_D(s) = \sum \sum \exp(-b_{ij}s^2) f_i(s) f_j(s) \sin(sr_{ij}) / sr_{ij} \quad \dots (5)$$

In 5, r_{ij} is the mean radial distance between atoms i and j , and the summation is over all atoms in the structure under consideration. A temperature factor $\exp(-bs^2)$ is included in 5; it takes into account the distribution of instantaneous interatomic distances about their means r_{ij} both in time and space. The coefficient b_{ij} is one-half the mean-square variation in the distance r_{ij} between atom pairs.

Intensity curve for intramolecular interaction was computed from⁵. The parameters used in this computation were then subjected to systematic refinement by iterative nonlinear least square to seek a satisfactory fit of the experimental data.

Four parameters were varied: The P-P and Se-Se distances and the mean amplitudes associated with them. The four adjustable parameters were sufficient to give a good fit to all but the low angle region of the intensity function. The refined intramolecular P-P, Se-Se, B-Se distances and their root mean square (rms) displacements are shown in Table I. The Se-Se distance is 2.39 Å which is in good agreement with the value proposed in the amorphous Se⁶ and amorphous $Ge_{0.1}As_{0.3}Se_{0.6}$ ⁷.

For nonbonding distances "intermolecular", we terminate the series of terms in eq. (5) at some arbitrary distance and assume a uniform distribution of distances (continuum) beyond. This corresponds to making a "hole" in the

Table I $P_{0.5}Se_{0.5}$ intramolecular distances and their associated root mean square (rms) displacements

i	j	r_{ij}	(rms)
Se	Se	2.39(2)	0.06
P	P	1.91(3)	0.05
P	Se	2.18(2)	0.03

uniform structureless medium in which to place a discrete interaction of the model structure. The contribution of the continuum to the reduced intensity can be calculated from the following equation:

$$i_i(s) = \sum_i \sum_k \exp(b_{ik}s^2) f_i(s) f_k(s) 4\pi \rho_0 [sr_{ik} \cos(sr_{ik}) - \sin(sr_{ik})] / s^3, \quad \dots \quad (6)$$

where r_{ik} is the radius of the hole for interaction between atoms of type i and atom of type k . The reduced intensity function is then equal to the sum of (5) and (6). The calculated reduced intensity and the corresponding radial distribution function is shown in Figs. 1 and 2 (lines). The fit of the calculated RDF to the experimental one is reasonably well since the observable intensity range is limited.

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