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Aggregation of tetrahedral and quartoctahedral Delaunay simplices in liquid and amorphous rubidium

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Abstract. Simplicial atomic configurations (four nearest atoms, defining the Delaunay simplices) are considered for molecular-dynamic models of liquid and quenched rubidium. The aggregates, involving simplicial configurations of a tetrahedral and quartoctahedral form, are studied. The problem is reduced by the general Voronoi–Delaunay approach to the study of clusters of the coloured sites on the Voronoi network in terms of percolation theory. The results of a detailed analysis of finite clusters, depending on the fraction of coloured sites for different colours, are proposed. The simplicial atomic configurations, close in shape to regular tetrahedra, determine the T-coloured sites on the Voronoi network and those close in shape to regular quartoctahedra determine the O-coloured ones. Small, medium and large clusters and the backbones of finite ones are studied for this model. The percolation thresholds are determined for the T and O colouring. A topological similarity between the aggregates of tetrahedral simplices in liquid and quenched states is revealed. The significant role of the quartoctahedral simplicial configurations in the quenched state structure is emphasized.

1. Introduction

The problem of structure has two aspects. First, it is a problem of the local order. It is necessary to determine the characteristic structural elements that will be the basic structural blocks of the system. These structural 'tiles' may be represented by atomic configurations which are typical of the given class of systems, composed of a few atoms. Second, one should be able to describe the rules of the spatial distribution of these structural elements. Up to now the former problem has been the focus of attention because a system without translational symmetry assumes the presence of local order only, and the absence of long-range order. However, it is clear that both amorphous and liquid phases are indicative of a certain extended structural order. Thus, studying the pair distribution function of the interstitial cavity of tetrahedral atomic configurations in disordered packing of hard and soft balls, Finney and Wallace (1981) showed them to form linear clusters with branchings. We have investigated the mutual arrangement of tetrahedral and quartoctahedral atomic configurations in Lennard-Jones models (Medvedev *et al* 1988). Tetrahedral configurations were observed (see figures therein)

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to contact by the faces to form branched chains and five-membered rings. The quart-octahedra (one fourth of a perfect octahedron) sometimes join into octahedra but more often form aggregates with quartoctahedra belonging to different octahedra. Thus, the models of dense disordered systems of spherical atoms have definite statistical motives in the arrangement of these structural elements. Unlike crystals, in which the structural motives are described in terms of the translational order, in this case the methods need to be different from those in crystallography. We think the methods and terminology of percolation theory to be most helpful here.

Percolation theory in its simplest classical variant deals with networks, containing some randomly coloured sites (the problem of site percolation). Small or large clusters of a stochastic nature appear due to the fraction of coloured sites. For a fraction larger than or equal to p_c there exists an infinite cluster, connecting the opposite network sides. Earlier (Medvedev *et al* 1988) we have shown how to formulate the problem of disordered atomic system structure in terms of percolation theory. Our approach is based on the mathematical theorems by Voronoi and Delaunay on covering the space for a system of discrete centres (Voronoi 1908, Delaunay 1947).

Thus, Voronoi networks have been used in structural studies. The sites of these networks are the vertices of the Voronoi polyhedra constructed around the atoms. The bonds are formed by their edges. The Voronoi polyhedron (VP) for a given atom in the system of atoms is known to be a convex polyhedron, binding the volume of space whose points are closer to the centre of this atom than to that of the others. In our models the Voronoi networks are four-coordinated (each site has four bonds) because the models of disordered phases (liquid or quenched) are 'non-degenerating' (only four VPs meet at each vertex (Delaunay 1947)). It is important that each site of the Voronoi network is the circumcentre of its Delaunay simplex whose vertices are formed by four atoms for which the Voronoi polyhedra meet at a given site of the Voronoi network. These four atoms are called the simplicial configurations. Another peculiarity of the Voronoi network is that two contiguous network sites (connected by a bond) correspond to the face-contiguous Delaunay simplices or, in other words, to two simplicial atomic configurations with three atoms in common. Thus the Voronoi network topology unambiguously reflects the mutual arrangement of the simplicial atomic configurations in the model.

In disordered phases the Delaunay simplices are commonly represented by a broad distribution of distorted tetrahedra. However, one can readily choose some classes of simplices with a definite structural meaning from a set of simplices of a given model. For instance, the Delaunay simplices with the largest circumradii are the local discharges in the structure, and those with small ones are the most dense local configurations (Delaunay 1947). The simplices may also be classified by their shape. The models of dense disordered systems of spherical atoms have two classes of Delaunay simplices which are close in shape to regular tetrahedra and regular quartoctahedra, respectively (Medvedev and Naberukhin 1987a).

Thus, the simplicial configurations with the structural properties of interest to us can be taken as a structural element. In this paper we restrict ourselves to tetrahedral and quartoctahedral simplices. We then use the Voronoi network on which the sites corresponding to the chosen simplicial configurations are coloured. Thereupon the clusters of the coloured sites are analysed in terms of percolation theory. In section 2 we discuss the rubidium models used in this paper. Section 3 reports the measurements for the tetrahedral and quartoctahedral simplices. Sections 4 and 5 contain the results of the analysis of finite clusters of coloured sites on the Voronoi network of the rubidium

models. In conclusion (section 6) the structural meaning of the results obtained is discussed.

2. Models

Two molecular-dynamic models, composed of 864 atoms, have been studied for liquid and quenched rubidium (Tanaka 1982). A liquid model (denoted below by (l)) corresponds to a temperature $t_l = 315$ K, that is slightly higher than the melting point. The self-diffusion coefficient determined from the mean square atomic displacement $D_l = 3.8 \times 10^{-5}$ cm^2 s^{-1}. The model of a quenched state has been created by cooling the liquid at constant density with a rate of about 10^{13} K s^{-1}. For details see Tanaka (1982). For a quenched state (model (q)) $t_q = 4.5$ K. The self-diffusion coefficient D_q is very small and determined with a large relative error. Tanaka gives the upper estimate for $D_q \leqslant 0.06 \times 10^{-5}$ cm^2 s^{-1}). Model (l) is a typical liquid, demonstrating the usual liquid-like radial distribution function. Model (q) corresponds to a solid (or highly viscous) phase. The second maximum of the radial distribution function is split into two sharp sub-peaks (Tanaka 1983) which allows it to be regarded either as a quenched or amorphous phase.

For each model the Voronoi and Delaunay tessellations have been constructed by taking into account the periodic boundary conditions. The numbers of sites N_0 on the Voronoi network inside the model box are 5381 for (l) and 5187 for (q) models.

Although only one instantaneous realization has been used for each thermodynamic state, we are sure of the authenticity of all the qualitative results obtained below. The Tanaka models are fairly large and the main structural features are reliably displayed already in one instantaneous realization (Tanaka 1986). We have performed a usual Voronoi polyhedra analysis of these models, and found that the result for the given individual configurations is very close to that obtained by Tanaka (1986) where he has employed a set of configurations for each thermodynamic state.

3. Statistics of the Delaunay simplices

The measure T (tetrahedricity) proposed by (Medvedev and Naberukhin 1987a, b) is used to determine the simplices close in shape to a regular tetrahedron:

$$T = \sum_{i>j} (l_i - l_j)^2 / 15\bar{l}^2.$$

Here l_i is the length of the ith edge; $\bar{l}$ is the average edge length for this simplex. With $T = 0$ the simplex is a regular tetrahedron. For a weakly distorted tetrahedron T is small, and vice versa, if the simplex has small T it is close in shape to a regular one. Another measure O (octahedricity) is required to determine the quartoctahedral simplices (Medvedev and Naberukhin 1987a, b):

$$O = \sum_{\substack{i>j \\ i,j\neq m}} (l_i - l_j)^2 / 10\bar{l}^2 + \sum_i (l_i - l_m/\sqrt{2})^2 / 5\bar{l}^2$$

where l_m is this simplex edge with the maximum length. A regular quartoctahedron (one fourth of a perfect octahedron) has one edge $\sqrt{2}$ times as long as the other five, which

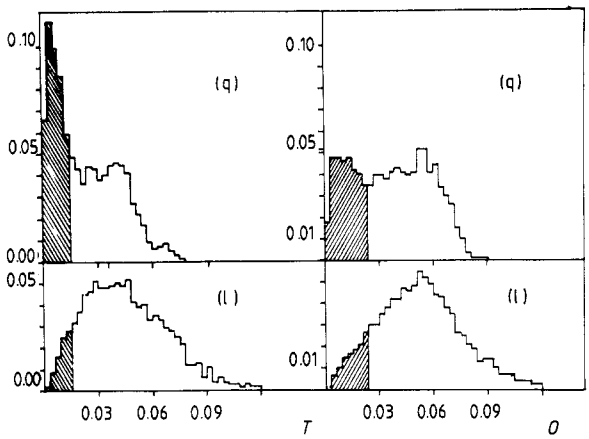

Figure 1. Histograms of the distribution of the Delaunay simplices by measure T (tetrahedricity, left) and O (octahedricity, right) for liquid (l) and quenched (q) rubidium. Hatched areas show 'good' tetrahedral ($T \leq 0.016$) and 'good' quartoctahedral ($O \leq 0.024$) simplices (see text).

are equal. Hence, $O = 0$, and only the simplices close in form to regular quartoctahedra have small values of O.

Note that one measure, e.g. tetrahedricity, is insufficient for our aims. For a regular quartoctahedron $T = 0.057$. This value, however, may belong to other distorted simplices of non-quartoctahedral form as well. Unambiguous correspondence between the simplex shape and measure value holds for the low measure values only (Medvedev and Naberukhin 1987b).

Figure 1 gives the T- and O-distributions of the Delaunay simplices for our rubidium models. These distributions are similar to those of the Lennard-Jones liquid and quenched models (Voloshin *et al* 1989). The liquid demonstrates the unimodal T- and O-distribution (figure 1(l)). The quenched state gives the maxima at the low measure values thus testifying the tetrahedral (figure 1(q) left) and quartoctahedral (figure 1(q) right) simplices to be a distinct type. The broken lines in figure 1 denote the boundary values $T_b = 0.016$ and $O_b = 0.024$ used to separate arbitrarily 'good' tetrahedra and quartoctahedra from the 'strongly distorted' ones. These boundary conditions were obtained by analysing the Lennard-Jones models of an FCC crystal near the melting temperature (Medvedev *et al* 1987). They separate the maxima, corresponding to the tetrahedral or quartoctahedral configurations, preserved in the crystal at a given temperature on the T- and O-distributions of the crystal. Note that the liquid phase has a noticeable fraction of good tetrahedra and quartoctahedra (figure 1(l), hatched) which, however, does not represent a distinct type.

In order to study clusters of the simplices of a given shape we use Voronoi networks, colouring all the network sites whose measured values are smaller than a certain chosen limit. This limiting value defines the fraction of coloured sites which is the integral of the distribution from zero to a given limiting value (figure 1). The fraction of coloured sites is a parameter which is highly important in percolation theory.

The curves in figure 2 show the correspondence between the fraction of coloured sites and the limiting measure value. The horizontal broken lines denote the boundary values T_b and O_b. The vertical intercepts indicate the fraction of coloured sites on the

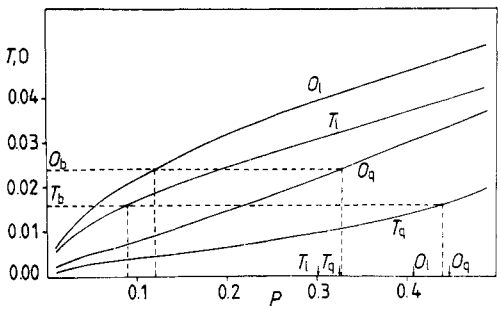

Figure 2. The values of measure T and O against the fraction of simplices P, with the measure value less than a given T (or O). Curves T_q and O_q for tetrahedricity and octahedricity in model (q). Curves T_L and O_L are for those in model (l). Horizontal broken lines denote the boundary values of measure $T_b = 0.016$ and $O_b = 0.024$ (see caption to figure 1). Vertical broken lines point to the corresponding fractions of coloured simplices. Arrows on axis P show the threshold values for the corresponding colouring and models (see table 1).

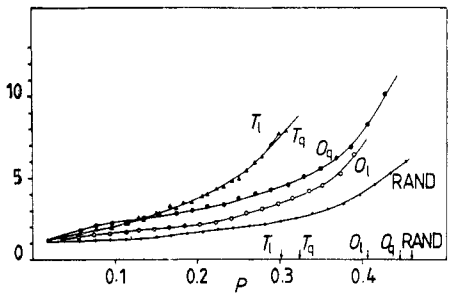

Figure 3. The dependence of the average number of sites in the finite clusters on the fraction of coloured sites P. Curve RAND for the random colouring averaged over the networks of models (l) and (q). Arrow RAND on P axis indicates the percolation threshold for the random colouring. See also the caption to figure 2. ▲, T colouring in model (q); △, T colouring in model (l); ●, O colouring in model (q); ○, O colouring in model (l).

network, corresponding to these limiting values of tetrahedricity and octahedricity. Note that in the liquid phase for both colours (curves O_l and T_l) the 'good' simplicial configurations comprise a fraction which is substantially lower than the percolation threshold. For the quenched state for O-colour the same situation is valid. Only the curve T_q shows that the number of 'good' tetrahedral simplices is sufficient to form a percolating cluster. Hence, one should remember that with an equal fraction P of the coloured sites, the simplices demonstrate the different quality of the form in the quenched and liquid phases.

4. Finite clusters

Figure 3 depicts the dependence of the average number of sites in finite clusters as a function of the fraction of coloured sites. In terms of percolation theory this characteristic is $\Sigma_s sN_s/\Sigma_s N_s$, where N_s is the number of clusters, containing s sites; the summation is carried out over all s values, beginning with unity. To simplify the figure, the curves have been constructed with fractions P not exceeding the threshold values P_c. When the percolating cluster appears, the average number of sites in the finite clusters decreases drastically with increasing P. First, we pay attention to a noticeable difference of the curves for both colours from the RAND one, corresponding to a random colouring. The RAND colouring was performed in the usual way. Each site, irrespective of the others, was considered as coloured with probability P (P being the fraction of coloured sites), i.e. here the coloured sites are non-correlated. In this case the curves of the average number of sites in the finite clusters practically coincide for the Voronoi networks of the (l) and (q) models; the percolation thresholds are reached at almost the same values, $P = 0.46$. The difference of curves T_l, T_q, O_l, O_q from the RAND one as well as from the

Table 1. The threshold fractions of coloured sites on the Voronoi network for the model of liquid (l) and quenched (q) rubidium. P_c^T for T-colouring, P_c^O - for O-colouring, $P^{\min(T,O)}$ for mixed colouring (see text). For random colouring P_c for the (l) and (q) models are approximately the same and equal to 0.46 ± 0.03.

	(l)	(q)
P_c^T	0.305	0.324
P_c^O	0.407	0.446
$P_c^{\min(T,O)}$	0.352	0.279

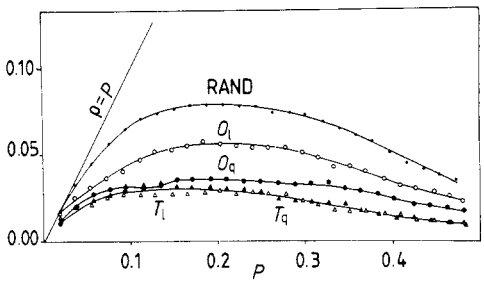

Figure 4. The probability of a given site to be isolated coloured. Straight line $\rho = P$ depicts the probability that a given site is the coloured one.

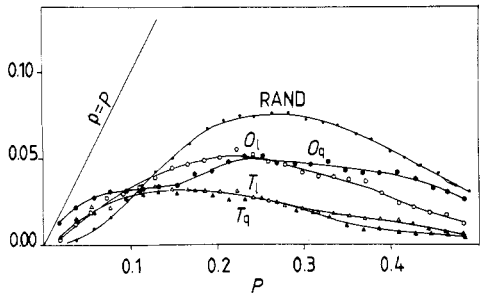

Figure 5. The probability that a given site belongs to a small cluster (consisting of two or three coloured sites).

percolation thresholds (see table 1) indicates that the T- and O-coloured sites appear on the Voronoi network not by chance, i.e. there is a correlation in the arrangement of the quartoctahedral and especially tetrahedral simplices. Of interest is that in the liquid and quenched states the curves for the T-coloured clusters (T_l and T_q) actually coincide, which does not hold for the O-coloured ones. However, the average number of sites in the cluster is a highly averaged characteristic. Below we analyse the finite clusters in more detail.

Figure 4 points to the probability that a given site is an isolated coloured site. This value is determined as N_1/N_0, where N_1 is the number of isolated coloured sites, and N_0 is the total number of network sites (see section 2). Here, as in figure 3, the RAND curve is very different from the T- and O-ones. The largest difference is observed for the T-colour, where the isolated sites are hardly probable. Note also that in this case the curves for the (l) and (q) models coincide. As in figure 3 the O-colouring for liquid is closer to the RAND one. The straight line $\rho = P$ depicts the probability that a given site is coloured (it is either isolated or belongs to any cluster). At small P our curves meet at this straight line thus testifying that only the isolated coloured sites are feasible in this case. Passing over the threshold fraction P_c, this characteristic has no jump.

Figure 5 demonstrates the probability that a given site belongs to a small cluster (involving two or three sites: $\Sigma_{s=2,3} sN_s/N_0$). Figure 6 depicts the probability that a given site belongs to a medium cluster (containing four, five or six sites: $\Sigma_{s=4,5,6} sN_s/N_0$). All the curves for small and medium clusters differ from each other and from the curves of the isolated sites. A common feature is the difference of the T- and O-curves from the

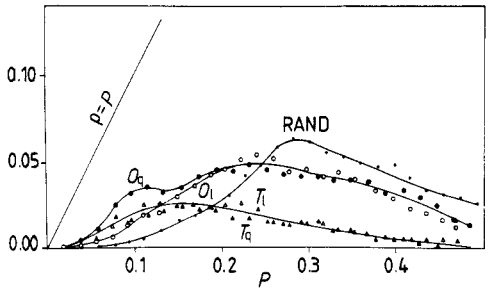

Figure 6. The probability that a given site belongs to a medium cluster (consisting of four, five or six coloured sites).

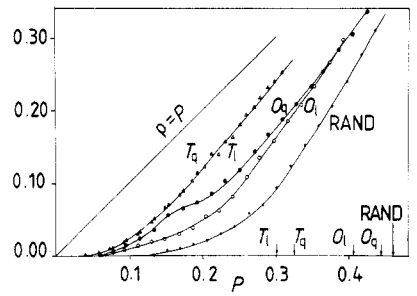

Figure 7. The probability that a given site belongs to a large cluster (consisting of seven or more coloured sites).

RAND ones, and an agreement between the results for liquid and quenched states for T-colouring. It is noteworthy that at a small fraction of coloured sites the quartoctahedra have the highest ability to form small and medium clusters (curves O_q). Finally, figure 7 shows the probability that a given site belongs to a large finite cluster, consisting of seven or more coloured sites ($\Sigma_{s\geqslant 7} sN_s/N_0$). The above properties are valid for this case as well. In addition, the tetrahedral simplices are observed to have a greater tendency to form large clusters (curves T_l and T_q) than in the case of the randomly coloured sites (curve RAND) and O-colouring. The curve O_q has a shoulder, which starts at about $P = 0.14$, just at the point where the maximum is observed for the medium clusters (figure 6). This means that an increase in the fraction of O-coloured sites makes the medium clusters join with the large ones.

5. Backbones of finite clusters

The backbone (the residue left after the removal of all dead ends) is an important feature of a cluster. It is a ring or a number of rings joined by common sites or bonds.

Analysis of the models used shows that in the clusters of the T- and O-coloured sites neither liquid nor quenched states contain the backbones, representing the rings of three sites. A small fraction of such backbones is observed at random colouring only.

Another situation is true for the four-site rings. Figure 8 depicts the curves for the probability that a given site belongs to a four-membered ring. This value was calculated to be $4N_4^C/N_0$ where N_4^C is the number of backbones of four sites. These backbones are most probable in the O-coloured clusters. Moreover, in the quenched state their number is three times as large as in the liquid one (curves O_q and O_l). A four-membered ring, consisting of good quartoctahedra, is a good octahedral atomic configuration. There are only traces of T-coloured four-membered rings in the liquid (curve T_l), which are completely absent in the (q) model. The curve RAND demonstrates the four-membered rings on the Voronoi network, revealed by random colouring of the sites.

It is not so for the backbones consisting of the rings with five sites ($5N_5^C/N_0$). The quenched phase contains the majority of such rings (curve T_q (figure 9)). Five good tetrahedra are readily packed in a ring to form a decahedron. The five-membered rings are not typical of the O-coloured clusters. These cannot be constructed by good tetrahedra, otherwise they must be strongly distorted. Therefore such backbones are

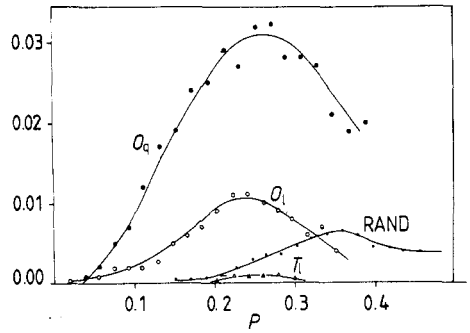

Figure 8. The probability that a given site belongs to a four-membered ring in the backbone of the finite clusters.

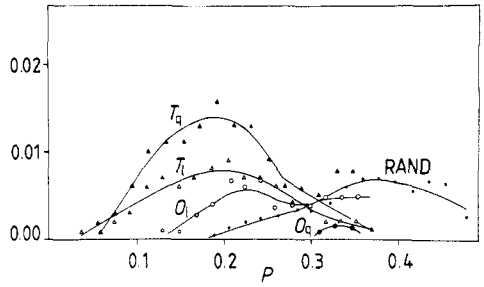

Figure 9. The probability that a given site belongs to a five-membered ring in the backbone of the finite clusters.

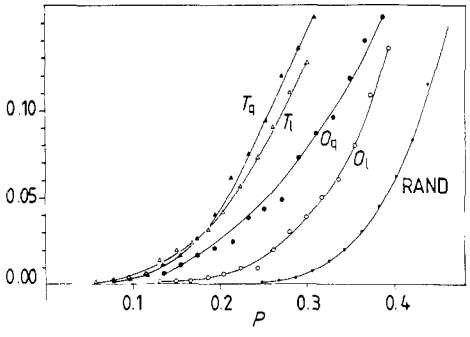

Figure 10. The probability that a given site belongs to the backbone of a finite cluster, consisting of seven or more sites.

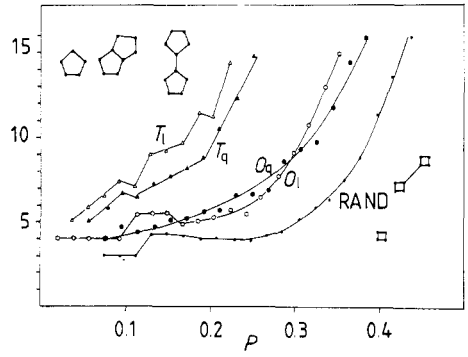

Figure 11. The dependence of the average number of sites in the backbone of the finite clusters on the fraction of coloured sites. At the upper left are the schemes of the simplest backbones at T-colouring. At the bottom right are those for O-colouring.

observable in liquids and are practically absent in quenched states. Rings consisting of six sites are quite rare in both types of clusters but there are backbones with a great number of sites.

Figure 10 contains the probabilities that a given site belongs to a ring with seven and more sites ($\Sigma_{s\geq 7} sN_s^C/N_0$) where N_s^C is the number of backbones with s sites. The curves for T colourings rise faster than the others. This implies that the T-clusters are much more cross-linked than the rest. With random colouring these backbones appear only near the percolation threshold, thus illustrating the statistical 'interlacing' of clusters with increasing number of coloured sites. Note that the curves T_q and T_l in this case are very close, which indicates the similarity between the T-clusters of liquid and quenched phases.

Figure 11 presents the dependence of the average number of sites in the backbones of the finite clusters $\Sigma_{s\geq 3} sN_s^C/\Sigma_{s\geq 3} N_s^C$ on the fraction of coloured sites. The curves are very different from those in figure 3, with an average size of whole clusters. The minimum

number of sites in the backbone is three. The mean size of the backbones for random colouring begins with this value (curve RAND). For O-colour the minimal backbones consist of four sites (curves O_q and O_l) and for the T-colour they consist of five sites, their size rapidly increasing (curves T_q and T_l). The three simplest backbones observed for the T-coloured clusters in our model are given at the upper left of the figure. Their sizes are five, eight and ten, respectively. The non-monotonic nature of the T_q and T_l curves seems to be due to the appearance of these discrete backbones rather than poor statistics of our data. The two simplest backbones (four and eight sites) in the O-coloured clusters present in our model are depicted at the bottom right. Thus, analysis of the backbones of finite clusters testifies the clusters of tetrahedral configurations to contain the five-membered rings (decahedron atomic aggregate) and those of quartoctahedral ones the four-membered rings (octahedra).

6. Conclusion

In this paper we have studied the properties of clusters consisting of the coloured sites on the Voronoi network of liquid and amorphous rubidium. Each site of this network corresponds to a simplicial atomic configuration. Therefore each cluster, composed of coloured sites, depicts an aggregate of atoms consisting of the simplicial configurations of a given type. In other words, the network clusters demonstrate the arrangement of the corresponding atomic aggregates. In the general case our clusters are the 'animals'. This variety of structural realizations is a property of disordered phases. Therefore we think that the structure must be studied by searching for the statistical laws of the mutual arrangement of the given structural elements and not only by searching for and enumerating some separate aggregate types.

It is quite suddenly that the T-clusters have the same topology at any fraction of coloured sites P for both liquid and quenched rubidium. The average cluster sizes are equal as are the probabilities for small, medium and large clusters. The same can be said about their backbones. This may be attributed to the fact that the aggregates of most tetrahedral configurations in the liquid are not basically reconstructed on removal of temperature perturbations (glass formation). Although the simplices in the liquid are strongly distorted, the T-coloured clusters correspond to the aggregates of most tetrahedral, i.e. most locally dense and energy profitable, simplicial configurations compared to the others in this liquid. With decreasing temperature the atoms of perturbed tetrahedral configurations may easily pass by small shifts to the deep local energy minima, corresponding to good tetrahedral configurations. The connectivity of these clusters may practically be the same.

For O-colouring the clusters in the quenched and liquid phases are different. In the liquid phase these are mostly close to that observed for random colouring, i.e. the correlations between quartoctahedra in this case are the least and the threshold fraction $P_c = 0.407$ which is substantially higher than for T-colouring and closer to the value of random colouring. Indeed, the quartoctahedral configurations are stable only at a spatial arrangement of the neighbouring atoms (e.g. being parts of the octahedral configuration). In liquids the temperature perturbations hamper the appearance of any special low-density octahedron-like configurations. Therefore the appearance of quartoctahedra in the liquid is rather random. In the quenched state the situation is quite different. The quartoctahedral simplices readily join in clusters to form many octahedral configurations. Although the correlation between the quartoctahedra is high,

the threshold fraction value is large ($P_c = 0.446$) because the quartoctahedra in the quenched state tend to be located in closed clusters, which hampers the appearance of the percolating cluster.

We believe a large fraction of good quartoctahedral configurations to be a result of a large number of good tetrahedral ones. This is likely to be a general fact. If the T-distribution has a peak at small values, the same system displays the peak of good quartoctahedra on the O-distribution. On the contrary, if there is no peak of good tetrahedra, the peak of good quartoctahedra is also absent (Medvedev and Naberykhin 1987a, Voloshin *et al* 1989, Medvedev *et al* 1987). The reason is that the tetrahedron and octahedron are mutually complementary figures. Alternating these, one can readily cover the space. The most dense crystalline packings (FCC, HCP) are constructed on this principle. In the disordered dense packings the octahedra, half-octahedra and even separate quartoctahedra may find the natural places between the clusters of tetrahedral configurations.

Thus, if the most dense tetrahedral configurations are an attribute to the dense packings of spherical atoms, the quartoctahedral ones are their results. The fact that the clusters of good tetrahedra are 'linked' by quartoctahedra is confirmed with the help of a new colour, determined as $\min(T, O)$. Now we are colouring the Voronoi network site that has the lowest measured value T or O, i.e. the most regular tetrahedral or quartoctahedral simplices are chosen. For liquid the threshold fraction, $P_c^{\min(T,O)}$ has an intermediate value between P_c^T and P_c^O, see table 1. For the quenched state, however, $P_c^{\min(T,O)} = 0.279$, which is substantially less than the threshold values for the T- and O-colourings. A low $P_c^{\min(T,O)}$ indicates that the good quartoctahedral simplices join the finite T-clusters to form the percolating $\min(T, O)$-colour clusters. For the liquid phase the simplex quality is worse; neither bad nor good quartoctahedra must be packed between bad tetrahedra. Therefore a new colouring fails to reveal any correlation between the T- and O-simplices in the liquid.

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