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Letter to the Editor

A PHASE-SEPARATED MODEL OF $Al_{0.23}Te_{0.77}$ AMORPHOUS ALLOY

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In this work we have tried to go more deeply into the short-range structure of amorphous $Al_{0.23}$ $Te_{0.77}$. On the one hand, earlier work on the structural model of this alloy was performed by Monte Carlo techniques [1]. Such a model only accounts for an average situation through the glass and the actual existence of phase separation cannot be discarded. On the other hand, one study on the kinetics crystallization by DSC technique shows that two peaks occur, one exhibiting an earlier excess Te crystallization and a later one of the remaining amorphous matrix [2]. Thus, a model with these characteristics has been built in order to compare the results.

The model was generated using the same shape and size as the previous one [1], i.e., spherical of 10 Å radius. The working procedure was very similar in both cases. The model was generated only on the basis of the results of the RDF (radial distribution function) preliminary analysis [3]. First, we look for atoms with maximum coordination creating the positions required to saturate the volume. After, the atom type was assigned to some positions following the hypothesis used for the RDF interpretation. The positions with less coordination were rejected till the number of atoms within the volume were in agreement with density and composition. A random process was used to assign atom type to the rest of the unallocated positions. The structure is refined with the help of the random technique of Metropolis–Montecarlo [4].

The separated phase was placed in an inner sphere. Its volume will be determined by the amorphous phase density of Te [5] as well as by the amount of Te atoms involved. To determine this, a testing procedure was followed. Firstly, if tetrahedral coordination for the Al atoms is admitted, 30% of the Te atoms would be left over, provided that the Te atoms have only Al atoms as first neighbours. To refine this model, breaking of Te–Te bonds of the separated phase is not allowed and also the bonding of these atoms with any

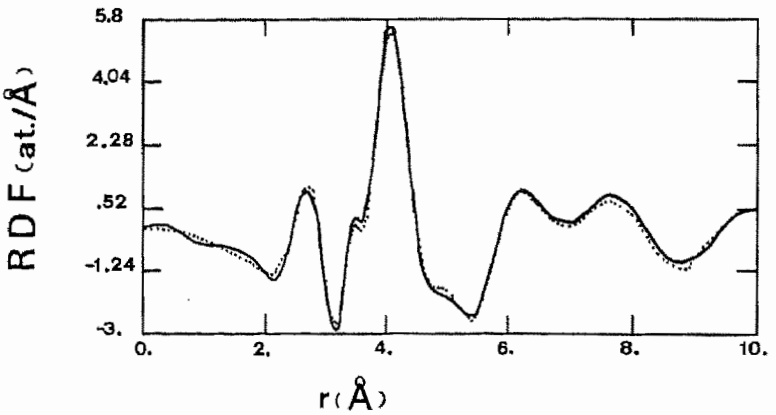

Fig. 1. Representations of the calculated RDF of the separated phase model (dotted line) and of the experimental one (continuous line).

other is avoided. The model built under these conditions turned out to be unsuccessful.

A second model, with an intermediate amount of Te atoms for the separated phase between extreme situations, was worked out imposing the same conditions in the refining process. The model involved 14% of Te atoms in the separated phase. It converged till a standard deviation value was obtained between the experimental and theoretical RDFs of 2.49% as opposed to 3.83% of the continuous model (figs. 1 and 2); thus it was considered more probable. It is worth noting that the improvement of the fitting arises from the 6–8 Å RDF interval. A spatial representation of the model can be seen in fig. 3.

Tables 1 and 2 collect the resulting coordination of the atoms. They present

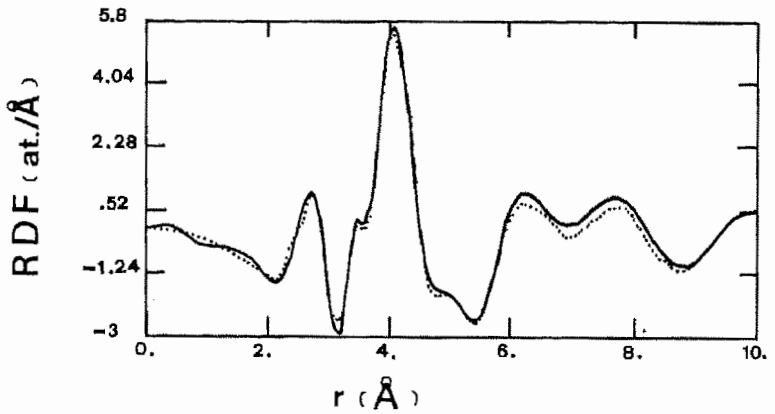

Fig. 2. Representations of the calculated RDF for the continuous model (dotted line) and the experimental one (continuous line).

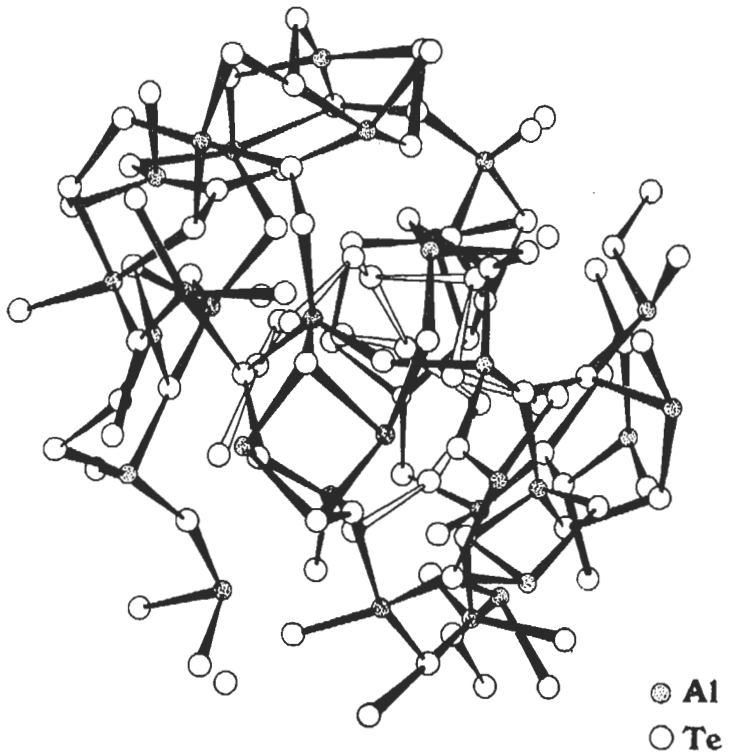

Fig. 3. Spatial representation of the separated phase model.

dangling bonds that, at a large extent, belong to atoms near the sphere's periphery and could be satisfied with hypothetical external neighbours. The amount of coordination defects of the Al atoms is smaller in the continuous model than in the separated phase one. That may be easily explained by taking into consideration that the present model has all the Al atoms in a spherical annulus, so it must be affected by a greater boundary (inner + outer). The amount of threefold coordinated Te atoms in this model is higher than that proposed for the RDF interpretation [3]. On the other hand, there are fewer twofold coordinated Te atoms than in the previous model. It can be noticed

Table 1
Separated phase model coordinations, the numbers in brackets correspond to the expected amount

Type	Coordinations					Total
	4	3	2	1	0	
Al	16 (30)	14 (0)	0 (0)	0 (0)	0 (0)	30
Te	–	30 (0)	26 (56)	25 (0)	5 (0)	86
Te (S.F.)	–	3 (0)	6 (14)	5 (0)	0 (0)	14

Table 2
Continuous model coordinations, the numbers in brackets correspond to the expected amount

Type	Coordinations					Total
	4	3	2	1	0	
Al	25 (30)	4 (0)	0 (0)	0 (0)	0 (0)	30
Te	–	16 (30)	60 (70)	22 (0)	2 (0)	100

Table 3
Dangling bonds percentage and defect per area unit

	Al	Te	Total	Defect/area (%/Å^2)
Cont. mod.	5.0%	17.3%	12.3%	9.3×10^{-3}
Mod. S. F.	11.7%	16.1%	14.6%	9.8×10^{-3}

that in the model built under the hypothesis of a continuous structure, threefold coordinated Te atoms was fixed in advance. On the contrary, in the present work, all the Te atoms could become threefold coordinated. Perhaps, it would be more illustrative to evaluate the percentage of dangling bonds in both models (table 3) since the suitability of this procedure lies in its validity from a statistical point of view. This percentage is smaller for the separated phase model in spite of its expected larger peripheral effect.

The total number of dangling bonds is greater for the present model than for the first one. Nevertheless, all the dangling bonds belong to atoms whose distances from the surface (outer or inner) is less that those corresponding to first neighbours. Beside this, if we take into account the surface of the volume containing the separated phase, the dangling bonds density per area unit (table 3) is, approximately, the same for each model.

The averaged bonding distances and number of bonds of each type can be found in table 4. The models are formed by 130 atoms, 30 being Al and 100 Te. It can be noticed that the averaged distance for Al–Te atoms is shorter in the separated phase model and closer to that found in the structural model of amorphous $Al_{0.10}$ $As_{0.20}$ $Te_{0.70}$ for which a separated phase structure has been proposed [6].

Table 4
Averaged bonding distances and bond quantity

Bond	Separated phase model		Continuous model	
	Distance (Å)	Number	Distance (Å)	Number
Al–Te	2.65 ± 0.17	106	2.72 ± 0.22	80
Te–Te	2.62 ± 0.17	31	2.71 ± 0.21	68
Te–Te(s. f.)	2.72 ± 0.13	13	–	–

Table 5
Percentage of second or higher order neighbour

Kind	Continuous model		Separated phase	
	1	2	1	2
Te...Te	43%	33%	26%	42%
Al...Te	13%	7%	8%	19%
Al...Al	7%	0%	3%	3%

Te–Te averaged atom distances belonging to the separated phase were almost unchanged. It is kept close to that resulting in the structural model of the mentioned ternary alloy.

Experimental RDF presents a small, but well-defined, peak between $r = 3.15$ Å and 3.60 Å [3]. An analysis of atom pairs forming this peak has been carried out.

Two kinds of atom pairs can be distinguished in this set:
(1) Second order neighbours.
(2) Higher order neighbours.

In table 5 the percentage of each pair type in the models is presented. Both show a majority of Te–Te pairs as may be expected in view of the alloy composition, but outline that in the separated phase model, the percentage of the second kind of Te–Te pairs is greater than that corresponding in the earlier one.

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