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![Fig. 1 and Fig. 2]

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DISTRIBUTION OF ELECTRON DENSITY IN ALUMINUM ARSENIDE AT 20 AND −100°

Among the arsenides of semiconductor compounds $A^{III}B^{V}$ with the sphalerite structure, AlAs is distinguished by a number of features: the greatest band-gap width, the highest melting temperature, and comparatively low values of mobilities. Unlike indium and gallium arsenides, aluminum arsenide is relatively unstable in an ordinary air atmosphere, reacting with water vapor. Knowledge of the nature of the interatomic bond in this compound is of considerable interest. In the course of a systematic study of the distribution of electron density in $A^{III}B^{V}$ compounds, we undertook the determination of the atomic scattering factors of aluminum and arsenic ions in aluminum arsenide at room temperature (20°) and at a temperature of −100°. The measurement and calculation procedure was analogous to that described earlier (^{1}).

[Fig. 1 and Fig. 2]

Fig. 1. *a*—change in the square of the structural amplitudes F^2 of aluminum arsenide at temperatures 20 and −100° as a function of $\sum_j^3 h_j^2$ (explanations in the text); *b*—change in the atomic scattering factors f of arsenic and aluminum ions at temperatures 20 and −100° as a function of $\sum_j^3 h_j^2$.

Fig. 2. Change in the logarithms of the atomic scattering factors (*a*) and f_2 (*b*) for arsenic and aluminum ions at temperatures 20 and −100° as a function of $\sum_j^3 h_j^2$.

An aluminum arsenide sample was obtained by melting the starting components in evacuated quartz ampoules by the two-temperature method. The part of the ampoule containing arsenic was in a furnace at a temperature of about 650°. The lower half of the ampoule, containing aluminum, was at a temperature of the order of 1150°. The synthesis lasted more than 5 hours. After synthesis the ampoule was slowly cooled to room temperature.

Examination of macrosections of the synthesized compound showed the presence of an admixture of a second phase—aluminum; however, no signs of a second phase were observed on the x-ray diffraction patterns. The aluminum arsenide crystals were crushed and then ground in an agate mortar in an argon atmosphere to the required sizes, not exceeding 15—20μ. A flat specimen was

Fig. 3. Electron-density distribution map in the (110) plane of the unit cell of aluminum arsenide at 20°

Figure 1: Fig. 3. Electron-density distribution map in the (110) plane of the unit cell of aluminum arsenide at 20°

Fig. 4. Electron-density distribution map in the (110) plane of the unit cell of aluminum arsenide at −100°

Figure 2: Fig. 4. Electron-density distribution map in the (110) plane of the unit cell of aluminum arsenide at −100°

prepared from the compound powder in an argon atmosphere. Recording both at room and at low temperatures was also carried out in an argon atmosphere.

Fig. 3. Electron-density distribution map in the (110) plane of the unit cell of aluminum arsenide at 20°

The low temperature (−100°) was produced by blowing over the specimen, located under a very thin rubber film, with a stream of nitrogen vapor supplied at a regulated rate from a Dewar vessel containing liquid nitrogen. Temperature control was carried out with a thermocouple attached to the irradiated surface of the specimen. Temperature regulation was achieved by regulating the intensity of the blowing*.

Fig. 4. Electron-density distribution map in the (110) plane of the unit cell of aluminum arsenide at −100°

The x-ray diffraction patterns were recorded on a URS-50I with a Geiger–Müller counter in Cu K_α radiation. In Fig. 1, *a* are shown the curves of the square of the structure amplitude for lines with even indices whose sum is divisible by four (1), with odd indices (2), and with even indices whose sum is not divisible by four (3), for temperatures 20 and −100°. In Fig. 1, *b* are shown the curves of the atomic scattering factors of arsenic and aluminum ions as a function of $\sum_j h_j^2$ at temperatures 20 and −100°. The curves for −100° lie somewhat higher. Judging from the data obtained, the averaged characteristic temperature approximately agrees with the result of work [2].

In Fig. 2, *a* the logarithms of the atomic scattering factors of the arsenic and aluminum ions of the compound AlAs are given for 20 and −100°. For the sum of the squares of the indices greater than 12, for both ions the logarithms of the atomic scattering factors fall on straight lines, which in this case also indicates the possibility of describing the distribution of part of the electrons by a Gaussian curve [3] $\rho_1 = Ae^{-\alpha r^2}$. Table 1 gives the principal quantities characterizing the electron-density distribution described by the part of the atomic scattering factors $f_{1\mathrm{As}}, f_{1\mathrm{Al}}$, whose logarithms are represented by the

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* E. M. Gololobov and A. U. Sheleg took part in developing the method of measurements at low temperatures.

straight lines mentioned above.

Table 1

Principal data characterizing the electron-density distribution ρ_1

Temp., °C	Ions	A, el/Å^3	α	$f_1(0)$	tg φ	Temp., °C	Ions	A, el/Å^3	α	$f_1(0)$	tg φ
20	Al	78.130	13.10	9.07	0.0236	−100	Al	84.71	14.01	8.99	0.0221
20	As	406.08	20.34	24.65	0.0152	−100	As	507.36	24.116	23.87	0.0128

Thus, with decreasing temperature the tangent of the angle of inclination of the linear part of the curves $\ln f_{\mathrm{As}}$ and $\ln f_{\mathrm{Al}}$ decreases, and the magnitudes of the intercepts cut off by the straight lines $\ln f_{1\mathrm{Al}}$ and $\ln f_{1\mathrm{As}}$, as functions of $\sum_j h_j^2$, on the ordinate axis at $\sum_j h_j^2 = 0$, decrease somewhat. The data presented show that, with decreasing temperature, the distribution ρ_1 changes in such a way that the height of the Gaussian curve near the center of the atom increases, while the curve itself becomes narrower (the dispersion of the curve decreases).

The distribution in the outer part of the ions is characterized mainly by the quantity ρ_2, determined by the difference $f - f_1$ of the experimentally determined atomic scattering factors (respectively for aluminum and arsenic ions) and the factors calculated for a Gaussian distribution of electrons, the logarithms of which are expressed by straight lines.

In Fig. 2, *b* the differences $f_2 = f - f_1$ are given for 20 and −100°, respectively, for the arsenic and aluminum ions. As can be seen from Fig. 2, *b*, there is a noticeable influence of temperature on the magnitude of f_2. With decreasing temperature the value of f_2 increases both for aluminum and for arsenic. This indicates that, with decreasing temperature, a change occurs in the electron-density distribution in the outer parts of the ions.

In Figs. 3 and 4 maps of the electron-density distribution are given for 20 and −100°, respectively. Analysis of the maps presented shows that, with decreasing temperature, the electron density between the nearest aluminum and arsenic ions in the [111] direction increases slightly. On the other hand, for example, in the (110) plane in the [110] direction between aluminum and arsenic ions, with decreasing temperature the region of low electron density expands noticeably.

The experimental data presented indicate the need for systematic studies of the electron-density distribution at different temperatures, especially at low temperatures.

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