Scientific session of the Division of General Physics and Astronomy and the Division of Nuclear Physics of the Academy of Sciences of the USSR (28–29 December 1983)

Usp. Fiz. Nauk 143, 492–500 (July 1984)

On December 28 and 29, 1983, at the A. B. Shubnikov Institute of Crystallography of the USSR Academy of Sciences and the P. N. Lebedev Physics Institute of the USSR Academy of Sciences there was held the Joint Scientific Session of the Division of General Physics and Astronomy and the Division of Nuclear Physics of the Academy. The following papers were heard at the session:

28 December (Institute of Crystallography)

1. *B. K. Vaĭnshteĭn*. Structure, physics, and biology of protein molecules.
2. *V. I. Simonov*. Precision structural studies of crystals with special physical properties.
3. *V. R. Regel'*. Some problems of contemporary research on mechanical properties of crystals.
4. *A. A. Kaminskiĭ*. Physics and spectroscopy of laser crystals.

29 December (Lebedev Institute)

5. *G. A. Gusev and I. M. Zheleznykh*. On the possibility of detection of neutrinos and muons on the basis of radio radiation from cascades in natural dielectric media (the antarctic ice sheet and others).
6. *B. A. Dolgoshein*. Exploration of the Earth by means of a neutrino beam.

A brief summary of four of the papers is given below.

B. I. Simonov. *Precision structural studies of crystals with special physical properties.* The qualitative changes which are occurring before our eyes in structural crystallography are due to the development of the theory of the interaction of radiation with matter, to creation of new methods of obtaining and processing experimental data on the diffraction of x rays, and to automation and computerization of all the principal steps of the study of atomic structures of crystals. Computer-controlled automatic diffraction apparatus permits optimization of the measurements at the level of each diffraction reflection. In processing the experimental data one takes into account the absorption of x rays in matter, anomalous components and diffuse thermal scattering, simultaneous reflections, extinctions, and other effects of interaction of the radiation with the crystal. The accuracy of a contemporary diffraction experiment and the methods for analyzing it permit localization of atoms in crystals with errors which do not exceed 10^{-3} Å. In anisotropic thermal vibrations of atoms one takes into account departures from harmonic motion. Special techniques permit separation of the anisotropy of thermal vibrations of atoms and the asymmetry of the spatial distribution of valence electrons due to chemical bonding of the atoms in crystals and molecules.

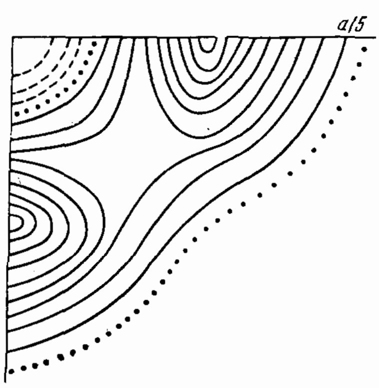

FIG. 1. Difference distribution of the probability density of finding a Cl atom on the cube face of a unit cell of the crystal $CsPbCl_3$ 5° away from a phase transition.

Precision structure studies permit one to learn the atomic mechanisms of the appearance of a number of physical properties of crystals. On the basis of analysis of the anharmonicity of atomic thermal vibrations in crystals it is possible, tens of degrees away from a structural phase transition of the displacement type, to establish that such a transition exists and to indicate which atoms will be displaced in which directions in the approaching transition.

Figure 1 shows the distribution in the plane of the cube face of the unit cell of the $CsPbCl_3$ structure of the probability density of finding a Cl atom at a given point of space; this distribution is due to the anharmonic component of the thermal motion of this atom. The maxima of the distribution indicate that during the approaching phase transition the Cl atoms will be displaced from the center of the cube face in directions parallel to the coordinate axes of the initial structure.

A precision analysis of the thermal motion of atoms in crystals of solid electrolytes permits investigation of the mechanisms of high ionic conductivity in these compounds.

In Fig. 2 we have shown the distribution of Na^+ ions in the conduction channels of the superionic conductor $Na_{0.82a}(Ti_{1.20}Mg_{0.80})(O_{3.22}F_{0.78})$. In this case detailed structural information turns out to be very important in searching for new solid electrolytes and in synthesis of compounds

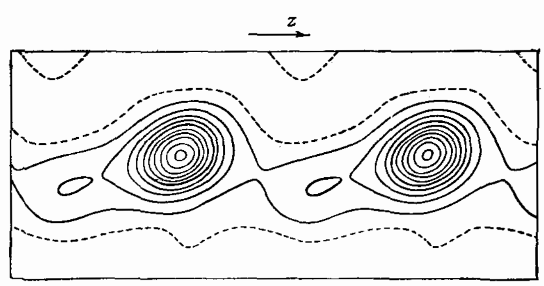

FIG. 2. Distribution of Na^+ ions in the conduction channels of the solid electrolyte $Na_{0.82}(Ti_{1.20}Mg_{0.90})(O_{3.22}F_{0.8})$ at $T = 153$ K.

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with some intended change of their structure and consequently of their properties.

In patterns of the distribution of valence electrons in crystals and molecules obtained on the basis of x-ray diffraction data it is easy to establish, for example, the spatial localization of the unpaired electron responsible for paramagnetism of the compound. Laser crystals pose for precision structure analysis of the problem of localization of small activating impurities in them.

The problem of establishing relations between the structure and properties of crystals was posed long ago, but only the contemporary level of precision structural crystallography permits an adequate solution of this problem.

[1]Computational Crystallography/Ed. D. Sayre, Oxford, Clarendon Press, 1982.

[2]V. I. Simonov, A. M. Golubev, and A. A. Rusakov, Pis'ma Zh. Eksp. Teor. Fiz. **35**, 59 (1982) [JETP Lett. **35**, 68 (1982)].

[3]A. A. Shevyrev, L. A. Muradyan, and V. I. Simonov, Pis'ma Zh. Eksp. Teor. Fiz. **30**, 107 (1979) [JETP Lett. **30**, 96 (1979)].

[4]B. K. Vaĭnshteĭn, V. I. Simonov, V. A. Mel'nikov, A. B. Tovbis, V. I. Andrianov, M. I. Sirota, and L. A. Muradyan, Kristallografiya **20**, 710 (1975) [Sov. Phys. Crystallogr. **20**, 435 (1975)].