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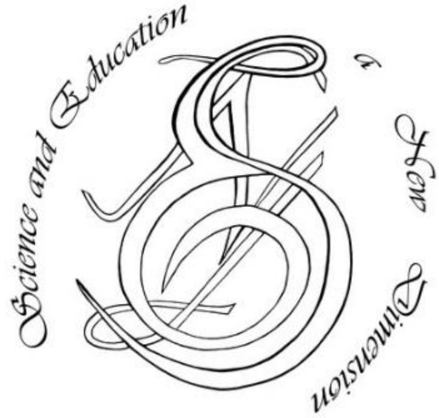

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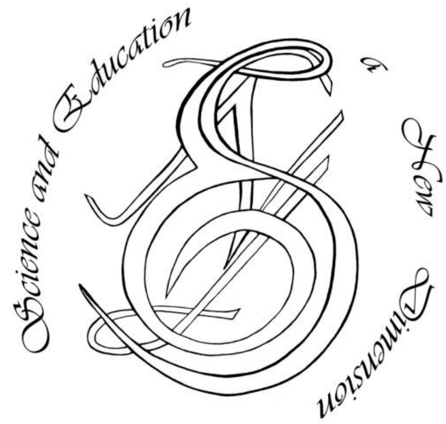

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CONTENT

PHYSICS

The use of the structural units for the description of the short-range order in the amorphous substances

V. P. Ivanitsky[1], V. S. Kovtunenko[2], M. M. Ryaboschuk[1], M. V. Stojka[1]

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Abstract. It is proposed to define the structure of the amorphous substance by the set of all realized structural units with the allowance made for the functions of their statistical distribution in the disordered atomic network. In the aggregate, all these elements make basis for constructing the minimal elementary structural fragment of the amorphous substance – an analog of the elementary cell in the crystal. Solution of this task is reduced to the correct choice of structural units and determination of their structural parameters. In this relation, the partitioning of the sample that expresses its structural and chemical composition using the minimal number of different-kind structural units seems to be optimal.

Keywords: *amorphous materials, disorder structure, short range order, structural unit.*

The atoms of different chemical elements are the primary structural particles that build any substance. However such structural particles are less informative for the description of the structure of the substances. The description of the atomic network structure in the language of chemical bonds between the atoms is also inadequate and insufficiently informative, though in some cases it may provide quite useful structural information. This requires the introduction of the secondary large-scaled structural particles, which are a certain spatial location of the group of atoms and, respectively, describe the real atomic environment, where the certain chemical bonds are realized. Thus, in such formations, the chemical composition of the substance is fixed and the set of constant parameters having the sense of characteristics of the forces of interaction between the atoms both in the above formations and at their boundaries is defined [1]. The procedure of partitioning the macrosample into the set of the structural particles leads to the important question concerning the choice of such structural particles. To describe the short range order (SRO) structure and the properties defined by SRO the use of traditional structural units (SU) as the structural particles is quite efficient [2]. The SU's are the groups of the adjacent atoms that correspond to the chemical composition of given substance and contain a fixed number of the chemical bonds. Binding with each other in different ways, they form the whole disordered atomic network of the amorphous substances. In some cases the separate chemical bond can be the structural unit. As a result, the condensed medium may be presented on the local structural level by the set of SU's with different types and structures. The structural units are the universal objects, which contain information on the topology and the character of the chemical bonds within the SRO of the substance. Therefore SU's describe simultaneously both topological and chemical SRO.

The chemical interaction parameters realized between the atoms in the disordered network, i.e. the type of the chemical bonds, the binding energy, the iconicity degree etc. are the driving forces of SU formation. The main parameter that determines the formation of the chemical bonds is, certainly, their energy. However, its action is revealed on the particular material basis – the system of atoms, which is defined by the chemical composition of the substance. Another quite important parameter of the influence on the formation of certain SU deals with the technological conditions of production of the amorphous substance. For example, the existence of the compound polyatomic complexes in the vapor phase may affect significantly the form of SU, which will be formed in the disordered atomic network of the condensed amorphous films. It should be noted that the chemical bonds themselves directly reflect the structure and the properties of the electron shell of the atoms. They define the SU's dimension and the character of their linkage in the disordered network (chains, clusters, layers, 3D networks etc.).

A detailed approach of pointing SU out in the region of the first coordination sphere was developed by R. L. Muller [3] when working on the methods of partitioning the atomic network of the oxide glasses into the structural particles. He suggested the correct combination of the formula notation of the chemical composition and geometric representation of the structure of SU, which allow the conditions of additivity of the composition and volume of the amorphous system to be satisfied. According to this method, SU's are mainly represented in a form of the central atom surrounded by the nearest neighbors. The central atom is usually chosen with the maximal coordination number, though the necessity of this choice is not substantiated [2]. Therefore, introduction of SU is assumed to be not completely clear and unambiguous. SU is defined by setting its spatial structure that reflects the geometry of the chemical bonds of the central atom with the nearest environment. If one denotes the central atom A, its neighboring atoms – B and the relevant coordination numbers Z_A and Z_B, then the formula notation of SU has a following form: AB_{Z_A/Z_B}. It is always assumed here that $Z_A > Z_B$. In the covalent amorphous substances (like in the crystals), the maximal numbers of the nearest neighbors of given atom in the most cases are equal to the number of the valence bonds, which it may form in the atomic network under the particular conditions.

The classical choice of SU in the atomic network of the oxygen glasses is stipulated by the dominant formation of stronger heterobonds as compared to the homobonds.

In the chalcogenide glasses, when oxygen is substituted by sulfur, selenium and tellurium, the difference between the energies of the homobonds and heterobonds is decreased. In these materials, the unambiguous choice of SU is more complicated. Therefore, more general and more formalized approach to the SU selection is usually suggested, which is normally used for the metallic glasses. In accordance with this approach, SU is expressed by the cluster with the chemical composition that corresponds to the atomic parts of each element with the allowance made for the pair interaction between them. Here the transition from choosing the classical SU of the covalent substances to setting the Voronoy's polyhedrons of metals and ionic substances is observed. Chalcogenides are the intermediate variant of the two extreme methods of setting SU, which can be widely used to describe their structure in the amorphous state. In particular, this allows one to include in SU the atoms of not only the first, but also the second and further coordination spheres.

More augmented interpretation of SU is given in Ref. [4]. SU's are considered there as the separate atoms or groups of chemically bound atoms with individual compositions and structure, which are multiply repeated in the glass matrix and are grouped in the rings, chains, layers etc. SU's are the carriers of information about the chemical composition of the glass and geometric location of the atoms within the SRO limits. They are suggested to be considered the elementary cells of the atomic network of the glassy substances, which define almost all physical and chemical properties of the glass. However, there are several comments on this definition. First, the notion of SU works efficiently for the description of not only the structure of glass but also of any other kind of the condensed state. Second, SU's themselves can hardly be the elementary cells of the amorphous substance in the sense used for the crystalline lattices. Third, the role of the elementary cell in the amorphous substances can be played by the large-scale structural fragment of the atomic network constructed of different SU's inherent in given substance.

Application of the above approach to introduce SU allows the structure of SRO of the atomic network in the region of first coordination spheres to be described only for the central, more coordinated, atom. The structure of the atomic network around the less coordinated atoms is completely indefinite, and this is quite inconsistent, because from the viewpoint of the properties and the structure of the amorphous substance no distinctions in the approaches to the description of SRO around different atoms should be found. The shortages of such approach were indicated in Ref. [2]. In particular, it was stated that the vibrational spectra of the quartz glasses couldn't be explained by the vibrations in the $SiO_{4}/_{2}$ SU only. For these purpose one has also to take into account the strong influence of the atomic network linkage around the bridge oxygen atoms, which requires the analysis of the Si–O–Si-like SU's as well. The similar problems exist when interpreting the vibrational spectra of the As_2O_3 glasses.

Thus, the description of the SRO structure in the amorphous substance with preset chemical composition could be reduced to identification of any SU's realized in it and to the search of their relative parts [4] or distribution functions. Solution of this task is reduced to the correct choice of SU's and determination of their structural parameters. The choice of SU is related to the construction of the boundaries that separate it from other SU's. In this relation, the partitioning of the sample that expresses its structural and chemical composition using the minimal number of different-kind SU's seems to be optimal.

There is also a possibility to introduce the same SU's in the amorphous substances with different chemical compositions. In Ref. [5], such SU's are suggested to be called the optimally close ones. Entering the atomic networks of different chemical compositions, they slightly modify their properties. The example of such optimally close SU's are the atomic formations of different chalcogenides, which keep their molar volume (shown below in brackets) independent of the chemical composition of the matrix: $AsSe_{3/2}$ (41,3 - 42,3); $GeSe_{4/2}$ (52,2 - 54); $SeSe_{2/2}$ (35,6 - 36,8); $SbSe_{3/2}$ (38,9 - 54,3); $PSe_{3/2}$ (34,8 - 59,7).

In Refs. [5, 6], the choice of the traditional SU's as the structural particles is also substantiated for the case of chalcogenides. The argument supporting this approach is the presence of mainly covalent short-range forces of the interatomic interaction. Then the manifold of all possible structures of the atomic network of this substance could be found by enumerating all combinations of the atomic linkage (or all chemical bonds combinations). Methodically, this can be done more conveniently and more efficiently by considering the set of all possible SU combinations in the system of preset chemical composition. By virtue of the additivity principle the macroproperties of the substance will be specified by the ratio of different SU's in its disordered atomic network. The changes of these ratios could be matched with the change of the structure and different properties of the substances, e.g., at the expense of the change of technological conditions of synthesis or the action of external factors.

The structure of the amorphous substance could be defined by the set of all realized SU's with the allowance made for the functions of their statistical distribution in the disordered atomic network. In the aggregate, all these elements make basis for constructing the minimal elementary structural fragment of the amorphous substance – an analog of the elementary cell in the crystal. Such elementary fragment will carry the whole information about the chemical composition and the structure of SRO. Thus, the physical and chemical pro-perties of the amorphous substance will be defined not only by SU's but also by the character of their linkage on the largescale levels in a form of a certain structural fragment.

Therefore, each SU combination in the amorphous atomic network, which we denote $\vec{R}_n$, will have its specific properties and certain fixed values of the physical and chemical quantities. The change of the ratio of different SU's, which can be described in terms of spontaneous or stimulated transitions between different $\vec{R}_n$ [6], will automatically define the change of the properties of the atomic network. It is important here to know also the specific mechanism, which provides certain change of the ratio of different SU's in the amorphous substance of specified chemical compositions with fixed structure. Obviously, the total number of different $\vec{R}_n$ for given system defines the limits of variations of its properties. As the change of the SU ratio for the system of fixed chemical composition means the change of the SU distribution function, then such changes automatically mean the transition from one amorphous matrix structure to another one (e.g., from the model of the total chemical disorder to the model of the total chemical order). The maximal variation of the properties will take place at the transitions between $\vec{R}_n$ with extreme possible SU distribution functions given the preservation of the system homogeneity (the lack of the secondary phases, eutectic or spinodal decay etc.). The changes in $\vec{R}_n$ are possible due to different structural transformations: the transitions of some SU's to other ones, the appearance of new SU's, the formation of defective SU's and so on.

The probability of realization of certain SU's in the substance is defined by the energy of the chemical bonds between the atoms involved in them. Respectively, the most probable will be those SU's, which have the maximal energies of the chemical bonds, while vanishing of some SU's and the appearance of other SU's must be accompanied by the energy absorption or release.

Determination of the elementary fragment of the atomic network in the particular amorphous substance corresponds to the certain description of its structure, since, using different translations of this fragment, one may obtain the whole volume of this sample. Such procedure is an analog of filling the space with the crystalline lattice by transferring its elementary cell along the translation vectors. However, the dimensions of the elementary amorphous fragment can be much larger as compared to those of the elementary cell of corresponding crystal. In addition, these elementary amorphous fragments must be related to the above vectors $\vec{R}_n$ setting. As a result, each elementary fragment will describe a certain structural state of the atomic network of given substance.

The number of different structural states, which can be realized in given amorphous substance, is specified by its chemical composition. At the same time the energy of each particular structural state, $U(\vec{R}_i)$, is determined by the average binding energy per one atom, $\overline{E}$, or by the ratio of different SU's in it. Availability of different structural states $\vec{R}_i$ for certain substance means the possibility of the structural changes due to the variation of SU's and their ratio. Respectively, for each disordered fixed-composition substance there exists a certain interval of internal energies $\Delta U = \overline{E}_{max} - \overline{E}_{min}$, within the limits of which different structural states can be realized and different structural changes may occur due to the change of the ratio of different SU's. For example, in the system this interval is maximal for the $As_2(S, Se)_3$ composition and equals to 34 kJ/mole [6].

Thus, not only identification of all SU's of the atomic network but also the studies of their statistical distribution functions and construction on their basis of the relevant elementary structural fragments are the important practical task. In this context, of special interest is the influence of mutual location and linkage of different SU's in the space on the structure and properties of the amorphous substances. To study all these peculiarities, it was suggested in Ref. [7] to take as the basis the structural chemical steric factors of different atoms that form given SU's. In such approach, SU's are to a great extent arbitrarily linked with the atomic network of a certain amorphous material. It is more expedient to point out SU's and the character of their mutual linkage in the atomic network of the amorphous material in accordance with its real structure and real properties [8]. In this case one has to take into account the peculiarities of the atomic network structure on any level: SRO, intermediate range order, mesoscopic and nanodimensional levels.

In many cases, the particular predictions of the amorphous atomic network structure, i.e. its model, are useful for solving such problems. This model can be taken as a certain theoretical approximation or as a result of the experimental data analysis. Furthermore, when determining the probability of realization of different SU's, the additional trivial regularities can be used, e.g. the condition of constancy of the number of chemical bonds in the system of certain chemical composition or the condition of total saturation of all bonds in the matrix. For each model of the atomic network the particular SU distribution function will exist. The number of the atoms included in the system under consideration, i.e. the size of the elementary fragment of the structure under study, is an important parameter of the above function. Besides the geometrical and combinatory factors, the probability of the SU realization will be defined by its internal energy. It is insufficient to take into account the energies of the chemical bonds only, like Ref. [6], but one has to make allowance for the energies of deformation of the angles between the bonds. At the same time, an essential role in the SU production is also played by the weaker interactions, e.g., Van-der-Vaals interaction. Their active influence is manifested in the effects of the atomic network clusterization, its phase separation on the molecular level, formation of the different-scale structural inhomogeneities. Accounting these components can change substantially the SU distribution function in given amorphous atomic network.

Thus, the chemical composition of the substance is a leading parameter that defines the type of SU's realized in this substance and the dimension of their linkage in the joint structural motive of the atomic network [9]. Since SU's are the carriers of all solid body properties, then the properties, in general, will be determined by the ratio of different SU's according to the additivity principle. It should be noted that different properties of the atomic network could be related to different structural carriers. After determining some structural carriers and studying their properties, one can find their statistical distribution functions and construct the elementary structural fragment, which will reflect all the properties of the amorphous substance as a whole. Translation of such integral structural fragment in the space allows the whole macrosample of given amorphous substance to be obtained. The paper [5] confirms this fact and demonstrates that any condensed quantum-mechanical macrosystem can be partitioned into the arbitrary number of microfragments identical by any finite set of properties with the accuracy up to the infinitely small positive number ε.

The problem of choosing SU is closely related to the strategy of distinguishing the equivalent (by the structural environment) atoms and equivalent (identical) SU's in the atomic network. The equivalent atoms are called the atoms of the same chemical element, which have equal number of electrons, equal (or quite close) structure of electron shells and type of their hybridization. Since it is rather difficult to determine the electron structure of the atoms, then, usually, the simplified definition of equivalence is applied: the equivalent atoms are those, which have the same set of characteristics of their nearest environment. The number of the neighbors, the lengths of the bonds and the angles between them lie within the narrow limits defined by the dispersions of the corresponding distributions. In many cases the equivalence of the atoms can be found according to the parameters of the first coordination sphere only, because often it makes no sense to take the large-scale structural formations as SU's [2].

In general case, when defining the atoms of the same type and their SU's in the atomic networks of solids, one has to take into account such specific feature inherent in them all, as SRO [8]. One has to take into account here the parameters of not only the first coordination sphere, but those of all coordination spheres that define this SRO. It is expedient to use the number of the neighbors of a certain chemical element in each coordination sphere, the lengths of the chemical bonds, the interatomic distances and the angles between them as the quantitative limits of atomic equivalence. A special attention should be drawn to those SU's, which are characteristic for the different molecules, clusters and stable and metastable condensed phases of the relevant chemical compositions. According to such equivalent atoms of the atomic network, the equivalent SU's will also be related. Obviously, the central atoms of the equivalent SU's could be considered identical from the viewpoint of their local environment within the SRO limits.

The equal SU's are related to the equivalent atoms as the central ones. Respectively, we shall call the atoms and SU's characterized by different local environment and different topological parameters, the different-type ones. The different-type SU's will be realized in the disordered atomic network of the particular amorphous substances with different probability.

The most optimal for the amorphous substances is the statistically probabilistic method of setting all SU's that reflects correctly their inherent entity [8]. According to this method, each atom of the disordered atomic network should be related to its own SU defined by this atom (as the central one) and its nearest neighbors. Then one has to distribute all SU's into the groups of equivalent SU's and to find the regularities of the statistical distribution of such equivalent SU's. Determination of the main different-type SU's and the probabilities of their realization or the statistical distributions in the atomic network is the principal problem of studying the atomic structure of the amorphous state of the substances.

Recently the structure of the atomic network of the amorphous state was considered quite stable and constant up to initiating the crystallization processes. Today a number of results are available indicating that even for the amorphous films of elementary Ge and Si the structure depends on the technologies of production and varies in the process of further storage and low-temperature processing. Such results show that in general case the amorphous substance may be in the three main thermodynamical states: the stable, the metastable and the labile states. The peculiarities of the structure of the amorphous substances are to a great extent determined by the energy parameters of atoms and SU’s in the disordered network.

It is assumed in the studies that the energy of certain atomic network subsystem depends both on its internal parameters and on the external parameters of the state. The potential energy is minimized according to the internal parameters, while its dependence on the external parameters of the state occurs in the potential parametrically. Since the internal parameters have fluctuations from one area (ensemble) to other one, some of these structural fluctuations correspond to the double-level or multi-level potentials. From the point of view of the phase transformations, these potentials arise in the amorphous structure due to the instability of a certain class of potentials to the fluctuations of microscopic parameters of SU’s.

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Использование структурных единиц для описания ближнего порядка в аморфных веществах

В. П. Иваницкий, В. С. Ковтуненко, М. М. Рябощук, М. В. Стойка

Аннотация. Предложено определять структуру аморфных веществ установлением набора всех тех структурных единиц, которые реализуются в неупорядоченной атомной сетке, с учетом статистической функции их распределения. Совокупность всех таких единиц есть основой для создания минимального элементарного структурного фрагмента аморфных веществ – аналога элементарной ячейки кристаллов. Решение этой задачи требует корректного выбора вида структурных единиц и определения их структурных параметров. В этом отношении оптимальным будет такое разбиение образца, которое выражает его химический состав и структуру с помощью минимального количества структурных едини разного вида.

Ключевые слова: *аморфные материалы, разупорядоченная структура, ближний порядок, структурная единица.*

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