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N. N. Sirota. Electron and Spin Density Distribution and the Physical Properties of Crystals. The report dealt mainly with the structure and physical properties of crystals, including semiconductors and semimetals. The structure and physical properties of these bodies are determined by the nature and energy of the interatomic interaction. The widespread solid-state band theory can, in this connection, only be considered as an element of the general theory of the chemical bond. We must apparently agree with Coulson that the determination of the bonds in any molecule and in a crystal simply consists in the description of the electron distribution in them.

The most direct methods for determining the electron density distribution functions in a crystal are the methods used in the study of x-ray, electron, and neutron scattering. Since the value of the electron density $\rho(x, y, z)$ at a given point in a crystal is numerically equal to the square of the modulus of the wave function $|\psi(x, y, z)|^2$, it is clear that the experimentally determined electron density distribution function is at the same time a function of the square of the eigenfunctions.

The experimentally determined electron and spin density distribution functions allow us, when using the methods of quantum mechanics, to determine more accurately the form of the eigenfunctions, to partially separate the wave functions according to the orbitals of the atoms, and find with the aid of the tools of quantum mechanics the correlations between the wave and spin density distribution functions and a number of physical properties, and even carry out quantitative computations of the magnitudes of some of these properties.

The possibility of finding the electron density distribution functions in a crystal from x-ray scattering was pointed out by Bragg. The first systematic experiments and computations were carried out in our country by N. V. Ageev and likewise by V. E. Loshkarev.

In recent years experimental methods have been developed which allow us to increase considerably the accuracy of the measurements and computations.

Investigations have been carried out at the BSSR Academy of Sciences Institute of Solid-State and Semiconductor Physics on the experimental determination of x-ray, electron, and neutron scattering form factors, of structure factors, and electron and spin density distribution functions on the basis of the measurements of the absolute, Bragg-scattering intensities. The magni-

tudes of the temperature factors and the root-mean-square displacements of various sorts of ions were also determined, and the anisotropy of the ion oscillations were taken into account. As a rule, the space of the ion oscillations in a crystal had the shape of a sphere or an ellipsoid. The electron and spin density distribution functions in a crystal were computed from the experimentally determined atomic scattering functions (form factors), which were scaled to absolute zero temperature and to the state of stationary atoms when eliminating the zero-point oscillations.

The electron density distribution functions were in this case found by means of a subtractive three-dimensional Fourier synthesis—summation of three-dimensional Fourier series comprising of the differences between the structure amplitudes which had been rigorously computed for a given known distribution function for largely inner-shell electrons (it is possible this distribution was close to the real one), and for experimentally determined structure amplitudes. In such a computational method one sums up small differences which form comparatively rapidly converging series, and series-cutoff effects are completely eliminated. The experimental measurement procedures and the computational methods developed at the Institute yield relatively high degrees of accuracy. The errors are of the order of 2–3%, or, expressed in absolute quantities, of the order 0.1–0.05 e/Å³. Electron density distribution charts were constructed for crystals of the group IV elements and for compounds of the type A^{III}B^V with the diamond, sphalerite, and wurtzite structures. The experimental methods developed have enabled us to distinguish comparatively clearly bridges of sp³-couplings in crystals with the diamond and sphalerite structures, and to find in crystals regions with depressed electron density.

For a number of substances, e.g., C, Si, Ge, and certain compounds of the type A^{III}B^V; potential distribution functions have been found for the lattice, and potential distribution charts have been constructed for different planes. The values of the mean potential, which are proportional to the diamagnetic susceptibilities, are in good agreement with independent magnetic measurements.

The effective charges of the ions were determined by integrating the electron density over the volume of the ions within the boundaries constructed from the electron density charts by comparing the theoretical structure amplitudes for neutral atoms with the experimentally determined amplitudes for neutral atoms with the experimentally determined amplitudes, as well as by determining the ionicity coefficient λ , assuming that the wave function comprises of component functions: $\psi = \psi_A + \lambda\psi_B$. The results of the estimates obtained by the three indicated methods are close to each other and coincide in sign. The magnitudes of the effective charges of the ions have been determined for the majority of the A^{III}B^V-type compounds. It has been established in this case that the A^{III} ions are always positive. For the A^{III}B^V-type compounds which have been investigated the values of the ionicity λ lie between the limits 0.745–0.715. A method has been developed for determining from x-ray patterns (from experimentally determined form factors f) the dia- and paramagnetic

components of the magnetic susceptibility of the elements with the diamond structure and of the compounds with the sphalerite structure and with ionic and semiconductor (ionic-covalent) types of bonding.

The results of the separate determination of the diamagnetic and paramagnetic components of the magnetic susceptibility are in good agreement with the experimental data. The working out and development of the method of separating the paramagnetic and diamagnetic components according to the values of the atomic scattering factors are of considerable interest for the problem of the chemical bond, a fact which was previously pointed out by Ya. G. Dorfman.

The magnitude of the paramagnetic Van-Vleck component of the magnetic susceptibility characterizes the anisotropy of the sp^3 covalent-bond bridges. In particular, for the $A^{III}B^V$ -type compounds, besides the estimate of the magnetic susceptibility, the separation of the diamagnetic and paramagnetic components according to the f -curves enabled us to give a method for the determination of ionic polarizability from x-ray analysis data. The possibility of determining the characteristics of the magnitude of the ionic radii from the electron density distribution charts deserves attention.

Of unquestionable interest is the analysis of the possibilities of determining the elastic constants of the crystallographic lattice and phonon spectra from the electron density distribution functions.

We have considered two methods of estimating the elastic constants: a method based on the statistical model of the atom, and one developed in the molecular orbit theory approximation. Both methods have not as yet led to good quantitative agreement with the experimental data, but the qualitative results obtained are encouraging.

Assuming that the total energy U_{12} of the pair interaction of the atoms in a diamond lattice is made up of a Coulomb U_C , an exchange U_a , and a kinetic U_K energy component and expressing them, within the framework of the statistical theory of atoms, in terms of the electron density, we have

$$U_{12} = \frac{Z_1 Z_2}{\delta} - e^2 \int \left(\frac{Z_1 \rho_2}{r_1} + \frac{Z_2 \rho_1}{r_2} \right) dV + \kappa_h \int [(\rho_1 + \rho_2)^{5/3} - \rho_1^{5/3} - \rho_2^{5/3}] dV - \kappa_a \int [(\rho_1 + \rho_2)^{4/3} - \rho_1^{4/3} - \rho_2^{4/3}] dV \dots$$

where for the diamond lattice $C_{11} - C_{12} = (1/\Omega)(\partial U_{12}/\partial \delta) \times (\alpha/\sqrt{3})$. By substituting the experimental value for $\rho(x, y, z)$, we found the elastic and force constants for C_{diamond} , Si, Ge, and a number of $A^{III}B^V$ compounds and computed the phonon spectra.

The magnetic properties of ferro- and ferrimagnetic crystals are due to the electron density distribution for all the electrons and, in particular, for a portion of the 3d-electrons with uncompensated spins. From the experimentally determined x-ray and coherent magnetic neutron scattering form factors we computed the total electron density distribution function and the density distribution function for the electrons with uncompensated spins for nickel, iron, manganese oxide, manganese arsenide, antimonide, and bismuthide, etc. The relations between the total electron density distributions and the density distributions for the electrons with uncompensated spins (a cloud of such electrons is situated inside the total electron cloud) were elucidated.

Correlations have been established between the degree of the spin density overlap and the magnetic transition temperature (the exchange energy); the temperature of transition to the phase MnBi - MnSb - MnAs decreases with increase of the degree of the Mn - Mn overlap. Using neutron-diffraction methods, we constructed magnetic phase diagrams for MnAs - MnSb solid solutions and a magnetic P-T phase diagram for MnAs. A connection was established at the same time between the variation of the magnetic and electronic transition ($\alpha_{\text{FM}} \rightleftharpoons \beta_{\text{PM}}$) temperature and the degree of overlap of the 3d-electron orbitals.

A transformation of the $\alpha \rightarrow \beta$ type is accompanied by a redistribution of the electron density and a change in the degree of overlap of the orbitals. This leads us to conjecture the possibility of radiation in $\beta \rightarrow \alpha$ transformations.

On the other hand, it was established jointly with G. A. Govor that excitation by light pumping is accompanied by a magnetic phase transition from the ferromagnetic α_{FM} to the paramagnetic β_{PM} state.

There is a thermodynamic explanation for this effect. The decrease in the equilibrium temperature of the magnetic transition when the ferromagnetic phase is excited, which is accompanied by an increase ΔZ in the free energy, is, for a transition energy Q , determined by the relation $\Delta T = Q\Delta Z/T_K$. In the case of phase transitions in which, besides an insignificant nonradiative transformation, a radiative transition occurs, the frequency of the radiation will be $\nu = (Q - q)/h$, where $q = \gamma Q$ and Q is the transition energy for a nonradiative-like transition.

Since in an electron excitation, induced, for example, by optical pumping, the ions distend—increase in size—and a redistribution of the electron density occurs. This phenomenon is accompanied by an increase in the diamagnetic component of the magnetic susceptibility.

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L. I. Kiselevskiĭ. Problems of Low-Temperature-Plasma Spectroscopy. The sphere of scientific and technological applications of low-temperature plasma (temperatures of up to 10^5 °K) is now steadily expanding. Connected with the plasma is the development of such promising directions as gas-discharge and gas-dynamical lasers, the treatment of materials by means of plasma jets, plasma chemistry, and plasma engines and energy converters. A low-temperature plasma may be produced as a medium accompanying some physical phenomena: a powerful explosion, the motion of bodies with hypersonic velocities in the atmosphere.

The progress made in plasma application is inseparably connected with the development and improvement of investigative and diagnostic methods. Occupying a special place among these methods are the spectroscopic methods which are noncontact methods and enable us to determine the most important plasma parameters with a high time and spatial resolution.

The spectroscopic methods of investigation are based on the utilization of the optical characteristics of atoms, ions, and the simplest molecules both in the absence and presence of interaction with the heavy particles and