

PHYSICAL AND MATHEMATICAL SCIENCES

Borkach E.I., Ivanitsky V.P., Kovtunenکو V.S. **Order and disorder in the aggregate states of the substance**

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Abstract. It is justified that in the material science the term 'disorder' must have the only meaning that the microscopic state of the system of many particles is assigned by a set of random quantities calculated on the basis of the probabilistic laws. At that point we must take the geometrical (topological) parameters of the ideal spatial linkage of the atoms as basis of division of the solids into the crystalline and amorphous ones. We also suggest calling the ideal structurally ordered substances the substances, in which fully determined functional dependence between the topological parameters of atomic network is observed. This stipulates the existence of determined short-range order, which, by virtue of their determined character, ensure the formation of large-range order as well. We shall call the ideal totally structurally disordered systems the systems, in which there is no correlation in the location of the structural particles in the space. We also suggest calling the structurally disordered (unordered) substances the substances, in which only the probabilistic correlation relation between the topological parameters of atomic network is observed. This stipulates the existence of the correlation short-range order and correlation medium-range order of the ideal atomic network, which, by virtue of their probabilistic nature, result in the loss of large-range order. Besides the topologic ordering and disordering, a number of other types of ordering and disordering are realized in the substances. Certain of them are inherent in the crystals only, other – in the amorphous substances and liquids only, some of them are typical for any condensed medium.

Keywords: *amorphous materials, order, disorder*

Largely, this is due to the fact that, according to the general estimates, the information merit of the most of experimental methods for the amorphous substances is about 20 percent as compared with those carried out for the crystalline materials. In such conditions, one has to seek the ways of compensating the above significant loss of information. In turn, the successful use of this approach requires the solution of a series of tasks, i.e. clear physical and mathematical definition of the following terms: 'ordering', 'disordering', 'amorphous substance', 'short-range order (SRO)', 'long-range order (LRO)' and others, providing them with not only qualitative but also strict quantitative sense; clear definition of various scale levels of the amorphous material structure and studies of general regularities of structure formation at each of them.

The notions of order, disorder, ordering and disordering are decisive in relating the amorphous substances to a specific class of objects. While the clear physical sense of the the ratio of the average kinetic energy of the structural particles to the potential energy of their interaction makes classification of the substances over aggregate states clear and vivid [1], the problem of distinguishing the substances by the degree of their ordering is solved in more complicated and controversial way. The categories of ordering in the condensed state physics are used now with no clear quantitative gradation with insufficient disclosure of the essence of the boundary values of the absolute (ideal) order and disorder. Therefore there is a necessity of a distinct determination of the physical essence of these notions concerning the amorphous substances.

What do the notions of order and disorder mean, how could they be defined? On the intuitive level, we first address to the images of the spatial or geometric order and disorder. Such their application does not require a clear quantitative description.

An important method of studying the ordering in any state of the substance is its correlation with other one, studied previously, more common ore more transparent. To study the quantitative relations between different

states one has to establish a certain reference point. A certain reference system or benchmark should be taken as the reference point [2, 3]. The unordered state is easy to be described by finding its deviation from the specified ideal. The reference system must satisfy at least two conditions: the condition of ideality and the condition of the maximal correspondence to the relevant real systems by the most general attribute(s).

In crystals, the ideal spatial periodic lattices with the translation symmetry serve as the above benchmark. The condition of ideality in this case means the lack of any violations of the structural particle locations in the spatial lattice nodes. This means that all the particles are located strictly in the nodes, and no node is empty.

Thus, by definition, the ideal LRO in crystals describes a strong consistency in the structural particle locations in the space, which is repeated at the infinitely large distances with the formation of the infinite three-dimensional geometrically correct crystalline lattice. The presence of the translation symmetry of their structure is a necessary attribute of the above lattices. In the substances with LRO, the distance to any atom of the lattice can be set through its elementary cell parameters [4].

The condition of the maximal correspondence between the benchmark and the real systems means that the spatial lattices and the crystals under comparison must have the same symmetry group. For example, when describing the structure of the crystals of the monocline syngony it is inappropriate to use the spatial lattices of the cubic syngony.

The spatial periodic lattices are the simplest example of the ideal LRO, which does not exist in reality and is a convenient reference point only. In the real substances, the total LRO is inaccessible, and the region of the real crystals is located next to the total boundary order limit. In these crystals, disordering results from the thermal motion of the particles, the statistical character of the regularities of filling up the crystalline nodes by the structural particles, the fluctuation processes and so on. The above

processes result in the certain quantitative deviations from the total order attributes, but the substance is considered crystalline, if these deviations do not exceed some boundary limit at which LRO vanishes. Thus, the topological disordering of the structural particles locations is allowed in crystals provided it does not destroy LRO.

The ideal gas is the example of the absolute or total disorder benchmark. In any real substance, it is impossible to reach the total disorder. This is due to the interaction between the structural particles, which necessarily leads to a certain ordering in their locations. The character and the degree of ordering in the mutual locations of the structural particles depend on the type, value and character of the forces acting between the particles, as well as on the external conditions, which the particle is in. Dependence of the relation of these parameters the topological ordering will extend to the certain distances in the space.

The region of the ideal gases with almost random location of the structural particles lies near the total boundary disorder. Only in case of their mutual approaching the certain correlations of their location are revealed and the relevant structural ordering occurs. Therefore the real gases also have SRO, and the character of this order depends on what is considered their structural particle. Thus, the topological order and disorder in the substances are revealed in the spatial correlations between separate structural particles that form the substance, i.e. in the character of distribution of the atoms and in the local 'geometric' details of the above distribution.

As a result, the real substances lie in the wide region between the total order states (ideal crystal) and the total disorder (ideal gas) [5]. Some of these states are such close to the absolute order and disorder that they can be compared to the reference systems. In this case the boundary states of the total order and disorder and the real systems close to them allow quite rigorous and exact description of their structure.

At the same time, a great number of topological and configuration distributions of atoms exist among the real substances, which are quite far from the ideal reference systems of the total order and total disorder. The amorphous solids belong to them as well. In the amorphous systems, relation between the order and disorder remains an unsolved problem. Description of these intermediate states in a form of the non-crystalline solids faces considerable difficulties [6]. However, the lack of the spatial periodicity in the atomic locations does not exclude the existence of the specific atomic configurations in the amorphous materials, which join the groups of atoms due to the chemical interaction between them. The character and the degree of such local topological ordering depend strongly on the type of atoms, the method of production of the material as well as on the different kinds of its processing.

As follows from the above analysis, correlations between the structural particles that form a system make the basis of the order. The order always competes with the disorder, which is internally inherent in the macroscopic system. This competition results from the action of the average energy of internal or external force field and that of the disordered motion of the structural particles. Here both order and disorder act as mutually complementary values: the increase of a certain value leads to the decrease of another one. The only way leads to the order – more close

correlation between the separate elements of the system, up to combining them into the single entity (e.g., into the crystalline lattice). At the same time, the disorder may have various forms [7]. The viewpoint of the authors of Ref. [8] is close to the above statements. According to them, the disorder could be defined as any violation of the totally ordered system revealed in the lack of correlations of certain physical value that describes this system at the distances defining the disorder scale. At the same time, they call the total order the visible non-vanishing correlations of all physical values revealed at any distances within the limits of the system. Thus, in the single crystals those configurations of atoms are realized, which correspond to the minimum of casualty: the number of the structural particles with strictly correlated mutual locations is macroscopically large. In the gas, where disordering is maximal, significant are the correlations between several closest structural particles only. In the liquids and amorphous solids, the problem of the relation between the order and disorder are still being studied intensively [9].

In our opinion, the above definitions are physically confined and terminologically incorrect. This is due to the fact that they are based on the order of completely ordered system – the notion that itself requires rigorous definition. Furthermore, in case of introduction of violations in the total order the type of ordering of the system must not change. This means that the introduced disorder is inseparably related to the initial total order, which must be kept within the limits of the distances that set the scale of disorder and vanish at larger distances. Thus, the above definitions do not cover the systems, in which in case of disordering the total order is not simply violated, but also the character of ordering is changed drastically. Therefore, the above definitions are related only to the systems, in which the particular disordering at the certain scale coexists with the total order of the same type at other spatial scale: the defective crystals, ferromagnetics, real disperse systems etc. Most of real unordered substances with realized disorder that exists itself and does not result from 'violations' in the totally ordered system of the same order type, which existed earlier, go beyond the limits of the above definitions. This means that the differences between the order and disorder cover not only quantitative relations. One should also take into account the possibility of realization of qualitatively different types of correlations that correspond to the order and disorder.

Thus, classification of the amorphous substances as simply the disordered systems and their comparison with the ideal order or atomic disorder benchmarks is not reasonable and directs researchers to the wrong way [2]. Such approach requires the existence of the totally ordered boundary state and disorder in each system. For the most real systems, especially for the condensed substances, this is very difficult and, sometimes, impossible. The glasses from the wide vitrification regions in many binary and more complicated systems are a bright example of this. To define the disorder in each particular glass one has to have an infinite number of the boundary total order models, which correspond to the set of the chemical compositions of the glasses and different technological conditions of their formation.

One important question arises: must the studies of the general nature of unordered condensed substances be also

based on the relevant benchmark, for example, on the notion of the ideal disordered atomic matrix (or atomic network/atomic carcass)? Must the above network set the defect-free amorphous structure similarly to the crystals?

To find an answer to the above question we shall focus ourselves on some moments. First, in the above definitions of the order and disorder the notion of correlations is not used sufficiently explicitly. According to Ref. [10], the correlation is the probabilistic or the statistical dependence between the certain system parameters. In this relation, it acts as the contradiction of the functional dependence, at which the strict unambiguous relation between these parameters is specified. Correlation occurs when the relation between the parameters in the system is complicated by the presence of a number of random factors. In this case the total order must be described not by the correlation terms but by those of the functional dependence. Second, the notions of the order and disorder must be interrelated to one specific physical (or chemical) value or parameter only. Third, in the particular systems, the order and disorder may exist by several parameters simultaneously. In this case, along with the vanishing of the order by one parameter, the order by other physical parameters or values may persist in the system. Such system will be ordered by one physical parameter and disordered by other ones.

In our opinion, it is reasonable to use the following definitions. The system with the total order by the parameter P is any system with strict functional dependence between the values of the parameter P of all its structural elements. The system with the partial order (the system with the partial disorder, the system with the partial order, the disordered system) by the parameter P has only the correlation (statistical, probabilistic) dependence between the values of the parameter P and its structural elements. In the system with the total disorder by the parameter P , there is no (neither functional nor correlation) dependence between the values of the parameter P and its structural elements. In this context, the systems with the total order are simply ordered or are the systems with the long-range order by the parameter P , whereas the systems with the partial order or partial disorder are the unordered (disordered) systems by the parameter P . In case of the lack of any order in the system the latter is totally disordered or is the system with the total disordering by the parameter P . That is, provided the rigorous physical and mathematical consideration, the term 'disorder' must have the only meaning that the microscopic state of the system of many particles is assigned by a set of random quantities calculated on the

basis of the probabilistic laws [11, 12]. In case of the total order these quantities are completely determined.

When analyzing the structure of the substances, in general case, the terms 'order' and 'disorder' mean, first of all, the topological ordering in the location of the structural particles, i.e. the possibility to determine the direct correspondence between the spatial locations of all structural particles of the system [9]. Therefore, the radius-vector \vec{r}_i that defines the location of the relevant i -th atom of the substance in the space with respect to the preset coordinate frame is considered to be the main structural parameter of ordering P . Then the positions of all atoms can be defined for the crystal in a form of the unequivocal determined functions $\vec{r}_i = k_1\vec{a} + l_i\vec{b} + m_i\vec{c}$, where k_1, l_i, m_i is a set of integer numbers that define the positions of the crystalline lattice nodes, and \vec{a} , \vec{b} , \vec{c} are the vectors of elementary translations of the basis cell in the relevant crystalline lattice. In this case the discrete diffraction pattern for the crystals is completely described by the representation of their atomic network over the determined set of translation vectors.

For the unordered substances the mutual location of all the structural particles is described by the specific correlation dependences. The main characteristics of these dependences are the correlation functions $Y(\vec{r}_i)$, i.e. the functions that define the probability of location of the structural particles at the distances \vec{r}_i in the preset coordinate frame [4]. The intensity distributions of radiation diffracted by the amorphous substances obey such probabilistic regularities. Therefore today one may consider conclusively proven that the correlation regularities describe the structure of the amorphous network of the amorphous substances and reliably reflect the character of its revelation in the diffractograms.

The binary radial correlation function (or the binary radial distribution functions) $W(r)$ occupies a special place among the correlation functions, because it may be determined experimentally using the electron, neutron and X-ray diffraction techniques. In case of the total topological disorder there are no correlations in the spatial location of the structural particles of the substance. This means [13] that the vector \vec{r}_i with the same unit probability takes any values (fig.1a). Certainly, one has to take here into account that the structural particles cannot approach each other at the distances less than their size d_a . The ideal gas is the model system with this total topological disorder. A lot of real gases are also close to it by their structure. The example of the radial distribution for these gases is shown in fig. 1b.

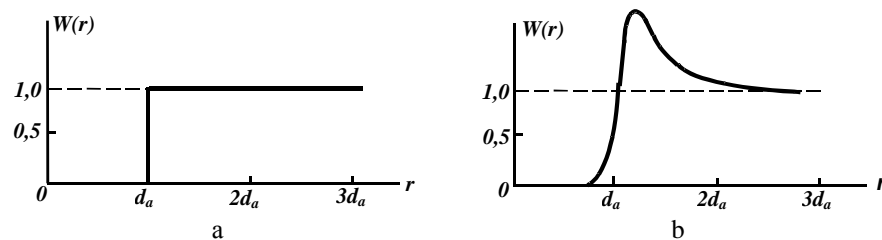


Fig. 1. Binary radial correlation function $W(r)$ for ideal (a) and real (b) monoatomic gas

Other order or disorder types will correspond to the other ordering parameters P as well, for example, the

chemical order or disorder, the order or disorder in the magnetic spin or dipole electric moment orientation of the

structural particles, the orientation order or disorder in the molecular substances. In this case the system may have the total order by one parameter and the total or the partial disorder by other parameters. The solid solutions are the example of such system with simultaneous realization of the topological order (the crystalline lattice is available) and the chemical disordering (i.e. there is no functional dependence in the distribution of the atoms of different chemical elements in the nodes of the above lattices). Examination of the disorder in the crystals is often non-separable from that of the phase transitions of the 'order-disorder' type, which result in the crystal transition from the state with the disorder by a certain parameter P to the state with the order by the same parameter P .

The above analysis testifies to the incorrectness of dividing the substances into structurally ordered and structurally disordered ones on the basis of the presence or the absence of LRO only. The latter is rather not a criterion of the above division but a partial manifestation of more general criterion that indeed makes a basis for dividing the substances into the ordered and disordered ones. The form of the dependence (i.e. functional or probabilistic) between the ordering parameters P of the structural particles can be such a criterion. In the topological relation, realization of a strict functional relation between the spatial locations of the structural particles leads to the topological LRO (both the short-range order and the intermediate-range order are realized automatically), while realization of the correlation dependence results in the LRO vanishing with the conservation of the topologic SRO (in some cases – the

topologic IRO as well, chart 2). The difference between the topologic SRO in the ordered and disordered substances is a significant consequence of the choice of the above criterion as the basic one. In the first case, we deal with the rigorous functional topological SRO, while in the second case – with the correlation probabilistic topological SRO. The first-type SRO being repeated along any direction results in the LRO realization, the second-type one – does not lead to the LRO formation.

Let us note also that different aggregate states of the substance have different character of the structural disordering. In the gases, this is purely dynamical disordering stipulated by the chaotic thermal motion of the structural particles. In the case of the condensed substances it is necessary to distinguish three different types of disordering. The first is the dynamic-static disordering, the value of which depends on the temperature of the system only and is equilibrium for it. This type of disordering is the most indicative for the liquids, where the disordered spatial distribution of the structural particles is combined with simultaneous dynamism of their spatial locations. In the solids, it is manifested in a form of the thermal oscillations of the atomic network. The second type is a purely statistical disordering determined by the disordered structure of the system and is typical for the amorphous solids, where the spatially unordered location of the structural particles is static and, in the limiting case is independent of time. The third type of disordering is related to the structural defects of the ideal system and is inherent in both crystals and amorphous solids.

Chart 2. Generalized diagram of the ordering degree variation in the aggregate states of the substance

The lack of any regularity in the spatial locations of the structural particles	There is a probabilistic correlation connection in the spatial locations of some closest structural particles	There is a probabilistic correlation connection in the spatial locations of rather large number of closest structural particles	There is a functional determined connection in the spatial locations of the most of structural particles of the substance	There is a functional determined connection in the spatial locations of all the structural particles of the substance
Ideal gas	Real gases	Liquids Amorphous solids	Real crystals	Ideal crystal
Total topological disorder				Total topological order

Of particular importance in the description of different condensed systems and phase relations is the degree of order or disorder in the system. In our notations, this parameter for the ordered (crystalline) and disordered (amorphous) substances must be different. Since the ideal lattice is a benchmark of the total order, then the degree of ordering in the real crystals will be determined by the measure of deviation of its structure from the above lattice. Such deviations are usually characterized by the type and concentration of different defects in the crystal. Occurrence of these defects distorts simultaneously the functional SRO and LRO in certain local sites of the crystal. In such defective areas, the correlation SRO and LRO arise. When the defect concentration exceeds a certain limit, the crystal transits from the ordered substances to the disordered ones. Disappearance of the functional dependences and appearance of the correlation

dependences in mutual locations of the atoms observed as the LRO vanishing is a criterion of the above transition. Thus, the degree of the crystal defectiveness can simultaneously serve the criterion of its ordering degree. Here this criterion describes the ordering degree of both SRO and LRO of the crystals.

In the non-crystalline substances, elucidation of disordering degree also requires introduction of relevant reference ideal systems but, as of today, there is no generally accepted benchmark. Therefore it is reasonable to speak about the ordering or disordering degrees in the amorphous substances in the qualitative sense only. To develop the strict quantitative criteria of the disordering degree in the amorphous substances one has to take into account the peculiarities of their structure. Figure 2 shows the generalized diagram that illustrates the character of ordering variation in different aggregate states of the substances.

The energy diagram of the substance is an important element in describing both order and disorder in the substances. In this context, especially principal in disordering analysis is that at correlation SRO several elements forming the macrosystem could be differently distributed between the predetermined set of a great number of the energy levels. As a result, the possibility of the existence of different microscopic states, which are almost identical from the viewpoint of the total energy of the system but differ by the methods of location of separate structural elements on the energy levels, i.e. in the different energy states, is provided. Therefore for any macroscopic system, which the substance is, the tendency to the internal disordering is always characteristic. This is explained by the fact that such macrosystem is related to a considerable number of microscopic states with almost equal energy, and they differ by the value of this energy.

Note that there are many partial notions of order and disorder in the disordered state theory related to a certain direction of their study or to different parameters P , which determine the order. Yu.N. Shunin and K.K. Schwarz [14] divide the disordered substances and the systems into four classes depending on the type of disorder.

1. The disorder in the regular lattices, when the physical properties of the elementary cells of the structural matrix vary randomly at the transition from one cell to another one. This disorder can be compositional due to the random fluctuations of the chemical composition of the cells. It is manifested as the substitution disorder in the alloys and solid solutions; the spin orientation disorder in the crystalline lattice nodes; the defect location disorder in the elementary cells and the diagonal disorder due to the local excitation parameter fluctuations in the lattice nodes. Other examples are the Anderson's disorder [15] – the one-dimensional distribution of regularly located potential wells of different depth and the spectral disorder that reflects the properties of the system in the reciprocal space and provides the statistically disordered set of harmonics. At the disorder of this type the total topological long-range order or the translation periodicity in the locations of the structural particles of the system may be kept. This class of disorder types relates also to the amorphous substances if one takes the ideal topologically disordered amorphous matrix as the initial structural unit.

2. The disorder in the irregular lattices with preserved topology characterized by a small shift of the lattice nodes with respect to the equilibrium positions. This results in the vanishing translation periodicity of the relevant parameters of the system and, respectively, this type of disorder is typical for different disordered systems. This includes the following types of disorder. The topological disorder in a form of deviations of the lengths and angles of chemical bonds as compared to the matrix of the ideal crystalline lattice. The positional disorder with random shifts of atoms with respect to the corresponding crystalline lattice nodes (hot solid body disorder). The Lifshitz's disorder [16] in the medium with irregularly located atoms having the same potential. The Gubanov's disorder (Gubanov's quasi-crystalline model) [17], at which the crystal topology is preserved, but due to the gradual bending and stretching the crystal becomes so deformed that orientation of the crystalline lattice planes at large distances is violated. The non-diagonal disorder due to the violation of the translation

symmetry of the interaction constants of the adjacent lattice nodes. The Kroning-Peny disorder [18], in which the total potential of the medium is a result of superposition of randomly located δ -like potentials. The media with these types of disorder could be brought to the total order by the continuous topological transformations.

3. The disorder in the irregular lattices with the broken topology is characterized by the irreversible structural changes, which may be accompanied by other violations of the local physical parameters. At this topological disorder the total order could not be restored by the continuous topological transformations. This includes [19] the polycrystalline disorder in the medium with the crystallite dimensions that greatly exceed the free path of electron or phonon. Dislocation disorder means violation of the polymer structure (polymer chain bending and intertangling). The gas-type disorder is an ideal topological disorder in the medium, where the structural particles are independently located in the volume. Bernal's disorder is a structure in a form of the randomly scattered spheres with no interaction within a certain space volume. In the most cases this type of disorder relates to the amorphous substances.

4. The disorder of inhomogeneous continuous medium based on the structureless concept of the substance as the permanent continuum. In such a medium, the distribution functions for the structural particles or their potential energies are of random and continuous character. In Ref. [20], the continuum disorder with the continuous unordered potential distribution; the Gauss's disorder in a form of a superposition of randomly located separate potentials and the Torp's disorder – a set of the 'hard' and 'soft' regions, which continuously transit from each to other – are pointed out.

The above classification is based on the geometrical and topological properties of the atomic lattices. In this case the spatial atomic structure (unordered or ordered) is superimposed by the certain-parameter disorder. Small distortions of the regular atomic structure, as a rule, preserve the topology of the regular object (e.g., the crystal). However, such irregular lattices are physically unstable and rapidly relax to the regular structure with the minimal energy. The irregular structures, which cannot be transformed to the regular analogs via the continuous topological transformations, are related to the higher degree of disorder. This requires essential energy consumption related to the bond rupture. In addition, the above lattices are quite stable and they could be considered the certain phase state of the substance. There are also the disorder models, which generally ignore the particular atomic structure and develop the concept of the continuous medium. They are based on the certain special random distributions (e.g., Gauss distributions) of the substance density or the energy potential. This approach is of general character and fails to provide the description of the particular structure of real substances.

Note also that classification of solids by two attributes – long-range order and short-range order – is rather schematic, because both order and disorder in the solids are never realized completely in a pure form. In the real bodies, the minor disorder elements appear against the main background of both short-range order and long-range order or vice versa the minor order elements appear against the main disorder background. In most cases one may neglect certain minor disorder/order elements in the ideal

system approximation, however in some cases the minor elements become the same essential as the basic structural background.

Summarizing the above analysis, one can make some important conclusions.

It is necessary to take the geometrical parameters of the ideal spatial linkage of the atoms as the basis of division of the solids into the crystalline and amorphous ones. We suggest calling such parameters of the atomic networks the topological ones and they are related to all scaling levels, i.e. SRO, IRO, mesoscopic ordering and LRO.

We also suggest calling the ideal structurally ordered substances the substances, in which fully determined functional dependence between the topological parameters of mutual location of the atoms in the space is observed. This stipulates the existence of determined SRO and determined IRO of the ideal atomic network, which, by virtue of their determined character, ensure the formation of LRO as well. We shall call the ideal totally structurally disordered systems the systems, in which

there is no correlation in the location of the structural particles in the space. We also suggest calling the structurally disordered (unordered) substances the substances, in which only the probabilistic correlation relation between the topological parameters of mutual location of the atoms in the space is observed. This stipulates the existence of the correlation SRO and correlation IRO of the ideal atomic network, which, by virtue of their probabilistic nature, result in the loss of LRO.

The general structure of the ordered and disordered substances is described mathematically by various objects. For the ordered substances this is the system of the translation vectors, while for the unordered ones – the correlation functions.

Besides the topologic ordering and disordering, a number of other types of ordering and disordering are realized in the substances. Certain of them are inherent in the crystals only, other – in the amorphous substances and liquids only, some of them are typical for any condensed medium.

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Боркач Е.И., Иваницкий В.П., Ковтуненко В.С. Порядок и беспорядок в агрегатных состояниях вещества

Аннотация. При анализе структуры веществ понятия порядок и беспорядок должны относиться лишь к одному конкретному физико-химическому параметру системы или к группе ее однотипных параметров. В частности, при разделении твердых тел на кристаллические и аморфные следует учитывать только геометрические параметры идеального пространственного увязывания атомов между собой – топологические параметры. Предлагается называть идеальными структурно упорядоченными те вещества, в которых реализуется полностью детерминированная, функциональная зависимость между топологическими параметрами атомной сетки. Это обуславливает существование в таких сетках детерминированных ближнего порядка и промежуточного (мезоскопического) порядков, которые в силу своей детерминированности обеспечивают образование в них и дальнего порядка. Идеальными полностью структурно разупорядоченными будут системы, в которых отсутствует любая взаимозависимость в размещении структурных частиц в пространстве. Для веществ этому условию соответствует только идеальный газ. Идеальными структурно разупорядоченными (неупорядоченными) предлагается называть такие вещества, в которых реализуется лишь вероятностная корреляционная зависимость между топологическими параметрами атомной сетки. Это обуславливает существование в них корреляционного ближнего порядка и корреляционного промежуточного порядка, которые в силу своей вероятностной природы ведут к потере дальнего порядка. Кроме этого, в реальных неупорядоченных веществах, так же как и в кристаллах, атомные сетки дополнительно разупорядочиваются тепловым движением структурных частиц, флуктуационными процессами и разными дефектами. Математически структура упорядоченных и разупорядоченных веществ описывается разными объектами. Для упорядоченных веществ это система векторов трансляций, а для неупорядоченных – корреляционные функции.

Ключевые слова: аморфные вещества, порядок, беспорядок