B. K. Vaĭnshteĭn, V. I. Simonov, and D. M. Kheĭker. The Project "Aroks" (Automatic X-ray Determination of Crystal Structures)

The modern apparatus of diffraction methods makes it possible to establish the atomic structure of metals and alloys, of minerals, of inorganic and organic compounds, of proteins and nucleic acids. The acquisition and interpretation of thousands (and in the case of biological objects also hundreds of thousands) of diffraction reflections is a laborious and complicated process. The complete cycle of investigation of the structure of a crystal containing on the order of 100 atoms per unit cell, called for more than one year of intense labor.

A project for the development of an automatic system of determining crystal structures has been developed and is now being realized at the Institute of Crystallography of the USSR Academy of Sciences. The automatic x-ray diffractometers models DAR, DAR-B (for biological objects), DAR-UM (computer controlled), and the controlling computer "Dnepr," developed by the Institute of Crystallography together with the Design Office of the Institute and the Design Office for x-ray Apparatus, make up the experimental stage of the system. The productivity of these instruments is larger by several dozen times than the productivity of photographic methods with manual reduction of the x-ray patterns; the intensity-measurement accuracy can be increased with their help by one order of magnitude.

A second stage of the system, based on the M-220 computer, should automatize the main steps in the determination of the atomic structure of crystals as obtained from the diffraction data. Known and newly-developed procedures for the construction of an approximate model of the investigated atomic structure with the aid of a computer are being perfected and combined into one unit. The realization of the process will make it possible to reduce the time of interpretation of a crystal structure of average complexity to two–three weeks.

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Kh. S. Bagdasarov and V. Ya. Khaimov-Mal'kov, New Procedures and Results of Synthesis of High-melting-point Single Crystals

It is known that the real properties of single crystals are determined not only by the physical and chemical properties of the given substance, but by the conditions of their synthesis, the control of which makes it possible to exert an influence on the real structure of the crystal, and primarily on the homogeneity of the stoichiometric composition, the impurity distribution, the distribution of dislocations and the distribution of other defects. The problem of high-temperature synthesis of perfect single crystals cannot be regarded separately from the concrete geometrical dimensions of the crystal, especially if one deals with relatively large crystals reaching several dozen centimeters. In this sense, the production of large homogeneous crystals is determined not only by the methodological problems of the synthesis, but also by the specific crystallography problems, since synthesis of large homogeneous crystals is not a direct counterpart of the synthesis of small crystals.

The problem of synthesis of large homogeneous crystals was solved using high-melting-point single crystals of sapphire, yttrium-aluminum garnet, yttrium orthovanadate, yttrium aluminate, and other crystals as examples. It must be emphasized that the problem of synthesizing sapphire crystals is an independent problem, which has no less an important significance in science and technology than, for example, the problem of quartz. This is connected with the fact that sapphire crystals are unique in a number of properties, namely the melting temperature, mechanical strength, wear resistance, optical transparency, and chemical stability.

Of equal fundamental significance is the solution of the problem of synthesis of crystals of yttrium-aluminum garnet, especially for quantum electronics.

An examination of the physical and chemical processes and of the kinetics of crystallization of the indicated substances has made it possible to develop corresponding procedures for synthesizing these crystals.

Among the common problems of high-temperature synthesis, an important place is occupied by the interaction of foreign inclusions in the melt with the crystallization front, for example, the problem of the interaction of the crystallization front with the products of the decomposition of aluminum oxide, and the problem of the distribution of the activator impurity in the volume of the crystal.

To solve the problem of the capture of particles by the crystallization front, nonstationary processes of crystallization, due principally to temperature fluctuations, have been considered. With regard to the problem of the distribution of the activator in the crystal, attention was paid to the dependence of the magnitude of the impurity capture coefficient and its anisotropy on the conditions and kinetics of the growth, including facet and non-facet crystallization. It was demonstrated that the appearance of anisotropy of the impurity capture coefficient depends on the magnitude of the axial temperature gradient.

The work culminated in the development of new procedures and apparatus for the synthesis of large perfect crystals of sapphire and yttrium-aluminum garnet, which are widely used in science and technology.

E. A. Turov, Certain Problems of Modern Theory of Magnetism

Using concrete example of nuclear magnetic resonance and electric resistivity, it is shown that the existence of "magnetic defects" of the type of transi-

tion layers between domains in ferromagnets can affect in most significantly many of the physical properties of magnetic crystals, and can lead to a number of new effects. In this connection, the author considers the energy spectrum of a ferromagnet with one domain boundary and with a periodic domain structure. A theory of nuclear magnetic resonance of nuclei in domain boundaries is developed, with allowance for the influence of the "two-dimensional" magnetic-moment oscillations that are typical of them.

The discussion concerns the electric resistivity of ferromagnetic metals at low temperatures, and the giant change in the resistance under the influence of weak external magnetic fields and of the magnetic field produced by the measuring current itself. The idea is advanced that the creation of superpure ferromagnetic metals can uncover new prospects for their applications in technology, in connection with the possibility of controlling strong internal magnetic fields in such metals with the aid of weak currents and fields.

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S. A. Al'tshuler, Electron-nucleon Magnetic Resonance (ENMR)

Ions of elements of the intermediate groups, having an even number of electrons, in solids under the influence of the crystalline field, the ground energy level frequently splits in such a way that the lower sublevel is a singlet. If such ions have a nuclear spin $I \neq 0$, then it is possible to observe magnetic resonance, with the resonant frequencies, intensities, absorption line widths and paramagnetic-relaxation times that are intermediate between those in electron paramagnetic resonance and in nuclear magnetic resonance. This is due to the fact that the electronic magnetic moment, which is zero in the first approximation of perturbation theory, produces in the second approximation an increment to the nuclear magnetic moment μ_N, of the order of $\mu_e = a\beta/\Delta$, where a is the hyperfine-interaction constant, Δ the interval between the lower electronic sublevels, and β the Bohr magneton. An estimate shows that in many cases

An experimental study was made of the ENMR spectra in ionic crystals, viz., on V^{51} in corundum, Pr^{41} in sulfate, Tm^{169} in ethyl sulfate and gallium and aluminum garnets and on Pr^{141} and Tm^{169} in the intermetallic compounds PrP, PrAs, PrBi, TmP, TmAs, and TmSb, and in Pr metal. The measured values of the gyromagnetic factors γ and of the quadrupole-coupling constants turn out to be much larger than the corresponding values for the nuclear spins. In low-symmetry crystals, on going over from one crystal axis to another, the components of the tensor γ change very strongly; in thulium ethyl sulfate, for example, $(\gamma_\perp/\gamma_\parallel) \simeq 75$.

It is shown theoretically and experimentally that in ionic crystals, if the number of paramagnetic impurities is sufficiently small, the most effective mechanism of spin-lattice relaxation is as follows: the lattice vibrations, modulating the electric field of the crystal, act on the orbital motion of the electrons, and thus change the orientation of the nuclear spins. Measurements of the temperature dependence of the spin-lattice relaxation time have shown that, unlike the ordinary nuclear resonance, an important role is played not only by the processes of Raman scattering of the phonons, but also by transitions via the intermediate Stark level. In metals and in intermetallic compounds, if account is taken of the exchange interactions between the conduction electrons and the atoms of the intermediate groups, calculation in accordance with the experimental data leads to very short relaxation times.

Substances containing rare-earth ions with lower singlet electron levels, as shown by an evaluation of the results, can be used to obtain very low temperatures, $\sim 10^{-4}$°K, by adiabatic demagnetization. The first experiment with PrBi has made it possible to decrease the temperature from 26 to 10 millidegrees.

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