

Quantitative electron diffraction structure analysis

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Keywords: electron diffraction, structure analysis, electrostatic potential.

The development of the electron diffractometry methods jointly the analytical methods of electrostatic potential (ESP) reconstruction and its topological analysis allowed one to proceed to the quality new level of electron diffraction structure analysis (EDSA): investigation inner crystalline electrostatic field, which knowledge permits to study the relation of the atomic structure with physical properties of crystals. The review of the last achievements in this direction, obtained particularly in the Institute of Crystallography of Russian Academy of Sciences, in which EDSA method was discovered, and elsewhere will be done. The possibility of the EDSA method to solve precise problems of quantitative analysis of the electrostatic potential will be shown on the examples of investigations of the ESP distributions and chemical bonding in crystals with NaCl-type structure and covalent crystal Ge. The reliability of experimental results obtained was confirmed by the *ab initio* calculations by the Hartree-Fock method. Quantitative data on the potential distribution in addition to the topological analysis of the electron density considerably enlarge conceptions on the nature of interatomic and intermolecular interactions in crystals. The importance of this circumstance promotes the EDSA to the leading position in physics and chemistry of solids.

So the main contents of the lecture is:

1. State of the methods of the precise EDSA:
 - Electron diffractometry;
 - Problem of kinematic – dynamic scattering in thin polycrystalline films;
 - Using of the precession technics for EDSA.
2. Reconstruction of the ESP by Fourier and analytical methods.
3. Quantitative investigations of the chemical bonding and ESP by EDSA.
4. Quantitative analysis of ESP in EDSA.
5. The perspectives of development of the quantitative EDSA.