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Applications to practical cases of the basic parameters for the local order of glassy ternary alloys

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Abstract

A procedure was developed for determining theoretical expressions for the area under the first radial distribution function (RDF) peak and of the relative coordination numbers, n_{ij}, which depend on the coordination hypotheses and on the numbers of bonds between elements of a single type of pairs. In this method two important facts were taken into account. The products of atomic factors are functions of s (the scattering vector module) and so they cannot always be assumed to be constant; they were therefore approximated by polynomial functions which best fitted the results obtained from the atomic factors given in the International Tables of Crystallography. We considered the affects of the structural hypotheses (coordination, existence of certain types of bond) on the area and coordination numbers mentioned which enable us to postulate the most probable local order. To test the reliability of this method, it was applied to a set of alloys, quoted in the literature and the theoretical results obtained agree satisfactorily with the data. © 1997 Elsevier Science B.V.

1. Introduction

A method which, to date, has proven to be efficient for structural research is the interpretation of the diffraction of radiation by the solid. X-ray diffraction has been used to obtain structural information on the glassy materials considered in this work [1–4]. When interpreting the radial atomic distribution function (RDF), obtained from the X-ray diffraction intensities, the area under the first peak is determined by the relative coordination numbers, n_{ij}. From these numbers the short-range order of a material can be deduced. This area also depends on the products of the atomic scattering factors, $R_{ij}(s) = f_i(s)f_j(s)/(\Sigma_i x_i f_i(s))^2$ (s is the scattering vector module), which, in some cases, varies considerably with s [5].

This work takes into account that the atomic scattering factors are functions of Bragg's angle [5] and also the coordination hypotheses for a certain element in the alloy. These two considera-

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tions made it possible to calculate from theoretical expressions the parameters which depend on the alloy and of the coordination hypotheses which appear in the theoretical expression of the area under the first peak and in those of the average coordination numbers [6–9]. The theoretical results were applied to an analysis of the short-range order of different glassy alloys; the results agree with experimental data.

2. Theoretical background

The classical theory of electromagnetic wave diffraction, for a three-dimensional configuration of atoms, makes it possible to deduce a relationship between the diffracted intensity in a given direction and the relative positions of the atoms in the material. When this relationship is applied to a glassy material in which it is possible to postulate that the positions are randomly oriented, the intensity diffracted in each direction, expressed in electron units (e.u.), is given by Debye's equation [10]

$$I_{\text{e.u.}}=\sum_{n,m} f_n f_m \frac{\sin sr_{nm}}{sr_{nm}} \qquad (1)$$

where $s=(4\pi/\lambda)\sin\theta$, f_m and f_n are the scattering factors of atoms m and n, respectively and r_{nm} is the distance between those atoms.

An evaluation of Debye's equation involves the atomic scattering factors as functions of Bragg's angle via the magnitude s, a consideration which was taken into account by Finbak [11] and later by Waser and Schomaker [12] and even later by Warren [5]. According to Warren, the following relationship is found for the RDF:

$$\frac{2r}{\pi}\sum_{ij} x_i \frac{n_{ij}}{r_{ij}} P_{ij}(r)=4\pi r^2\rho_0+rG(r), \qquad (2)$$

where x_i is the atomic fraction of element i, $G(r)$ is the Fourier transformation of the interference function, ρ_0 is the average atomic density of the material, r_{ij} is the distance between an i-type atom and a j-type atom and the function $P_{ij}(r)$ is defined by

$$P_{ij}(r)=\frac{1}{2}\int_0^{s_m} R_{ij}(s)\cos\left[s(r-r_{ij})\right]\mathrm{d}s, \qquad (3)$$

where s_m is the maximum s for which experimental data are available. By defining a function, $\rho(r)=(2\pi^2 r)^{-1}\sum_{ij} x_i n_{ij} r_{ij}^{-1} P_{ij}(r)$, representing the local atomic density affected by the Fourier transformation of the atomic factor products, Eq. (2) changes to

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

which represents the average number of atoms surrounding a reference atom at a distance r.

When evaluating the average number of first neighbours of an arbitrary atom (that is, its average coordination), it is necessary to obtain the area under the first RDF peak given by the expression

$$\text{Area}=\frac{2}{\pi}\sum_{ij} x_i \frac{n_{ij}}{r_{ij}}\int_a^b rP_{ij}(r)\mathrm{d}r, \qquad (4)$$

where a and b are the abscissae of the limits of the peak.

There are practical cases in which it may be observed that the approximation of considering the function, R_{ij}, to be constant and equal to $Z_iZ_j/(\sum_i x_iZ_i)^2$ is sufficiently inaccurate to affect the short-range order postulated for the material. In relation to this, Fig. 1 shows the functions $P_{ij}(x)$ vs. $x=r-r_{ij}$ for all possible pairs of elements in amorphous SiO_2 [5]. In addition to the ripples due to the errors in finishing the series, the curve for Si–Si is observed to have a negative wing just outside the main peak and the curve for O–O has a positive region at the end of the main peak. These positive or negative regions are a consequence of the shapes of the $R_{ij}(s)$ curves. A relatively broad, though not complete, analysis of cases such as amorphous SiO_2 seems to make it advisable to express the products, $R_{ij}(s)$, through the functions which best fit the results obtained from the atomic scattering factors given in the International Tables of Crystallography. In this sense, Vázquez and Sanz [6] have developed an analytical method for evaluating the area under the first RDF peak in which the products, $R_{ij}(s)$, are expressed by n-order polynomials in s, i.e. $R_{ij}(s)=\sum_{\varphi=0}^{n} A_{\varphi} s^{\varphi}$. When these polynomials are of the first order, as is frequently the case, the authors [6] propose the following expression:

$$\mathrm{Area}\frac{2}{\pi}\sum_{ij} x_i n_{ij} A_{ij} \tag{5}$$

with $A_{ij}=r_{ij}^{-1}\int_a^b rP_{ij}(r)dr=(2r_{ij})^{-1}[B_{1ij}+B_{2ij}+r_{ij}(B_{3ij}+B_{4ij})]$, and the addends, $B_{uij}(u=1,2,3,4)$ being given by the relationships

$$B_{1ij}=(A_{1ij}s_m+A_{0ij})(\cos s_m a'_{ij}-\cos s_m b'_{ij})s_m^{-1},$$

$$B_{2ij}=\left(A_{1ij}\ln|a'_{ij}|b'^{-1}_{ij}\right),$$

$$B_{3ij}=\int_{a'_{ij}}^{b'_{ij}} x^{-1}\sin s_m x\,\mathrm{d}x,$$

$$B_{4ij}=A_{1ij}\Big[(1-\cos s_m b'_{ij})b'^{-1}_{ij} -(1-\cos s_m a'_{ij})a'^{-1}_{ij}\Big],$$

where A_{1ij} and A_{0ij} are the slope and the zero-ordinate, respectively, of the regression line corresponding to the product of the scattering factors of atoms i,j and $a'_{ij}=a-r_{ij}$ and $b'_{ij}=b-r_{ij}$.

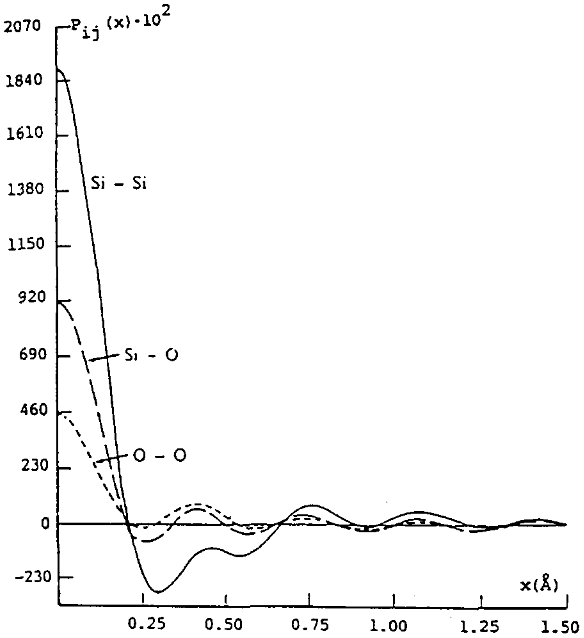

Fig. 1. Representation of functions $P_{ij}(x)$ vs. x for the different pairs of elements in amorphous SiO_2.

It should be noted that Eq. (5) is a function of the relative coordination numbers, n_{ij} and therefore it is a function of the number of the chemical bonds, a_{ij}, between the i-type and j-type elements of the alloy. This fact made it possible to develop analytical methods [7,8] for expressing the area under the first RDF peak as a function of the coordination of one type of element in the material and of the number of bonds between pairs of atoms.

2.1. Basic parameters which depend on the alloy and on the coordination hypotheses

A theoretical evaluation of the average coordination of a glassy alloy, from its RDF involves determining the area under the first peak of this function as accurately as possible. This area will enable a coordination to be attributed to a certain element, according to its properties and to the coordination proposed in the literature for the same element in similar alloys. The postulated coordination is substituted in the theoretical expression of the area and the area obtained for this coordination is compared to the area enclosed by the first experimental RDF peak. If the difference between the two areas is within experimental error, the coordination hypothesis may be considered adequate, otherwise, the hypothesis should be rejected and another one tested. On the other hand, it is a well-known fact that, in glassy alloys, the absence of bonds between certain types of elements may be postulated and therefore, it is important that the theoretical expression for the area should include this possibility in order to compare the experimental area to the theoretical areas obtained through different hypotheses of bonding of the elements in a glass.

To obtain the above-mentioned expression for the area, which permits hypotheses on the local order of solid, a ternary glassy alloy $A_{a'_1}B_{a'_2}C_{a'_2}$ assuming 100 atoms of material, has been considered and the hypotheses are

1. Element A has coordination N, irrespective of the composition of the alloy and the average coordination numbers of this element with all those bonded to it are proportional to their respective percentage concentrations.
2. The total number of i-type bonds, a_i, is given by
$$a_i = 2a_{ii} + \sum_{i \neq j} a_{ij}, \qquad (6)$$
where a_{ij} is the number of chemical bonds between i-type and j-type elements.
3. If the normal coordination of the different elements in the sample are called C_i and it is assumed that element A has a coordination N $(N \neq C_1)$, the number of bonds of this type of atom is
$$a_1 = Na_1' = C_1 a_1' \pm |x|,$$
$|x|$ being the variation in the number of bonds of the element, when its coordination changes from C_1 to N.
4. When the coordination of element A changes, the coordinations of elements B and D may increase or decrease, so the number of bonds of these elements is given by
$$a_i = C_i a_i' \pm |y_i|, (i \neq 1),$$
where $|y_i|$ represents the variation in the number of i-type bonds.

Taking these hypotheses into account, Vázquez et al. [9] deduced the following relation using Eq. (4) and results from Vázquez et al. [7,8]:

$$\mathrm{Area} = \frac{1}{50\pi}\left[(h + \beta A_{22} - \delta Q)N + \alpha A_{22} + \gamma Q + P\left(\sum_{i=j\neq 1} A_{ij} - \sum_{i,j\neq 1, i\neq j} A_{ij}\right)a_{ij}\right], \qquad (7)$$

where h, α, β, γ and δ are characteristic parameters of each alloy; P is a parameter equal to 2 when, $i = j$ in the variable a_{ij} and equal to -1 if $i \neq j$; and Q is defined by the relationship

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

in which δ_{ij} is Kronecker's delta.

The previous expression for the theoretical area enables, according to the experimental area, the variation interval of the number of bonds between the elements of a certain pair to be found, for each coordination hypothesis. This fact is useful when choosing the best coordination for the elements which usually make up compounds with different coordinations.

2.2. *Relative coordination numbers*

The relative coordination numbers, n_{ij}, of the different pairs of elements of a compound, are a set of parameters useful in postulating the short-range order of a glassy solid. These parameters, which represent the average number of j-type atoms surrounding an i-type atom, can be related to the coordination, N, attributed to a certain element; bearing in mind the restrictions imposed by the intrinsically positive nature of n_{ij}, it is possible to choose an appropriate N.

When postulating the absence of bonds between certain types of element, the corresponding n_{ij}'s are zero. As it is always possible to assign the subscript 1 to one of these types, considering the hypothesis mentioned above to the effect that the average coordination numbers of this element with all the elements, k, bonded to it, are proportional to their respective percentage concentrations, the following expressions are obtained:

$$n_{1k} = \frac{a_k' N}{\sum_k a_k'}, \quad n_{k1} = \frac{a_1' N}{\sum_k a_k'},$$

which depend on the coordination attributed to element A. Bearing in mind that the relative coordination numbers are given by $n_{ij} = a_{ij}/a_i'$, expressions can be deduced for the n_{ij} $(i,j \neq 1)$ enabling the short-range order of the solid to be hypothesized.

From Eq. (6), Vázquez et al. [9] deduced the following expressions for the coordination numbers n_{ij} $(i,j \neq 1)$ as functions of the number of a_{ij} bonds:

$$\begin{aligned} n_{22} = {} & \Bigg\{ \alpha + \gamma(1-\delta_{ij}) + \Bigg[\Big(\beta - \delta(1-\delta_{ij}) \Big) \sum_k a'_k \\ & + a'_1(\delta_{ij} p a'_3 - q a'_2) \Bigg] N \Big(\sum_k a'_k \Big)^{-1} \\ & + P a_{ij} \Bigg\} a'^{-1}_2, \\ n_{23} = {} & \Bigg\{ \Bigg[\gamma - \Big(\delta \sum_k a'_k + a'_1 p a'_3 \Big) N \Big(\sum_k a'_k \Big)^{-1} \Bigg] \delta_{ij} \\ & + (1-3\delta_{ij}) a_{ij} \Bigg\} a'^{-1}_2 n_{33} \\ = {} & \Bigg\{ \Bigg[\gamma - \Big(\delta \sum_k a'_k + a'_1 p a'_3 \Big) N \Big(\sum_k a'_k \Big)^{-1} \Bigg] \\ & \times (1-\delta_{ij}) - (1-3\delta_{ij}) a_{ij} \Bigg\} a'^{-1}_3 \end{aligned} \tag{8}$$

condensing, by δ_{ij}, the two possible expressions for each of the coordination numbers deduced. The fact that these numbers must be positive or zero makes it possible to find the variation of the number of bonds, a_{ij}, for each N that is chosen. The intersection of this interval with the interval deduced from the experimental area, is useful for choosing an N which best agrees with the structural information supplied by the RDF, when postulating the local order of the material.

3. Application to practical cases

The method described in the literature [9], for determining the parameters enabling postulation of the short-range order of an amorphous solid, was applied to a relatively wide set of glassy alloys for which experimental data are found in the literature. Different structural hypotheses were used and the theoretical results obtained agree with the experimental data mentioned above, confirming the reliability of this theoretical method. This work shows the theoretical analysis of five alloys chosen from the set considered; their experimental values are shown in Table 1. The constituent elements of each alloy were given the subscripts 1, 2 and 3 in the order in which they appear in the alloy. The coordination hypotheses used for obtaining the parameters which define the possible local order are shown in Table 2, C'_i $(i = 2,3)$ represents the coordination of element i in the compound. The existence of bonds between all pairs of elements in all alloys was postulated, except in M2, where the absence of Al–Al bonds was assumed [13].

Bearing in mind the structural hypotheses mentioned and using the theoretical expressions of the above-mentioned parameters [9],

$$\alpha = C_2 a'_2 - C_3 a'_3 - C_1 \beta, \beta = a'_1(a'_3 - a'_2) / \sum_{i \neq 1} a'_i, \gamma$$
$$= C_3 a'_3 + C_1 \delta, \delta = a'_1 a'_3 / \sum_{i \neq j} a'_i,$$

the values shown in Table 3 were calculated, corresponding to parameters that depend on the specific characteristics of each alloy and on the coordination variations of its elements. Table 4

Table 1
RDF characteristics of the analyzed alloys

Alloy	First peak		Area (atoms)	Refs.
	a (Å)	b (Å)		
$As_{0.20}Se_{0.30}Te_{0.50}$ (M1)	2.05	2.90	2.10	[14]
$Al_{0.10}As_{0.20}Te_{0.70}$ (M2)	2.25	3.05	2.04	[15]
$Ge_{0.20}Bi_{0.06}Se_{0.74}$ (M3)	2.00	3.05	2.62	[16]
$Ag_{0.04}As_{0.38}Se_{0.58}$ (M4)	2.01	2.81	2.60	[17]
$Cu_{0.20}As_{0.35}Te_{0.45}$ (M5)	2.20	2.95	3.21	[18]

Table 2
Coordination hypotheses

Alloy	N	C_1	C_2	C_3	C'_2	C'_3
M1	4	3	2	2	< 2	< 2
M2	4	3	3	2	> 3	> 2
M3	4	4	3	2	3	2
M4	4	1	3	2	> 3	> 2
M5	4	1	3	2	> 3	> 2

Table 3
Parameters related to the coordination hypotheses

Alloy	α	β	γ	δ
M1	−55	5	137.5	12.5
M2	−190/3	−50/9	350/3	−70/9
M3	−130	0	148	0
M4	−7/6	−5/6	1363/12	−29/12
M5	17.50	−2.50	78.75	−11.25

Table 4
Average bond lengths for each alloy

Pair	r_{ij} (Å)					Reference				
	M1	M2	M3	M4	M5	M1	M2	M3	M4	M5
1–1	2.49	2.86	2.52	2.68	2.58	[19]	[22]	[26]	[20]	[29]
1–2	2.38	2.43	2.68	2.55	2.60	[20]	[23]	[20]	[28]	[30]
1–3	2.62	2.53	2.37	2.50	2.64	[13]	[20]	[27]	[20]	[31]
2–2	2.34	2.49	2.92	2.49	2.49	[20]	[19]	[20]	[19]	[19]
2–3	2.54	2.68	2.62	2.38	2.62	[20]	[24]	[20]	[20]	[13]
3–3	2.71	2.83	2.34	2.34	2.71	[21]	[25]	[20]	[20]	[21]

shows the average bond lengths used for calculating the parameters A_{ij}, shown in Table 5, together with the h parameter.

Table 5
Values of the parameters A_{ij} and h obtained for $s_m = 12$ Å^{-1}

Alloy	A_{ij}						h
	1–1	1–2	1–3	2–2	2–3	3–3	
M1	0.8284	0.9135	1.6232	0.9929	1.4400	2.6731	21.9112
M2	0.1097	0.2976	0.5099	0.8381	1.3768	2.3253	−10.6937
M3	1.1255	3.3849	1.3022	8.8966	3.3136	1.4356	74.0821
M4	2.9856	2.2810	2.3198	1.4744	1.5164	1.5673	12.3192
M5	0.7886	0.9106	1.4979	1.0460	1.7068	2.8178	14.2346

Using Eq. (7) and the set of parameters obtained, the theoretical expressions of the area shown in Table 6 were deduced. These expressions, together with the experimental areas (Table 1) with an error of ±0.1 atoms, made it possible to determine the variation intervals for a_{ij} $(i,j \neq 1)$, shown in Table 6. The quoted error has been evaluated bearing in mind the inherent errors with the determination of the limits of the RDF peak and analyzing the propagated error in the numerical integration used for the evaluation of the experimental area. Eq. (8) supplies the relative coordination numbers, which, due to their intrinsically positive values, define the new limits

Table 6
Theoretical results obtained for the different alloys

Alloy	Theoretical area	Coordination numbers n_{ij}, $i, j \neq 1$	Variation intervals for parameter $a_{ij}, i,j \neq 1$		
			Defined by the n_{ij} parameters	Defined by limits of error of the experimental area	Intersection of intervals
M1	$1.9410 + 10^{-2}a_{33}$	$n_{22} = (-19 + 2a_{33})/30$ $n_{23} = (47.5 - 2a_{33})/30$ $n_{33} = 2a_{33}/25$	$9.5 \leq a_{33} \leq 23.75$	$5.9 \leq a_{33} \leq 25.9$	$9.5 \leq a_{33} \leq 23.75$
M2	$2.2473 - 2.6 \times 10^{-3}a_{33}$	$n_{22} = (53.33 - a_{23})/20$ $n_{23} = a_{23}/20$ $n_{33} = (116.66 - a_{23})/70$	$0 \leq a_{23} \leq 53.33$	$41.27 \leq a_{23} \leq 118.19$	$41.27 \leq a_{23} \leq 53.33$
M3	$0.7677 + 47.2 \times 10^{-3}a_{33}$	$n_{22} = -12.6 + a_{33}/3$ $n_{23} = 14.8 - a_{33}/3$ $n_{33} = a_{33}/37$	$37.8 \leq a_{33} \leq 44.4$	$37.13 \leq a_{33} \leq 41.36$	$37.8 \leq a_{33} \leq 41.36$
M4	$2.6511 + 1.1 \times 10^{-4}a_{33}$	$n_{22} = (-1.3 + 2a_{33})/38$ $n_{23} = (113.97 - 2a_{33})/38$ $n_{33} = a_{33}/29$	$0.65 \leq a_{33} \leq 56.99$	$0 \leq a_{33} \leq 444.55$	$0.65 \leq a_{33} \leq 56.99$
M5	$3.1017 + 5.7 \times 10^{-3}a_{33}$	$n_{22} = (15.5 + 2a_{33})/35$ $n_{23} = (87.75 - 2a_{33})/35$ $n_{33} = 2a_{33}/45$	$0 \leq a_{33} \leq 43.88$	$1.46 \leq a_{33} \leq 36.54$	$1.46 \leq a_{33} \leq 36.54$

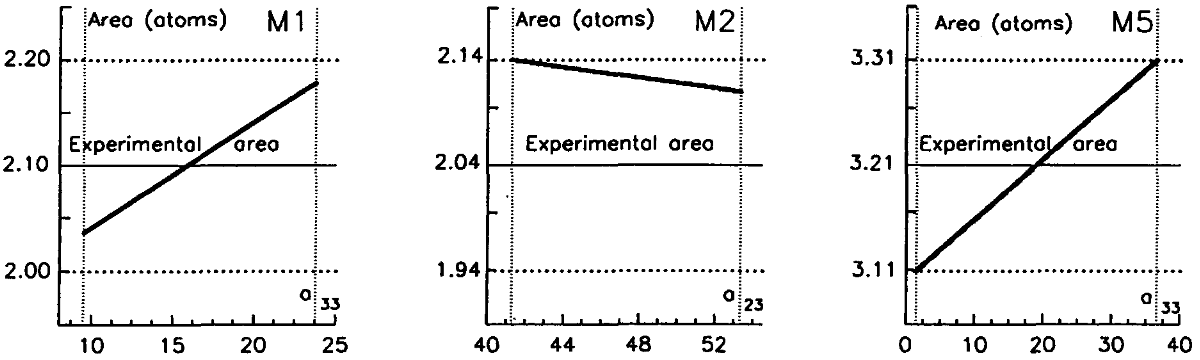

Fig. 2. Area of the first RDF peak vs. the number of a_{ij} bonds ($i, j \neq 1$) for alloys M1, M2, and M5.

for the magnitude a_{ij}, shown in Table 6, together with their intersections with the intervals corresponding to the margin of error of the experimental area.

To illustrate the theoretical calculations, Fig. 2 shows the theoretical areas obtained vs. the numbers of a_{ij} bonds ($i, j \neq 1$) for three of the alloys studied. Fig. 2 shows the intervals in which the theoretical areas are simultaneously compatible with the experimental area and the corresponding coordination numbers.

4. Conclusions

This theoretical method enables different structural hypotheses to be tested in relation to the coordination numbers or the absence of some types of bonds, since the expressions for the relative coordination numbers and for the area under the first RDF peak depend on these hypotheses. On the other hand, when deducing this area, polynomial functions were used which best fitted the products of the atomic factors in those cases in which said magnitudes differ from the approximate values, $Z_iZ_j/(\Sigma_i x_i Z_i)^2$; this fact is of great interest when accurately evaluating the average number of first neighbours in a glassy alloy.

Because of the procedure used, it is possible to postulate certain structural properties and to obtain the average theoretical coordination of atoms in a solid from them. If the difference is within the experimental error, we can assume that the hypotheses describes the most probable local order of the material.

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