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Fig. 2. Change in the logarithm of the atomic scattering factor of germanium as a function of $\sum_i h_i^2$

Figure 2: Fig. 2. Change in the logarithm of the atomic scattering factor of germanium as a function of $\sum_i h_i^2$

Abstract

Full Text

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Distribution of Electron Density in Germanium

In our laboratory a systematic investigation is being carried out of the distribution of electron density in semiconductors—elemental substances and compounds. In the present article some results are presented of determinations of the atomic scattering factor for various values of $\sum_i h_i^2$ and of the distribution of electron density in germanium.

Along with the study of the distribution of electron density in diamond ($^{1-3}$) and silicon (^{4,5}), the investigation of the distribution of electron density in germanium, which is also in the fourth group of D. I. Mendeleev' s periodic system and is a semiconductor material of practical importance, is of considerable interest.

Fig. 1. Change in the atomic scattering factor of Ge as a function of the sum of the squares of the indices of reflections of diffraction maxima $\sum_i h_i^2$

Fig. 2. Change in the logarithm of the atomic scattering factor of germanium as a function of $\sum_i h_i^2$

The investigation of the distribution of electron density in the diamond—silicon—germanium series is also of considerable interest for elucidating the nature of interatomic interaction in semiconductors—elemental substances—and for establishing the connection between the character of the electron-density distribution and semiconductor properties. In the work of Yu. N. Shuvalov (^{6}) only relative values are given, which do not make it possible to draw any quantitative conclusions about the distribution of electron density in germanium.

Fig. 3. Map of the distribution of electron density in one quarter of the (110) plane of the unit cell of germanium

Figure 3: Fig. 3. Map of the distribution of electron density in one quarter of the (110) plane of the unit cell of germanium

The object of the investigation was germanium powder obtained by grinding single-crystal germanium in an agate mortar with subsequent

by grinding in toluene to a particle size of 5-8 μ. To prepare the powders, an n-type germanium single crystal with a resistivity of 60 Ω/cm was used. The x-ray diffraction patterns were recorded at room temperatures in CuK_α radiation on a URS-50I recording apparatus with a Geiger-Müller counter. Nickel foil 20 μ thick, placed in front of the counter, was used as a filter. The intensities of the reflections I_{hkl} were determined from the areas of the peaks recorded on an automatic electronic potentiometer EPP-09.

To determine the absolute values, the intensity of the primary beam I_0 was determined and, in addition, a method was used in which the intensities of the hkl lines of germanium were compared with the intensities of the 220 and 311 lines of silicon and NaCl, taken as standard substances.

To determine the absorption coefficient of germanium, the attenuation of the intensity of the primary beam after its passage through plates of various thicknesses from 50 to 200 μ was measured. The plates were prepared by pressing, without the use of any binders.

From the experimental data obtained, the curve of the atomic scattering factor was constructed. In constructing the curve, a correction for dispersion was introduced; the other factors were taken into account in the usual way. Since the powders used for the measurements had a sufficiently high degree of dispersion, and the absorption coefficient was relatively large, extinction was not taken into account.

Fig. 3. Map of the distribution of electron density in one quarter of the (110) plane of the unit cell of germanium.

Figure 1 shows the obtained curve of the atomic scattering factor of germanium as a function of $\sum_i h_i^2$ up to $\sum_i h_i^2 = 48$. The experimental points fit the smooth curve comparatively well. A certain deviation from the smooth curve of the points corresponding to the lines 422, 531, and 620 may be attributed to experimental errors. All points represent the average of 5 experimental values.

Since the distribution of the greater part of the electrons located near the nuclei can be approximated by a Gaussian function, most of the points of the curve

$$\ln f - \sum_i h_i^2,$$

Fig. 4. Distribution of electron density in the directions [111] and [113] in the (110) plane of the unit cell of germanium

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corresponding to values $\sum_i h_i^2 > 8$, lie on a straight line (Fig. 2).

From the data of the given f-curve, the distribution of electron density in the volume of the unit cell was calculated by the method described earlier (^{3}). Figure 3 gives a map of the distribution of the electron density of germanium in the (110) plane of the unit cell. Figure 4 gives the distributions of electron density between the nearest atoms in the unit cell along the directions [111] and [113].

Consideration of the results obtained makes it possible to draw a number of conclusions about the features of the electron-density distribution and about the ionic radius of germanium ions. The ionic radius of germanium, determined at the electron-density level of 1.5 el/Å^3, is 0.5 Å; in this case, outside this volume there lay 6 electrons. The radius of germanium ions at the electron-density level

0.05 el/Å^3 is equal to 2 Å; within this volume there is a very small number of electrons. Let us note that the ionic radii determined in this way are, respectively, 0.20-25 and 1.25 Å for diamond and 0.4 and 1.75 Å for silicon.

Fig. 4. Distribution of electron density in the directions [111] and [113] in the (110) plane of the unit cell of germanium

In the [111] direction, at the position ${}^3/_4\ {}^3/_4\ {}^3/_4$, the electron density is small, not exceeding 0.03 el/Å^3. In the interval between the position 000 and ${}^1/_4\ {}^1/_4\ {}^1/_4$, the smallest electron density is equal to 0.6 el/Å^3.

As is seen from the electron-density map in the direction [111], the segment 000–${}^1/_4\ {}^1/_4\ {}^1/_4$ corresponds to a certain electronic "bridge" of increased electron density. The segment between the points with coordinates ${}^1/_2\ {}^1/_2\ {}^1/_2$–${}^3/_4\ {}^3/_4\ {}^3/_4$ corresponds to a minimum ("trench") of electron density, practically equal to zero.

Department of Solid-State and Semiconductor Physics
Academy of Sciences of the BSSR

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CITED LITERATURE

1. R. Brill, H. G. Grimm et al., *Naturwiss.*, **26**, 479 (1938).

2. R. Brill, H. G. Grimm et al., *Ann. Phys.*, **34**, 393 (1939).
3. N. N. Sirota, N. M. Olekhnovich, A. U. Sheleg, *DAN*, **132**, No. 1, 160 (1960).
4. S. Göttlicher, R. Kuphal et al., *Zs. phys. Chem.*, Neue Folge, **21**, 133 (1959).
5. N. N. Sirota, N. M. Olekhnovich, A. U. Sheleg, *Dokl. AN BSSR*, **4**, No. 4 (1960).
6. Yu. N. Shuvalov, *Fizika tverdogo tela*, **1**, 1959, p. 208.

Note: Figure translations are in progress. See original paper for figures.