JOURNAL OF MATERIALS SCIENCE 29 (1994) 3316–3322

Local order hypotheses and atomic arrangement in the glassy alloy $Cu_{0.20}As_{0.35}Te_{0.45}$ by X-ray diffraction

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An analysis of the atomic radial distribution function of $Cu_{0.20}As_{0.35}Te_{0.45}$ amorphous alloy obtained from quenching of the molten mixture of the elements, has been performed. The short-range order was determined by interpreting the radial distribution function (RDF), using a theoretical expression which takes into account the variation in the atomic scattering factors with the scattering vector module, *s*, and approximates them to polynomial functions. The tetra- and di-coordinated copper hypotheses, quoted in the literature for glassy alloys containing this element, have been considered. It was found that only the tetra-coordinated copper hypothesis is compatible with the structural information that was experimentally obtained. A spatial atomic distribution model was generated in accordance with this copper coordination, using a conveniently modified MonteCarlo random method. A comparative analysis of the structural parameters of this model revealed good agreement with the values given in the literature for similar materials.

1. Introduction

Traditionally, solid-state physics has meant crystal physics. Solidity and crystallinity are considered as synonymous in the texts on condensed matter. Yet, one of the most active fields of solid-state research in recent years has been the study of solids that are not crystals; solids in which the arrangement of the atoms lacks the slightest vestige of long-range order. The advances that have been made in the physics and chemistry of these materials, which are known as amorphous solids or as glasses, have been widely appreciated within the research community. Glassy alloys of chalcogen elements were the initial object of study because of their interesting semiconducting properties [1] and more recent importance in optical recording [2]. Recording materials must be stable in the amorphous state at low temperature and have a short crystallization time. Tellurium alloy films, in particular, are used as recording media because they have a low melting temperature and high absorption coefficients for the wavelengths of semiconducting lasers; promising materials with these characteristics have recently been studied [3, 4]. Glassy materials exhibit a characteristic transition temperature [5] from the more energetic glass phase to the minimal energy crystalline phase. The temperature at which the glass–crystal transition takes place is proportional to the average coordination of the material [6], so an understanding of its local order is very important, because it can be related to other physical properties of the material.

This work analyses the short-range order of the glassy alloy $Cu_{0.20}As_{0.35}Te_{0.45}$ from radial distribution function (RDF) data determined from X-ray diffraction intensities. The experimental value of the area under the first RDF peak was compared to the one obtained theoretically [7–9] as a coordination function of the copper, and bearing in mind that the products of the atomic scattering factors, $R_{ij}(s) = f_i(s)f_j(s)/[\Sigma_i x_i f_i(s)]^2$, depend on the Bragg angle, θ, through the scattering vector module, *s*, and cannot always be approximated by the constant value $Z_iZ_j/(\Sigma_i x_i Z_i)^2$. The aforementioned comparison shows that, for this alloy, the tetra-coordinated copper hypothesis quoted in the literature [10–12] can be considered as valid. Based on this copper coordination hypothesis, a spatial atomic distribution model was generated, using a semi-random method which takes into account the geometrical restrictions imposed by the experimental RDF. An analysis of the parameters (bond lengths and angles) of this model shows good agreement with the values quoted in the literature for similar alloys.

2. Experimental procedure

2.1. Preparation of the samples

The samples were prepared in bulk form, from 99.999% pure copper, arsenic and tellurium, pulverized to grains smaller than 40 μm. The three elements were homogeneously mixed in adequate proportions in order to obtain 7 g of the composition desired. The samples were put into quartz ampoules and subjected to an alternating process of filling and vacuuming of inert gas (helium) until a residual pressure of 10^{-3} torr (1 torr = 133.322 Pa) was reached. The ampoules were sealed with an oxyacetylene burner, in order to avoid a possible oxidation of the alloy during the thermal process, and put into a rotary furnace at 900° C, quaranteening the melting of the three elements. The rotation device of the furnace turned the ampoules at 1/3 rev min^{-1}, in order to ensure the homogeneity of the molten material. After 5 h under these stirring and heating conditions, the ampoules were quenched in ice–water, producing the glassy material.

The quartz capsules were corroded in a mixture of hydrofluoridic acid and hydrogen peroxide, in order to remove the alloy. Part of the samples was pulverized and pressed into $20 \times 20 \times 1$ mm^3 bricks; it was checked by X-ray diffraction that the compound did not exhibit the characteristic peaks of a crystalline phase. Fig. 1 shows the diffractogram of alloy $Cu_{0.20}As_{0.35}Te_{0.45}$. The density of the material was determined by a pycnometric method at a constant temperature, the average value of the series of measurements being 5.98 g cm^{-3}, with a relative error less than 3%.

2.2. X-ray diffraction intensity measurements

The intensities of the radiations diffracted by the samples were measured in an automatic Siemens D500 powder diffractometer with Bragg–Brentano geometry by reflection. The proper selection of an X-ray wavelength was obtained using a bent graphite monochromator. The device was equipped with a scintillation detector, with a thallium-enriched photosensitive NaI window.

Because the detection system used consists of counting the number of photons randomly received, whose statistical error depends on the number of photons that reach the detector, the intensities were measured by determining the number of counts and digitally registering the time it took to carry them out, so the error is kept constant throughout the whole series of measurements. The number of pulses was determined as 4000, so the relative error was kept below 1.5%. The intensities diffracted by the samples were measured in the range of s ($= (4\pi/\lambda) \sin\theta$) from 7.7–144.8 nm^{-1} using a radiation of MoK_α ($\lambda = 0.071\,069$ nm), supplying the generator with a power of 50 kV, 30 mA. Four series of measurements were carried out, two with ascending and two with descending Bragg angle. The average of the four measurements carried out for each angle was taken as the intensity of the radiation diffracted by the samples.

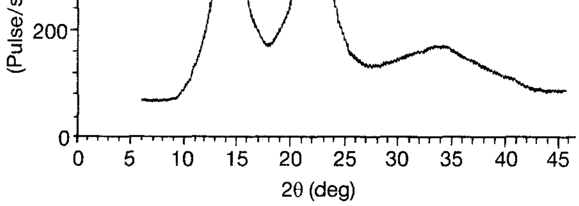

Figure 1 Diffractogram of glassy alloy $Cu_{0.20}As_{0.35}Te_{0.45}$.

2.3. X-ray intensity treatment

The intensities mentioned above were corrected, as usual, for background, polarization and multiple scattering [13], in order to eliminate that part of the radiation which does not carry structural information. Fig. 2 shows these corrected intensities in arbitrary units for the alloy studied.

The normalization of electronic units (e.u) was done bearing in mind the high-angle technique [13], according to which, for high values of s, the experimental intensity curve should oscillate around the independent scattering curve of the structure. The normalization method [7] consisted of fitting by least-squares, the experimental curve $I(s)$ in arbitrary units to the independent scattering curve $f(s)$, by minimizing the function (S is square deviation)

$$S = \sum_{i=1}^{M} [f(s_i) - k_1 I(s_i) \exp(-k_2 s_i^2)]^2 \quad (1)$$

where k_1 and k_2 are two adjustment parameters, and the factor $\exp(-k_2 s_i^2)$ is used as an adequate mathematical function for simulating a reduction in the amplitude of the oscillations for increasing angles. The normalized intensities were corrected for the Compton effect, the coherent spectrum $I_{e.u}(s)$ being obtained from which the reduced intensities are, in turn, obtained

$$i(s) = \frac{I_{e.u}(s) - \Sigma_i x_i f_i^2(s)}{[\Sigma_i x_i f_i(s)]^2} \quad (2)$$

where x_i and $f_i(s)$ are the atomic fraction and the atomic scattering factor of an i-type atom, respectively.

The application of a Fourier transformation to the interference function, $F(s) = s \times i(s)$, resulted in the relationship

$$G(r) = \frac{2}{\pi} \int_0^{s_{max}} F(s) \sin(sr)\, ds \quad (3)$$

s_{max} being the maximum limit for which there are experimental data.

From Equation 3, the radial distribution function is immediately deduced

$$4\pi r^2 \rho(r) = 4\pi r^2 \rho_0 + rG(r) \quad (4)$$

where $\rho(r)$ is the local atomic density which is affected by the Fourier transformation of the products $R_{ij}(s)$,

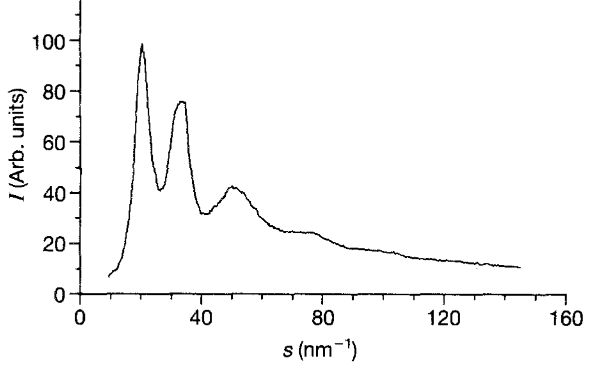

Figure 2 Corrected intensities in arbitrary units.

and ρ_0 is the average experimental atomic density of the material expressed in atoms per cubic nanometre. The spurious oscillations which appear in the radial atomic distribution function for small values of r, due to the lack of experimental data for high values of s, make it necessary to extend the interference function up to 300 nm^{-1}, a value for which function $F(s)$ tends towards zero. The extension was carried out using the method described in the literature [14], based on that proposed by Shevchick [15] according to whom, for high values of s, the experimental interference function can be approximated by

$$F_{\text{theoretical}}(s) = \frac{C}{r}\exp\left(\frac{-\sigma^2 s^2}{2}\right)\sin(sr) \qquad (5)$$

where C, r and σ are parameters obtained by least-squares adjustment from the initial values C_1, r_1 and σ_1, which represent the area, the position and the half-width of the first RDF peak, deduced from Equation 3 for $s_{\max} = 144.8\ \text{nm}^{-1}$, the maximum value for which data have been obtained with the device used. The Fourier transformation was applied to the extended interference function, resulting in the RDF shown in Fig. 3, which supplied the following structural information: position of the first two maximum value: 0.264 and 0.418 nm; limits of the first peak: 0.220–0.295 nm; area under the latter: 3.21 ± 0.1 atoms; average bond angle 104.7°.

3. RDF analysis and copper coordination hypotheses

Analysis of the structural data supplied by the radial atomic distribution function shows, among other things, that the definition interval of the first peak, corresponding to the first coordination sphere of alloy $Cu_{0.20}As_{0.35}Te_{0.45}$ (Cu = 1, As = 2, Te = 3), is such that all types of bond are possible between the different elements in the compound, as may be observed by comparing the mentioned interval to the bond lengths, r_{ij}, of all possible pairs quoted in the literature and shown in Table I.

Bearing in mind that the Te–X bonds (X = Cu, As, Te) ought perhaps to contribute most to the diffraction spectrum, it seems reasonable to assume that the first maximum RDF value is within the values defining the bond lengths of the corresponding pairs, which agrees with the average weighed value, 0.261 nm, of these three types of bond. Owing to the character of the RDF as a probability function, the positions of its maximum values can be interpreted as the average distances between the different coordination spheres and an arbitrary reference atom. Specifically, the abscissa of the first maximum value represents the average distance between first neighbours.

A parameter of great interest, when postulating short-range models of a glassy solid, is the area enclosed under the first RDF peak, because it represents the number of atoms which, on average, surround an arbitrary reference atom, in other words, the average coordination number of the material. Bearing in mind the physical meaning of this area, and the fact that the products of atomic factors, $R_{ij}(s)$, are functions of the scattering angle, Vázquez and Sanz [22], following the method described by Warren [13], have come to the conclusion that the area under the first RDF peak is related to certain structural parameters, the relative coordination numbers, n_{ij}, through the expression

$$\text{Area} = \frac{2}{\pi}\sum_{i,j} x_i \frac{n_{ij}}{r_{ij}} \int_a^b r P_{ij}(r)\,\mathrm{d}r \qquad (6)$$

r_{ij} being the average distance between an i-type atom and a j-type atom, a and b the limits of the first RDF peak and $P_{ij}(r)$ a function defined as

$$P_{ij}(r) = \frac{1}{2}\int_0^{s_m} R_{ij}(s)\cos\left[s(r - r_{ij})\right]\mathrm{d}s \qquad (7)$$

where s_m is the upper measurement limit.

The structural information obtained from the analysis of the experimental RDF, together with the physiochemical properties of the alloys and their constituent elements, allow us to hypothesize the local order of glassy materials. These hypotheses, reflected in the relative coordination numbers and therefore in

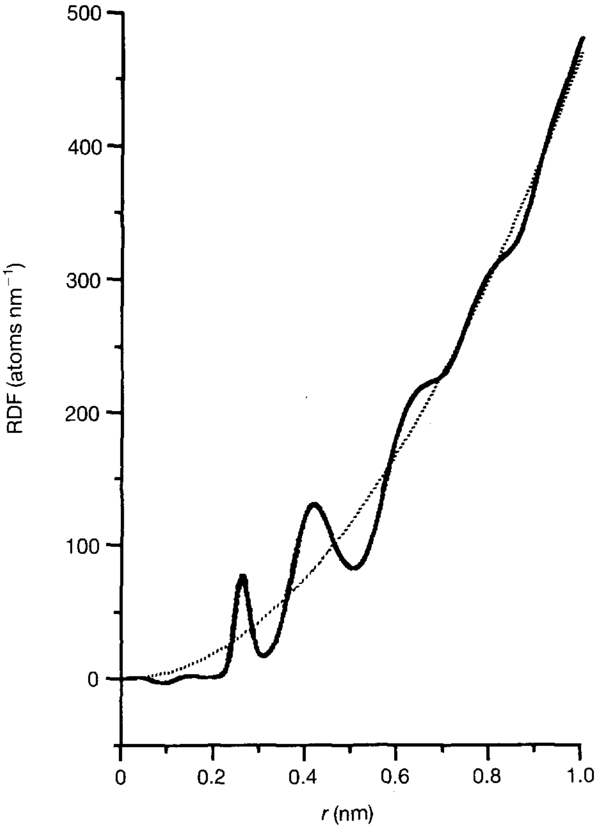

Figure 3 Radial distribution function.

TABLE I Bond lengths

Pair	r_{ij}(nm)	Reference
Cu–Cu	0.258	[11]
Cu–As	0.260	[16]
Cu–Te	0.264	a
As–As	0.259	[18, 19]
As–Te	0.258	[20]
Te–Te	0.262	[21]

[a] Estimation by means of Schomacker and Stevenson's formula [17].

the number of chemical bonds, a_{ij}, between the different pairs of elements in the material, led Vázquez *et al.* [9] to deduce from Equation 6, the following relationship

$$\text{Area} = \frac{1}{50\pi}\Big[(h + \beta A_{22} - \delta Q)N + \alpha A_{22} + \gamma Q + P\Big(\sum_{i=j\neq 1} A_{ij} - \sum_{\substack{ij\neq 1\\ i\neq j}} A_{ij}\Big)a_{ij}\Big] \qquad (8)$$

where h, α, β, γ and δ are parameters that depend on the alloy and on the coordination hypotheses, N is the coordination attributed to a certain element in the material, P is a parameter equal to 2 when, in the variable a_{ij}, $i = j$ and equal to -1 if $i \neq j$, and A_{ij} is determined by

$$A_{ij} = \frac{1}{r_{ij}}\int_a^b rP_{ij}(r)\,\mathrm{d}r \qquad (9)$$

being

$$Q = \delta_{ij}\sum_{\substack{ij\neq 1\\ i\neq j}} A_{ij} + (1-\delta_{ij})\sum_{i=j\neq 1} A_{ij}$$

(δ_{ij} = Kronecker's delta).

A theoretical evaluation of the area under the first RDF peak according to Equation 8, as function of the coordination, N, attributed to the copper, requires calculation of the parameters A_{ij}. According to the literature [22], the calculation of these parameters involves establishing the order of the polynomes in s, which approximate the functions $R_{ij}(s)$; in this work, the mentioned functions were adjusted to the straight regression lines of the corresponding pairs of elements in the alloy, whose equations, $F_{ij}(s) = A_{0ij}s + A_{1ij}$ are given in Table II. Parameters A_{ij}, given in Table II, were calculated according to the literature method [9] from the bond lengths, r_{ij}, given in Table I and the coefficients A_{0ij} and A_{1ij} of the aforementioned straight regression lines.

In order to express the area in question as a function of the coordination, N, assigned to the copper atoms in this alloy, the characteristic parameters ($h = 14.2338$, $Q = 3.4137$) and those depending on the coordination hypotheses were calculated [9]: $\alpha = 17.50$, $\beta = -2.50$, $\gamma = 78.75$, $\delta = -11.25$, for $N = 2$ and 4. From these data and the tabulated A_{ij}s, and using Equation 8, the following expressions were obtained

$$\text{area} = 2.4649 + 5.7\times 10^{-3}a_{33} \qquad \text{for } N = 2 \quad (10\text{a})$$

$$\text{area} = 3.1018 + 5.7\times 10^{-3}a_{33} \qquad \text{for } N = 4 \quad (10\text{b})$$

TABLE II Straight regression lines fitted to values of $R_{ij}(s)$ and A_{ij} parameters

Pair	$F'_{ij}(s)$	A_{ij}
Cu–Cu	$-6.30\times 10^{-3}s + 0.4885$	0.7886
Cu–As	$-6.09\times 10^{-3}s + 0.5598$	0.9106
Cu–Te	$-3.02\times 10^{-3}s + 0.9014$	1.4979
As–As	$-5.65\times 10^{-3}s + 0.6414$	1.0460
As–Te	$-1.02\times 10^{-3}s + 1.0325$	1.7068
Te–Te	$1.31\times 10^{-2}s + 1.6594$	2.8178

which may be used for postulating the short-range order of the alloy. These relationships are functions of the number of Te–Te bonds, a_{33}, limiting the variability field of the theoretical area.

In order to generate a local-order model of alloy $Cu_{0.20}As_{0.35}Te_{0.45}$, it is necessary to establish the average coordination of its constituent elements, which involves attributing a certain coordination to the copper. This is a relatively difficult question, because there is no single-coordination hypothesis in the literature for this element in other compounds. Whereas some authors [11, 23] propose two-fold coordination for the copper in similar compounds, others [12, 16] propose tetrahedral coordination for copper in ternary alloys with chalcogens; both hypotheses must be taken into consideration.

Bearing in mind that, for each value of N, Equations 10a and b vary linearly with the number of Te–Te bonds, and that the relative coordination numbers, n_{22} and n_{23}, also depend on N, it is possible to obtain, according to the literature [24], the suitable coordination of copper by determining the variation interval of a_{33} for which the relative coordination numbers are positive and, at the same time, the theoretically obtained area is within the margin of error of the experimental area. In order to do this, the relative coordination numbers that contain parameter a_{33} are given [9] by

$$n_{22} = \frac{\alpha + [100\beta + a'_1(a'_3 - a'_2)](N/100) + 2a_{33}}{a'_2}$$

$$n_{23} = \frac{\gamma - [100\delta + a'_1 a'_3](N/100) - 2a_{33}}{a'_2} \qquad (11)$$

which allow us to obtain for $N = 2$ an average $\langle a_{33}\rangle = 20.8$. Considering Equations 10a with $N = 2$, a value of 2.58 is obtained for the area under the first RDF peak; 2.58 atoms, as may be observed, is considerably less than the value obtained experimentally, a fact that led to the rejection of coordination 2 for the copper in the alloy studied.

In the present work, tetracoordinated copper ($N = 4$) has been assumed, accepting the necessary electrons for the sp^3 hybridization of some arsenic and tellurium atoms which increase their coordination by one unit [16]. Under this hypothesis, the coordination numbers n_{22} and n_{23} are positive for values of a_{33} within the interval [0–43.88], and Equation 10b gives for the area under the first RDF peak an expression that is in good agreement with the experimentally determined value, within the ± 0.1 atom margin of error. This analysis leads us to the conclusions that in the alloy in question, the most probable short-range order can be described as a network of tetrahedral units centred on copper atoms together with other tetrahedra centred on arsenic atoms. All of these structural units would be joined by ramified chains, made up of an excess of tellurium atoms.

4. Generation of the spatial model and discussion of the results

The basic aim of determining the structure of glassy solids is to build spatial atomic distribution models which verify the experimentally obtained structural information and, at the same time, agree with the physiochemical properties of the materials. This model was generated using a variation of the Monte Carlo method, similar to the procedure followed by Rechtin *et al.* [25], which seems to be the most adequate for describing the short-range order of a glassy material obtained through quenching. The variations of this procedure refer to the geometrical and coordination conditions imposed by the experimental RDF, which imply a certain semi-randomness in the building of the atomic configuration.

The mathematical space considered suitable for generating the possible structural model of the alloy $Cu_{0.20}As_{0.35}Te_{0.45}$ is the volume limited by a 1 nm radius spherical surface, which is large enough statistically to represent the sample, and small enough not to require too much calculation time. The number of atoms which, according to the experimental density, can be located in this volume is 156, distributed as follows: 31 copper atoms, 55 arsenic atoms and 70 tellurium atoms.

The atomic positions were generated by finding their cartesian coordinates from three random numbers [26] and bearing in mind all the geometrical and coordination conditions deduced from the analysis of the experimental RDF, and which in this case are the following:

(i) the distance between first neighbours must be within the interval defined by the first experimental RDF peak;

(ii) the bond angle between an atom and two of its first neighbours may vary between 60° and 180°, as may be deduced [27] from the extreme radii of the first two coordination spheres represented by the limits of the first two RDF peaks;

(iii) the coordination attributed to each element must be such that the average coordination of the model agrees with the experimentally obtained coordination.

Considering the aforementioned geometrical and coordination conditions, 200 positions were generated and reduced to 156, the number predicted from the experimental density, by eliminating those with the lowest coordination. The next step was to assign the atoms to their positions, placing the copper atoms in the positions with maximum coordination, the other elements being randomly placed in the rest. The reduced RDF, $rG(r)$, was determined for this configuration, and compared to the experimental RDF, modified by the finite size simulation function [28]. The initial model was considered to be suitable for obtaining a relatively speedy adjustment of the theoretical and experimental reduced RDFs; so the positions were refined by successive atom movements, of arbitrary amplitude P and in random directions, adding the restrictions of not allowing movements which break copper atom bonds, thus keeping the coordination postulated for this element.

During the position refining process, the model evolved as shown in Table III where the mean square deviation refers to the last movement in each interval. The position-refining process was considered finished when the number of rejected movements became too high and the mean square deviation did not significantly improve. Fig. 4 shows the experimental reduced RDF and the model RDF, after the process of refining the positions and the thermal factors was completed.

The spatial representation of the generated atomic distribution is shown in Fig. 5, where tetrahedric units centred on copper atoms may be observed to coexist with other tetrahedric units centred on those arsenic atoms whose coordination has increased to four. Fig. 6 is a spatial representation of the network of tetrahedra centred on copper atoms. Both structural units are interlinked, forming a framework that constitutes the possible structure of the alloy.

TABLE III Position refining process

$P(10^{-1}$ nm)	Movement intervals	Squared deviation (nm)
0.5	1–417	0.003 12
0.3	418–439	0.002 75
0.1	440–476	0.001 93

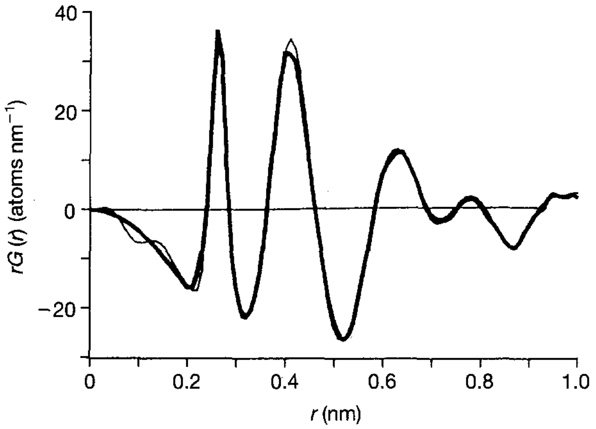

Figure 4 Representation of (——) calculated and (——) experimental RDFs.

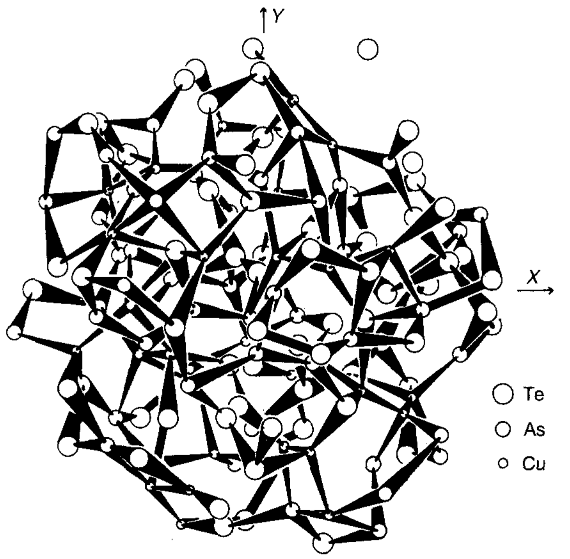

Figure 5 Spatial representation of the model of alloy $Cu_{0.20}As_{0.35}$-$Te_{0.45}$.

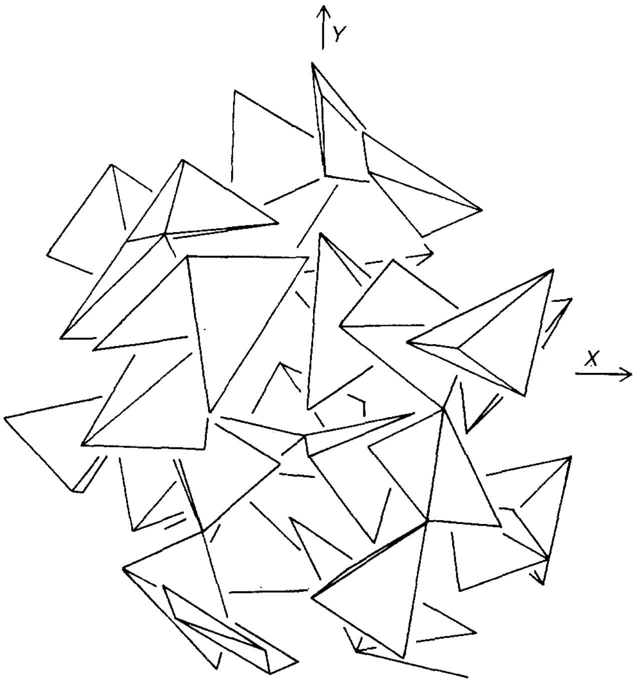

Figure 6 Spatial representation of the network of tetrahedra centred on copper atoms.

This theoretical model, which is randomly generated and which takes into consideration the structural information obtained from the experimental RDF, must be as representative as possible of the real structure of the alloy in question. One way of estimating the agreement between this model and the atomic distribution of the compound is by analysing its main structural parameters (coordinations, average bond lengths, etc.).

An important point to bear in mind when statistically analysing the generated model is the comparison of the resulting coordinations of its elements and those of the structural units, which, according to the established hypotheses, can be postulated from the information supplied by the experimental data. Table IV shows the coordinations of each element in the atomic model of the alloy and, in parentheses, the coordinations which were theoretically predicted based on the tetracoordinated copper hypothesis. Dangling bonds are observed in this spatial distribution, indicating the presence of atoms with unsaturated bonds; this can be partly justified by the finite size of the model. In this case, 75% of unsaturated atoms are less than 0.2 nm away from the spherical surface, and cannot, therefore, be considered infra-coordinated, as they can bond with external atoms. However, the existence of dangling bonds is inherent to the method of preparation of chalcogenide glasses.

An interesting aspect of the generated model is the average bond lengths in the different pairs of elements in the material, which in this case are as follows: Cu–Cu 0.255 nm, Cu–As 0.258 nm, Cu–Te 0.262 nm, As–As 0.259 nm, As–Te 0.257 nm, Te–Te 0.264 nm. The agreement between these lengths, which were theoretically calculated from experimental data supplied by the alloy in question, and those known for similar compounds, is a criterion for establishing the validity of the model. In this work, a comparative analysis of the mentioned distances and the bibliographical data was carried out as follows.

TABLE IV Model coordinations

Atom	Coordination				
	4	3	2	1	0
Cu	31(31)	0(0)	0(0)	0(0)	0(0)
As	15(41)	25(14)	15(0)	0(0)	0(0)
Te	0(0)	30(53)	31(17)	7(0)	2(0)

(i) The average value of the Cu–Cu length, theoretically calculated, is very close to 0.258 nm quoted in the literature [11] for this bond length.

(ii) The theoretically calculated average length of the Cu–As bond is approximated, by defect and by excess, to the 0.260 and 0.255 nm which are the lengths of this bond in alloys $Cu_{0.05}As_{0.50}Te_{0.45}$ [16] and $Cu_{0.15}As_{0.40}Te_{0.45}$ [16], respectively.

(iii) The average value of the Cu–Te length in this model is slightly higher than the 0.261 nm which is the length of this bond in alloy $Cu_{0.15}As_{0.40}Te_{0.45}$ [16], and equal to the value quoted in the literature [16] for the Cu–Te bond in the glassy solid $Cu_{0.05}As_{0.50}Te_{0.45}$.

(iv) In the case of the As–As bond, the theoretically calculated length coincides exactly with the As–As distance in the molecular unit As_4S_4 [19] and is slightly higher than the covalent distance of this element [10]. It is possible that As–As bonds are present in the alloy studied, these being relatively longer than the typical covalent bonds, due to circumstances similar to those found in the As_4S_4 molecule.

(v) The theoretical model gives an average value of 0.257 nm for the As–Te bond, a value which is very close, in defect and in excess, to 0.258 and 0.255 nm, the length of this bond in alloys $As_{0.45}Se_{0.10}Te_{0.45}$ [20] and $As_{0.20}Se_{0.50}Te_{0.30}$ [18] respectively, and exactly the same as the value found for this bond [16] in the glassy composition $Cu_{0.05}As_{0.50}Te_{0.45}$.

(vi) The generated spatial structure supplies an average Te–Te length which is somewhat lower than the 0.267 nm found for this bond in alloy $As_{0.45}Se_{0.10}Te_{0.45}$ [20] but very similar to the 0.262 nm in alloys $Cu_{0.15}As_{0.40}Te_{0.45}$ [16] and $Al_{0.20}As_{0.40}Te_{0.40}$ [29], so it can therefore be considered adequate in this study.

As we have seen, a detailed analysis of the theoretical values shows their good agreement with the bibliographical data; they can therefore be considered representative of the bond lengths in the real structure of the alloy.

Another parameter that is often used for obtaining information on the structure of a glassy solid is the average bond angle of each element with two of its first neighbours. The average values of the bond angles are as follows: Cu 107.1°, As 108.3°, Te 109.5°; a great similarity between these values and the characteristic angle of the typical tetrahedral disposition is observed. The most probable atomic configuration of the alloy studied may, therefore, be basically made up of tetrahedral structural units.

5. Conclusion

Considering the radial atomic distribution function of the alloy in question, obtained from the X-ray diffraction data, and from the copper coordination hypotheses quoted in the literature, the tetracoordinated copper hypothesis was found to most correctly explain the average number of first neighbours determined experimentally for this composition.

The use of the most approximate expression of the area under the first RDF peak has made it possible to discard two-coordination for the copper, as it has in copper oxide, as this coordination implies a considerably smaller theoretical area than that obtained experimentally for the alloy.

Bearing in mind the tetracoordinated copper hypothesis, a spatial atomic distribution model of the alloy was built, using the MonteCarlo random method and taking into account the geometric conditions deduced from the radial atomic distribution function obtained by X-ray diffraction of the samples.

From the analysis of the generated model, the three-dimensional structure of the studied alloy can be described as a network of tetrahedra centred on copper atoms, coexisting with other tetrahedra whose centres are occupied by tetracoordinated arsenic atoms, making the network more compact. These tetrahedral units can be joined together either directly or by chains of tellurium atoms.

Acknowledgements

The authors are grateful to the Junta de Andalucia and the Comisión Interministerial de Ciencia y Tecnología (Project MAT 92-0837) for their financial support.

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Received 30 March 1993
and accepted 10 January 1994