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## Abstract

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## PHYSICAL CHEMISTRY

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# ON THE DISTRIBUTION OF ELECTRON DENSITY IN INDIUM ARSENIDE

Among semiconductor compounds of elements of the third and fifth groups, $A^{\mathrm{III}}B^{\mathrm{V}}$, with the sphalerite structure, arsenides are of considerable interest, above all because of their semiconductor properties, and also because of the combination of high values of the mobilities of charge carriers with comparatively large values of the forbidden-band width. Therefore, investigation of the distribution of electron density in compounds of the indicated type is of great importance both for understanding the character and energy of the interatomic bonds in them and for elucidating the factors determining their special physical properties.

[Figure 1 and Figure 2: graphs showing changes in structural amplitudes and atomic scattering factors as functions of $\sum h_i^2$.]

**Fig. 1.** $A$—change of the square of the structural amplitude $F^2$ of indium arsenide as a function of $\sum h_i^2$. $B$—change of the atomic scattering factors $f$ of indium and arsenic ions in indium arsenide as a function of $\sum h_i^2$.
1—$F_1^2$, 2—$F_2^2$, 3—$F_3^2$

**Fig. 2.** Change of the logarithm of the atomic scattering factors of indium and arsenic ions as a function of $\sum h_i^2$

A powder was studied that had been obtained by grinding polycrystalline indium arsenide in an agate mortar, followed by elutriation in toluene. The particle size of the powder lay within the range 6—8 $\mu$. Polycrystalline indium arsenide was obtained by direct synthesis from purified components in evacuated and sealed quartz ampoules, as was described previously ($^1$).

Radiographs were taken at room temperature in CuK$\alpha$ radiation on a URS-50-I unit, by a method analogous to that described in ($^2$). From the experimental data obtained, the values of the square of the structure amplitude $F^2$ were calculated for various values of $\sum h_i^2$ for lines with even indices $hkl$, the sum of which is divisible by four (1), is not divisible by four (3), and for lines with

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

Figure 1: Fig. 3. Map of the electron-density distribution in the (110) plane of the unit cell of indium arsenide

odd indices (2) (Fig. 1 A). Figure 1 A gives the values of the squares of the structure amplitude calculated per molecule (per one pair of InAs atoms).

Since $F_1^2 = (f_{\text{In}} + f_{\text{As}})^2$, $F_2^2 = f_{\text{In}}^2 + f_{\text{As}}^2$, and $F_3^2 = (f_{\text{In}} - f_{\text{As}})^2$, then $F_3^2 = 2F_2^2 - F_1^2$.

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

Then, taking into account only $F_1^2$ and $F_2^2$, we obtain

$$f_{\text{In}} = \frac{F_1}{2} + \frac{1}{2}\sqrt{2F_2^2 - F_1^2}, \tag{a}$$

$$f_{\text{As}} = \frac{F_1}{2} - \frac{1}{2}\sqrt{2F_2^2 - F_1^2}. \tag{b}$$

It should be borne in mind, however, that in reality for each given value of $\sum h_i^2$ there exists only one line. Thus, the separate determination of the components $f_{\text{In}}$, $f_{\text{As}}$ is always associated with interpolation between neighboring points.

Figure 1 gives the values of the atomic scattering factors of indium ions $f_{\text{In}}$ and arsenic ions $f_{\text{As}}$ in the compound InAs. The initial portions of the $f$-curves are shown by a dashed line, since at $\sum h_i^2 = 0$ only the value of $F_1^2$, equal to the square of the sum of the ordinal numbers of the components of the compound under study, is known exactly, while the values of $F_2^2$ and $F_3^2$, which depend on the degree of ionization of the In and As atoms, are not exactly known.

Since the curve $F_3^2$ can be extrapolated to zero with a sufficient degree of reliability, it is possible to obtain the zero values of $f_{\text{In}}$ and $f_{\text{As}}$. Note that the dashed portions of the curves $f_{\text{In}}$ and $f_{\text{As}}$ do not affect the results of calculating the electron-density distribution in the lattice of the compound InAs, because the values $f_{\text{In}}$ and $f_{\text{As}}$ at $\sum h_i^2 = 0$ enter into the zero term of the three-dimensional Fourier series in the form of a sum equal to the sum of the ordinal numbers of the elements In and As in the periodic system of D. I. Mendeleev.

The logarithms of the atomic scattering factors of indium and arsenic ions at $\sum h_i^2 > 12$ fall well on straight lines (Fig. 2).

From the values of $f_{\text{In}}$ and $f_{\text{As}}$, the distribution of electron density in the unit cell of InAs was calculated by summing a three-dimensional Fourier series, using the method described earlier ($^3$); in doing so the edge of the unit cell was divided into 60 equal parts.

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

Figure 2: Fig. 4. Distribution of electron density in the [111] and [113] directions in the (110) plane of the unit cell of indium arsenide

Figure 3 gives a map of the electron-density distribution in InAs in the (110) plane of the unit cell. Figure 4 shows the distribution of electron density between indium and arsenic ions in the [111] direction and in the [113] direction in the (110) plane.

The experimental results obtained make it possible to draw certain conclusions about the features of the distribution of electron density in the unit cell of indium arsenide, as well as about the sizes of the ionic radii and the degree of ionization of indium and arsenic.

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

Of considerable interest is the character of the change in electron density along various directions. In the [111] direction, in the interval $\frac{1}{2}\,\frac{1}{2}\,\frac{1}{2}$—$\frac{3}{4}\,\frac{3}{4}\,\frac{3}{4}$, a certain "bridge" of electron density is observed, reaching values of 0.20 el/$\mathring{A}^3$ near the point $\frac{5}{8}\,\frac{5}{8}\,\frac{5}{8}$ and decreasing to values of 0.03 el/$\mathring{A}^3$ near the point $\frac{3}{4}\,\frac{3}{4}\,\frac{3}{4}$. This "bridge," as is seen on the electron-density map (Fig. 3), is elongated in the (110) plane along the [113] direction between the arsenic and indium ions. Let us note that in germanium no similar "bridge" is observed.

In the interval between the coordinates 000 and $\frac{1}{4}\,\frac{1}{4}\,\frac{1}{4}$ in the [111] direction there is a "bridge" of increased electron density appreciable in magnitude, similar in form to those observed in germanium ([2]), silicon ([4,5]), and diamond ([3]). The smallest electron density in this region is 0.45 el/$\mathring{A}^3$.

Let us also note that at half the distance between the nearest metal ions (In) in the [110] direction the electron density is of the order of 0.15 el/$\mathring{A}^3$, and in the [001] direction, of the order of 0.07 el/$\mathring{A}^3$. At half the distance between arsenic ions, the electron density is of the order of 0.15—0.10 el/$\mathring{A}^3$ in the [110] direction and less than 0.03 el/$\mathring{A}^3$ in the [001] direction.

The results obtained are of considerable interest for clarifying the character of interatomic interaction in indium arsenide.

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