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On the Physical Foundations of Polymorphic Transformations of Crystals

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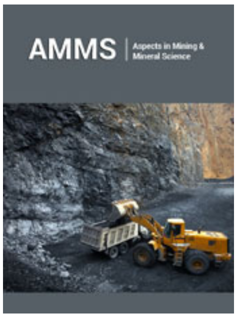

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Abstract

The paper discusses the application of the previously formulated principle of commensurability of conserved quantities to the classifications of polymorphic transformations of crystalline substances under the influence of external factors on these substances (temperature, pressure, magnetic field, etc.). To describe the crystal structure of a substance, it is more productive to think of electrons as localized entities, rather than wave packets. A physical model is proposed to explain, accepted in the scientific literature, the requirement of coprime for the Miller index numbers, which denote the crystallographic planes that come out on the surface of the crystals.

Keywords: Polymorphic transformations; Crystallography; Atomic structure; Lattice spacing; Principle of commensurability of conserved quantities; Emission spectra of hydrogen-like atoms

Introduction

Mineralogy is the ancient science of matter in its most universal sense. Physics, chemistry, crystallography and even astronomy come together here. Therefore, any new idea can be tested in the best possible way precisely on experimental samples created by nature, so to speak. In other words, minerals are not far-fetched structures, but structures that were formed according to the natural laws of nature. The task of the researcher is to understand these laws. So, despite the almost three hundred years of history of crystallography, in all textbooks, encyclopedias and reference books one can read that crystallographic plane are expressed by Miller indices, which are coprime, i.e. do not have common factors, for example, they can have values of 2,4,7, but not 2,4,8. And everywhere it is noted that these numbers never have large values. But nowhere is the physical reason for this firmly established empirical fact discussed. Although it should be noted that in [1] the cases are considered when in a centered unit cell there are crystallographic planes with Miller numbers that have common factors. Such planes pass through the centering atoms and cross the crystallographic axes not along the nodes of the lattice, but along the internodes.

However, firstly, the author himself notes that the special choice of coordinate axes for this case takes us beyond the limits of translational symmetry, and if there are no translations, then such cases cannot represent a structure in the broad sense of this concept (perhaps, some particular problems symmetries can be solved for a particular structure). And, secondly, and this is the main thing for us now-the group analysis of symmetries, as such, does not contain the physico-chemistry of the structure of matter, it is based on the geometry of crystals. And if so, then we can state that there is no physical explanation for the fact of the requirement of coprime of the Miller numbers-indexes that designate crystallographic planes. In conclusion, we add to this part three phrases from the work of the Nobel laureate on symmetry Wigner

[2]: "It is painful, on the other hand, to admit that the symmetry cannot be formed in terms of our present, quantum mechanical theory, that it is surely only approximate. Approximate in the sense that it is valid if classical, that is nonquantum, theory is a valid approximation for the motion of the nuclei. It is also painful to admit that none of us has succeeded in finding the limits of the validity of the concept of crystal symmetry and to point to phenomena in which the approximate nature of the symmetry would manifest itself." After this quotation, it seems obvious to us that the search for physical reasons for the observed symmetry of crystals is completely justified. The problem of the symmetry of crystals can be approached from a completely different angle if we ask ourselves the question: why is Nature arranged according to quantum laws? The usual answer is that it follows from the totality of the laws of quantum physics. But these laws only answer the question: how the world works, but do not answer the question: why is it so arranged? Actually, the lack of an answer to this particular question is the reason for well-known statements, in particular, by the outstanding contemporary physicist S. Weinberg, for example: "But I admit that I feel some discomfort, all my life using a theory that no one really understands" [3].

The actual reason for such "discomfort" for physicists was pointed out by Lee Smolin in his book [4], having formulated five most important problems of quantum mechanics, which, in his opinion, should be solved by it. Of these, PROBLEM 2, in his opinion, the central one, sounds like this: "The solution to the problem of the foundations of quantum mechanics, either by giving meaning to the theory in its current form, or by inventing a new theory that makes sense." Perhaps this is the most accurate definition of the difficulties in understanding the theory that everyone now uses to describe the World. But we can say that this is more a problem for philosophers than physicists, because the vast majority of physicists use the apparatus of quantum mechanics to obtain specific results, and do not delve (precisely because of the success of the results obtained) into the reasons why this apparatus works so well. According to the famous Nobel laureates in physics R. Feynman and S. Weinberg, the successful description of the world with the help of the apparatus of quantum mechanics is a "fatal inevitability" [5]. However, the imaginary fatalism in quantum mechanics can be avoided if we give physical meaning to the very principle of quantization of the states of physical objects of the World. This can be done by postulating the principle of commensurability of conserved quantities [6]. The proposed "principle of commensurability" is formulated as follows: during the interaction of physical objects, the conserved homogeneous quantities (energies, momenta, moments of momentums, magnetic moments, etc.) are redistributed between objects so that before and after the interaction these quantities have a common measure. And what does it mean to have a "common measure" for some homogeneous quantities? This means that the values of these quantities can be determined by measuring these quantities with the same "meter" (i.e., the unit of measure) and thus expressing their values with integer numbers of units of measure. From foundations of mathematics, it is well known that two or more of the same type of quantities (for example, a and b) always have a common measure when their relations (i.e., a/b) are expressed by integer (rational) numbers [7]. For example, side and a diagonal of a square do not have a common measure, the ratio of their lengths cannot be expressed in whole numbers of units of their measure because this ratio is expressed by the irrational number $\sqrt{2}$. This was established by ancient Greeks, which is why the Pythagorean school of integer perished [8]. One can formulate the condition for presence of a common measure in several quantities differently: in order for a certain number of the same type of quantities to have a common measure, it is necessary that value of each of the quantities can be measured by any other quantity, using it as a "meter".

Thus, Nature is arranged in such a way that during interactions physical objects convey one to another not any value of a conserved quantity, but only its "segments" (parts, shares) that have rational relations between their values, that is, have a common measure. At first glance, this greatly limits the options for exchanging physical entities between interacting objects, and such a hypothesis even causes an unconscious protest. To confirm this hypothesis by methods of the theory of integers, applying the principle of commensurability, in [9] the results of solving two central physical problems are presented in detail: the problem of scattering of a test particle on a force center with the simplest scattering potential in the form of a δ-function and another problem, which for our work now more important is the problem of emission of a hydrogen-like atom. In the last problem, the simplest mechanical model of an atom is considered, namely, as a proton with a localized electron rotating around. Three physical objects are involved in the process of radiation of an atom (i.e., interaction of physical objects): proton, electron, photon. By applying the principle of commensurability to the solution of the problem of radiation of a hydrogen-like atom, it was possible to obtain all the spectral series of the hydrogen atom (Lyman, Balmer, etc.) and the most important conclusion follows from the solution of this problem: the allowed radii of the electron orbits in the hydrogen atom, which determine the size of the atom in any of its excited states, have a common measure with the smallest value of the radius when the atom is in the ground state. In other words, the need to have a common measure for the orbital momenta of an electron in a hydrogen atom leads to the need to have a common measure of the possible radii of its rotation, i.e., to the total measure of the possible sizes of the hydrogen atom. It is natural to assume that the principle of commensurability, confirmed by the example of a hydrogen atom, in particular, the angular momentum of an electron in an atom (and for circular symmetric s-orbits of an electron in a hydrogen atom, this is automatically transferred to the radii of the orbits) also applies to all multielectron atomic structures. Of course, additional physical phenomena take place in multielectron atomic structures: the Pauli principle manifests itself, then, in addition to the spherical orbitals (s-orbitals) of atomic electrons, ellipsoidal orbitals appear, the so-called "penetrating" ones, when the electron orbits go beyond the outer electron shell of the atom (p, d etc. orbitals). But it is important to remember that in the structure of a crystalline substance, the distance between neighboring atoms and their chemical bond is determined by the valence electrons located in the outer electron shell, and the possible values of the trajectories of the orbits of the valence electrons are determined by the need to have commensurability not in terms of distances between atoms, but in terms of the values of angular momentum, which are the result of integrating the variable value of the electron momentum along the ellipsoidal trajectory of its motion. It is important to understand this, because the distances between atoms along different coordinate axes can be incommensurable, and only the angular momentum of electrons (as a conserved quantity) is commensurable. Finally, the most important: any new state of interacting atoms must have a common measure with their ground (or previous) state in all conserved quantities: energies, momenta, momentum, magnetic moments, etc. It is this universal requirement for the physics of interacting systems that governs absolutely all possible types of realized crystal structures.

Physics of Polymorphic Transformations

Now polymorphic transformations are classified according to the principle of grouping external changes or properties of crystals under the influence of external factors (temperature, pressure, magnetic field, etc.) [10]. But there must be some unifying principle that would demonstrate the physical causes of polymorphic transformations of crystals under various influences on them, i.e. it would be more correct for the classification of morphological transformations to be based not on a change in the external features or properties of a crystal-a change in volume, anisotropy of properties, or the appearance of new ones, but on changes in the internal state of the atoms that form the structure. All morphological changes are, of course, based on the physics of interacting atoms of matter. And there is no separate physics of high and low temperatures, high and low pressures, etc.-physics is the same for the world around us. The concept of electrons in atoms as averaged values of the electric charge in the space around the atom (spatial charge density) is not productive enough when building a model of the interaction of atoms inside a crystal, and this was noticed in [2], especially considering that a complete description of the crystal would be description of the interaction of all atoms that make up an conventional cell. (Since an ideal crystal of any size is only a translation of a conventional cell, we will not receive any new information when studying the interaction of a larger number of atoms in a crystal than is contained in a conventional cell, therefore, to describe a crystal, there is no need to increase the number of interacting atoms).

Much more productive is the idea of electrons in interacting atoms in a crystal as localized entities. If we assume that the physical laws that determine the magnitude of the measure of angular momentum for an electron inside a hydrogen atom (which we considered above) are the same for atoms with any number of electrons (i.e., for interacting atoms inside a solid body), then phenomenologically it is possible understand that whatever the nature of the bond between the atoms of the conventional cell (metallic bond, ionic, covalent), a new bond is realized only for such new states, when the conserved quantities during the transitions of matter from one state to another have common measures for the previous and new states. (Of course, there is no doubt that from the point of view of the physics of commensurability of states, any quantum states of an arbitrarily complex free atom (not connected with other atoms) have a common measure in all conserved quantities with its ground state). The unit of measure for each conserved quantity can be the absolute value of these quantities when the strongest bond between atoms is realized. For example, with an increase in the temperature of iron, i.e., with an increase in the level of electronic excitations of the interacting atoms, in order to agree on the commensurability of their new states in all conserved quantities, they can change the orientation of the spin magnetic moments, and, from a ferromagnet, iron becomes, for example, a paramagnet. Those the real reason for the change in the magnetic state of iron is not disorder due to the thermal motion of iron atoms, but the need for commensurability of the previous and new states of iron atoms in a new state of matter either with a new lattice or with new excited states of atoms. It is clear that for a complete description of a crystalline substance, it is necessary to describe the interaction of all atoms that make up a conventional cell (and, accordingly, seek commensurability in terms of conserved quantities for all interacting atoms in a conventional cell). This is a difficult task, but it seems to us that it is possible to solve it.

Principle of Commensurability and Coprime of Miller Numbers-Indexes

Let us return to the empirical phenomenon of the requirement of coprime of Miller numbers-indexes, which denote crystallographic planes. As noted above, to designate some specific crystallographic planes, Miller index numbers are possible, which have common factors. These planes do not come out on the surface of crystalline polyhedral and formally they could be called virtual planes, but Lauegrams from them are recorded in X-ray diffraction studies [1], i.e., inside the crystalline structure, there physically exist real ordered atoms of the substance that make up such planes (i.e., the corresponding flat grids of atoms-knots). The question arises: why do they never come to the surface morphologically? And if, for example, we had the opportunity to make an artificial cut along such a plane, would it be possible to grow a single crystal from this plane from the liquid phase of the molten material? If we consider the physics of the interaction of atoms on such an artificial plane with a low reticular density of nodes on it, then phenomenologically it can be understood that at large distances between atoms (a small number of atoms per unit area leads to large distances between them), the bonds between them are provided by valence electrons, whose trajectories go far beyond the electron shell, i.e. these are highly excited p, d, etc. - orbitals. This means that such planes would have to be built almost from the atoms of the liquid, which are in highly excited states. But the most important thing is that in order to ensure the structure of any synthesized crystal, each atom must be surrounded by other atoms with certain quantum states, then each atom that is embedded in the structure must coordinate its internal quantum state with the existing potential field of atoms that have already been structured, or this the embedding atom already has the desired quantum state, which is commensurate in conserved quantities with other atoms.

One can only guess that when the desired atom is selected from the melt, the remaining atoms of the formed structure induce the desired state into the incoming atom (i.e., the existing potential field forces it to adjust its electron shells so that its state is comparable in all conserved quantities! with the rest of the atoms already formed structure). This means that if we tried to synthesize and bring to the surface the quasi-virtual plane indicated by us, then it would be necessary to select from the liquid melt not only very highly excited atoms, but due to the low reticular density of nodes on this plane, the inducing effect of the existing atoms on each atom, which comes again, would be lower than for a plane with a high reticular density. Probably, these two conditions are very hard and do not allow nature to realize the exit of the plane we are discussing on the surface of a crystalline polyhedron. But it should also be noted that the study by Fedorov, Schoenflies [11,12] of real polyhedral (where only planes with index numbers that did not have common factors came to the surface) led to the discovery by them of the now known 230 space symmetry groups. For this reason alone, we can say that this requirement for the mutual simplicity of index numbers actually has a deep physical reason. So, the physical reason remains unclear why for the planes that come to the surface, the index numbers are always coprime. From the point of view of the principle of commensurability, the point is that the measure of the angular momentum of electrons that provide the chemical bond of atoms in the structure must have the same value for all interacting atoms of the conventional cell of a crystalline substance. If there were common factors, then this would mean that there is another measure for measuring the values of the conserved quantities for all atoms that have built a unit cell. If such another measure exists for the atoms that build the quasi-virtual plane mentioned above, then we can state that it is a multiple! the main measure and less than the main measure. In fact, a unit of measure for some conserved quantity can only be determined as a result of the interaction of physical objects, and its value is determined for connected objects, as the value of a conserved quantity with the greatest connection of objects (their least free energy). As it seems to us now, each time to determine the magnitude of the measure for the conserved magnitudes of interacting objects, it is necessary to study such a physico-chemical state of these objects, when the connection between them is greatest.

Conclusion

Based on the previously obtained results on the calculations of the states of hydrogen-like atoms using the principle of commensurability, the physics of polymorphic transformations of crystalline substances is explained as new physical states that must have common measures for all conserved quantities (energies, momenta, momentum, magnetic moments) with the main (previous) state. The unit of measure for each conserved quantity can be defined as its value at the greatest connection between interacting subjects. The fact of the existence of the mutual simplicity of the Miller numbers-indexes, denoting crystallographic planes that come on the surfaces of crystalline polyhedral, follows from the need to have one value of the measure for each conserved quantity that is related to a given structure of a crystalline substance. The authors are grateful to Litvin P.M. for valuable advice.

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