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Abstract

Full Text

PHYSICAL CHEMISTRY

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DISTRIBUTION OF ELECTRON DENSITY IN GALLIUM ARSENIDE

This paper presents the most essential results of a study of the distribution of electron density in gallium arsenide. The research method was, in the main, analogous to that described earlier ([1], [2]). Finely ground in an agate mortar powder of polycrystalline gallium arsenide, subjected to zone purification, was elutriated in toluene to a particle size of 5-8 μ. X-ray patterns were recorded at room temperature in CuK_α radiation on a URS-50 X-ray recording apparatus with a Geiger-Müller counter. The intensities of the lines were determined from the areas of the peaks recorded on an automatic EPP-09 potentiometer.

Using the experimentally obtained absolute values of the reflection intensities I_{hkl}, the squares of the structure amplitude F^2 were calculated for three types of lines—lines with even indices whose sum is divisible by four (F_1^2), lines with odd indices (F_2^2), and lines with even indices whose sum is not divisible by four (F_3^2) (see Fig. 1a). From the given squares of the structure amplitudes, the values of the atomic scattering factors of the gallium and arsenic ions were calculated (Fig. 1b). Figure 2 shows the values of the logarithms of the atomic scattering factors for various values of Σh_i^2. As is seen from Fig. 2, at $\Sigma h_i^2 > 12$ for arsenic ions and at $\Sigma h_i^2 > 10$ for gallium ions, the logarithms of the atomic scattering factors as functions of Σh_i^2 fall well on straight lines. This circumstance indicates the possibility of applying the previously described ([3]) method of summing three-dimensional Fourier series and calculating the electron-density distribution throughout the entire volume of the elementary cell of gallium arsenide, using the obtained values of the atomic scattering factors.

Figure 3 gives a map of the electron-density distribution in the (110) plane of the GaAs elementary cell. Figure 4a,b shows the distribution of electron density between Ga—As—Ga ions in the [111] direction (Fig. 4a) and between Ga—As ions in the [113] direction (Fig. 4b) in the (110) plane. In the (110) plane, between neighboring gallium and arsenic ions in the [111] direction, between the points 000 and $^1/_4\,^1/_4\,^1/_4$, a "bridge" of increased electron density is observed with a minimum value of 0.49 el/Å^3. Similar "bridges" are observed in crystals of silicon, germanium, and indium arsenide. In indium arsenide the minimum value of the electron density in the "bridge" is 0.45 el/Å^3, and the width of such a "bridge" is somewhat smaller.

Figure 1 and Figure 2: graphs of structural amplitudes and atomic scattering factors

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Between arsenic and gallium ions in the [113] direction there is not observed so clearly pronounced a "bridge" of increased electron density as occurs in indium arsenide. At the same time, no minimum of electron density ("groove"), characteristic of germanium and silicon crystals, is observed here either. In contrast to indium arsenide, in gallium arse-

somewhat larger values of the electron density occur between the metal ions Ga—Ga in the directions [001] and [110].

In gallium arsenide, as also in indium arsenide, in the [111] direction near the point 3/4 3/4 3/4 the electron density is close to zero. In gallium arsenide the nonsphericity of the arsenic ion is most clearly noticeable. In indium arsenide the nonsphericity of the arsenic ion is also noticeable, but is less distinctly expressed. It should also be noted that the maximum of the electron density

Fig. 1. Change in the square of the structure amplitude F^2 of gallium arsenide (a) and of the atomic-scattering factors (b) of arsenic ions (I) and gallium (II) in gallium arsenide as a function of $\sum h_i^2$

Fig. 2. Change in the logarithm of the atomic-scattering factors of arsenic ions (I) and gallium (II) as a function of $\sum h^2$

at the position of the center of the arsenic ion in gallium arsenide is significantly higher than in indium arsenide. It is possible that this circumstance is to some extent connected with the difference in the characteristic temperatures of these compounds.

The data obtained on the distribution of the electron density make it possible to make some estimates of the ionic radii of gallium and arsenic.

At an electron-density level of 0.5 el/Å^3, the ionic radius of gallium is 0.8 Å, and the ionic radius of arsenic is 1.65 Å. At the same time, in the [113] direction the ionic radius of arsenic is somewhat smaller—of the order of 1.3 Å. If the radius is determined at a somewhat higher electron-density level, then the ionic radius of gallium changes comparatively little, whereas the ionic radius of arsenic decreases noticeably.

At an electron-density level of 0.25 el/Å^3, the ionic radius of gallium is 1.3 Å, and the ionic radius of arsenic is 1.45 Å. In indium arsenide, at an electron-density level of 0.5 el/Å^3, the ionic radius of indium is 0.9 Å, and the ionic radius of arsenic is 1.2 Å—1.10 Å. At an electron-density level of 0.25 el/Å^3, the ionic radius of indium is approximately 1.5 Å, and the ionic radius of arsenic is

Fig. 3

Figure 2: Fig. 3

Fig. 4

Figure 3: Fig. 4

approximately 1.35 Å.

The values given for the ionic radii, although they are approximate and preliminary in character, are of considerable interest and, in particular, indicate that sphalerite structures, as structures of closest packings, can be considered only in a first approximation, taking into account the character of the electron-density distribution.

Fig. 3. Map of the electron-density distribution in the (110) plane of the unit cell of gallium arsenide.

Fig. 4. Distribution of the electron density in the direction [111] (a) and [113] (b) in the (110) plane of the unit cell of gallium arsenide.

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REFERENCES

1. N. N. Sirota, N. M. Olekhnovich, *DAN*, **136**, No. 3 (1961).
2. N. N. Sirota, A. U. Sheleg, *DAN*, **135**, No. 5 (1960).
3. N. N. Sirota, N. M. Olekhnovich, A. U. Sheleg, *DAN*, **132**, No. 1, 160 (1960).

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