Scientific session of the Division of General Physics and Astronomy and the Division of Nuclear Physics of the Academy of Sciences of the USSR (26–27 November 1986)

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A joint scientific session of the Division of General Physics and Astronomy and the Division of Nuclear Physics of the USSR Academy of Sciences was held on November 26 and 27, 1986 at the S. I. Vavilov Institute of Physical Problems of the USSR Academy of Sciences. The following reports were presented at the session:

November 26

1. G. E. Volovik. Quasicrystals.

2. V. Sh. Shekhtman. Icosahedral symmetry and the diffraction experiment.

3. P. A. Kalugin, A. Yu. Kitaev, and L. S. Levitov. Structure of quasicrystals.

November 27

4. V. S. Shpinel'. Nuclear-spectroscopic studies of hyperfine interactions for impurities in metals.

5. G. B. Khristiansen. Apparatus for studying extremely high energy cosmic rays.

Summaries of four of the reports are presented below.

G. E. Volovik. Quasicrystals. The first quasicrystal was discovered by Shechtman et al.¹ (National Bureau of Standards, USA) in 1984 under conditions of rapid cooling of the alloy $Mn_{0.14} Al_{0.86}$. Since then the number of quasicrystals has been continuously increasing. This new class of ordered materials falls between the regular classical crystals and amorphous materials. Unlike amorphous bodies the x-ray diffraction picture contains sharp Bragg peaks which are characteristic for a regular crystal, but it has a fifth-order symmetry axis, which is incompatible with the translational invariance of the crystal. Most quasicrystals belong to the point symmetry group of the icosahedron, but there exists a quasicrystal consisting of periodically repeating planes, each of which has a fifth-order axis.²

The physical reason for the appearance of quasicrystalline structures lies in the incompatibility of two tendencies: at the microlevel crystal chemistry requires icosahedral or pentagonal short-range order in the packing of atoms and therefore fixes in the medium distinguished fifth-order axes in the direction of chemical bonds, which counteracts the tendency for the establishment of translational long-range order. A mathematical model of an ideal quasicrystal, reconciling these tendencies, has been developed in two independently published theories,^{3,4} which later turned out to be equivalent.

Levine and Steinhardt³ constructured a model of a quasicrystal starting not from one unit cell, like in a crystal, but rather from two unit cells with an irrational ratio of their numbers. This is a generalization to the three-dimensional case of the two-dimensional aperiodic pentagonal Penrose tilings, in which the plane is filled by two rhombi with acute angles of $\pi/5$ and $2\pi/5$, respectively, in a ratio equal to the golden mean $(\sqrt{5} + 1)/2$ (see, for example, Ref. 5). Definite construction rules, based on the Fibonacci series, gave a

structure in which there is no periodicity in the arrangement of the atoms, but a series of properties characteristic for a crystal does exist: 1) long-range orientational order; 2) the atoms lie in "crystalline" planes; 3) δ -function Bragg peaks, corresponding to reflection from these planes, exist; 4) there exists a similarity symmetry—the structure obtained by eliminating a certain set of sites differs from the starting structure by a change in scale by a factor of $(\sqrt{5} + 1)/2$. But there are also differences: 1) the "crystalline" planes are not equidistant, but rather quasiperiodic, i.e., the distance between them assumes two values, alternating in the Fibonacci sequence; 2) the point Bragg peaks densely fill space, but the principal peaks are well distinguished because of the sharp difference in the intensities of the close-lying peaks.

The model constructed by Kalugin, Kitaev, and Levitov,⁴ who constructed an icosahedral quasicrystal starting from a "cubic" crystal in six-dimensional space, has the same properties. From this crystal a channel-an atomic layer whose thickness is of the order of the interatomic distance and which is sandwiched between three-dimensional hyperplanes---is cut out and then projected into the physical space. This method enables the construction of a continuum theory of quasicrystals which can describe dislocations and clarify the character of the low-frequency collective modes: aside from the usual phonons, which appear because there are three degrees of freedom for the motion of atoms along the channel, in a quasicrystal there are three "phasons," associated with the transverse motion of the channel in sixdimensional space. The phason modes, though they have an arbitrarily low energy, contain displacements of separate atoms by large distances and, unlike phonons, they have a diffusive character.

Both models explain well the arrangement and intensity of the Bragg peaks in the electron and x-ray diffraction patterns. However there is also disagreement with experiment, which gives peaks of finite width, corresponding to a distance of ~ 100 Å at which the translational order is lost. In addition, this is unrelated with the size of microcrystallites, which, judging, for example, by the correlation length of the orientational long-range order, is two orders of magnitude greater (see Refs. 6 and 7).

The disagreement is most likely attributable to the fact that a real quasicrystal differs from the mathematical model of an ideal quasicrystal, namely, the atoms in an ideal quasicrystal are located in nonequivalent and unsymmetrical environments and their positions at the sites of an ideal quasilattice are not positions of equilibrium. Therefore, in order to construct a real quasicrystal the atoms must be displaced into equilibrium positions by irregular forces exerted by neighbors. At the same time the quasiperiodic long-range order is destroyed, which broadens the δ function peaks of an ideal quasicrystal, and this is linked with phason variables, as can be easily followed in a continuum model of the quasicrystal.

Irregular forces acting on the phonon variables do not broaden the spots in precisely the same way that impurities in an ordinary crystal do not destroy the long-range translational order. But the same forces, acting on the phason modes, cause the correlation function of the phasons to diverge: the channel in six-dimensional space becomes bent and the amplitude of the deviation from the basal hyperplane diverges. This is what causes the finite width of the peaks. The orientational long-range order is not destroyed in this case; dislocations also remain well defined, so that a Berezinskiĭ phase with topological translational order is possible: in a circuit along a contour of length L Burgers' vector increases as $L^{1/2}$. This distinguishes a real quasicrystal from an amorphous body with orientational long-range order. The complete classification scheme for solids and liquids has yet to be constructed. It is possible that this scheme will be based on an extended symmetry group, including, for example, statistical symmetry and the group of diffeomorphisms.

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- ²L. Bendersky et al., Scripta Metall. 19, 909 (1985).
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- ⁴P. A. Kalugin, A. Yu. Kitaev, and L. S. Levitov, Pis'ma Zh. Eksp. Teor. Fiz. **41**, 119 (1985) [JETP Lett. **41**, 145 (1985)].
- ⁵A. L. Mackey, Kristallografiya **26**, 910 (1981) [Sov. Phys. Crystallogr. **26**, 517 (1981)].
- ⁶P. A. Bancel et al., Phys. Rev. Lett. 54, 2422 (1985).
- ⁷D. R. Nelson, Sci. Am. 255, No. 2, 42 (August 1986).

V. Sh. Shekhtman. Icosahedral symmetry and the diffraction experiment. The discovery of new packing principles for atoms in solids requires a more detailed analysis of the group relations between the quasicrystal model and the crystal lattice. Thus systems with fifth-order symmetry adjoin families of crystallographic point groups, unified by the seven limiting Curie figures. Moreover, if there are no restrictions associated with the Bravais lattice, the two groups of the icosahedral system are the natural and only addition to the standard 32 groups. At the same time the minimum requirement-the finite rotation group constructed on nonorthogonal rotational axes-is satisfied. Thus only two systems are added to the hierarchy of higher-order limiting groups of the sphere $(\infty/\infty \text{ and } \infty/\infty mmm)$: the cubic system (the groups 432, 23, m3m, $\overline{4}3m$, and $m\overline{3}$) and the icosahedral system (the groups 532 and $m\overline{5}m$).¹ We can immediately indicate important subgroup chains



It is useful to describe next the geometric relationships between the Bravais lattices and the quasicrystalline packing, taking into account the general properties of regular polyhedrons. It is well known that there exist only five socalled Plato bodies² with 4, 6, 8, 12, and 20 faces. In the language of crystallography they are all simple shapes (particular shapes) of the cubic or icosahedral system (Fig. 1). For the present discussion it is significant that there exist methods for mutual embedding of the indicated figures; for example, a cube can be inscribed into a dodecahedron with pentagonal faces. Let the cube belong to the group $m\overline{3}$, i.e., among its symmetry elements there are no fourth-order axes. Then the pentagon-dodecahedron is formed as a simple shape, if the starting face is given the indices $\{10\psi\}$ (where $\psi = (1 + \sqrt{5})/2$). We call attention to the fact that in this procedure the application of the symmetry operations of a cube to a plane in a unique (irrational) orientation results in a figure which is a simple shape of the supergroup $m\overline{5}m$.

L. Pauling's³ alternative interpretation of diffraction observations for annealed aluminum-manganese alloys can be regarded as a consequence of this construction. Indeed, right angles between the fifth-, third-, and second-order axes in electron diffraction pictures may be regarded as indications of a quasicrystalline cluster; but these angular relations could equally well characterize a system of 12 domains of the cubic phase, oriented during growth along planes close to $\{10\psi\}$ (for example $\{305\}, \{508\}$, etc., from the Fibonacci sequence). In this case the experimental observations of fifth-order symmetry can also be regarded, as an indication of the existence of icosahedral packing, as a prephase, whose symmetry is inherited in the diffraction picture of a polydomain crystal according to the Zheludev-Shuvalov principle.⁴

In concluding this presentation we call attention to the metal systems, in which unusual results, which served as the beginning of the "icosahedral catastrophe" in solid-state physics, were obtained. It is by no means accidental that among aluminum-manganese and aluminum-iron-silicon alloys there exist intermetallides whose structure belongs to the space groups Im3 and Pa3, respectively. Here there is also the possibility of second-order phase transitions out of the icosahedral group $m\overline{5}m$ into its subgroup m3.

Proceeding now to diffraction problems, we point out