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ATOMIC SCATTERING FACTORS AND THE DISTRIBUTION OF ELECTRON DENSITY IN GALLIUM ANTIMONIDE

With the present investigation we have begun a series of studies of the distribution of electron density in the antimonides of elements of the third group of D. I. Mendeleev' s periodic system. Gallium antimonide as a semiconductor compound is characterized by a considerable mobility of charge carriers–electrons and holes. Among other compounds $A^{\mathrm{III}}B^{\mathrm{V}}$ it has the lowest value of the ratio of these mobilities. The width of the forbidden band of GaSb is of the order of 0.8 eV ([1]), somewhat greater than that of germanium. In connection with the problem of the nature of interatomic bonding in $A^{\mathrm{III}}B^{\mathrm{V}}$ semiconductor compounds, the study of the distribution of electron density in gallium antimonide is of great scientific interest.

The object of the investigation was gallium antimonide obtained in the laboratory of the Institute of Rare Metals by direct fusion in quartz ampoules and subjected to zone leveling. The polycrystalline specimen was ground in an agate mortar. The powder was then soaked in toluene. For the investigation a powder with particle size 5–8 μ was taken. The particle size was checked under a microscope.

X-ray photographs were taken on a URS-50I apparatus with Cu K_α radiation. The unit-cell constant determined by us, $a = 6.087$ Å, agrees well with the literature data ([2]). The method of photographing and the calculations were analogous to those described earlier ([3–5]). On the basis of the determination of the absolute values of the intensities of reflections reflected from planes with even indices whose sum is divisible by 4, from planes with odd indices, and from planes with even indices whose sum is not divisible by 4, curves of the squares of the structure amplitude, referred to the formula unit GaSb, were constructed (Fig. 1a). From the data on the squares of the amplitudes, values of the atomic scattering factors of antimony ions and gallium ions were calculated (Fig. 1b).

The logarithms of the values of the atomic scattering factors of antimony and gallium ions, beginning with the value

Fig. 1

Figure 1: Fig. 1

$$\sum_{i=1}^{3} h_i^2 > 8,$$

fall on straight lines (Fig. 2).

For the logarithms of the atomic scattering factors only the first two points for antimony ions and the first three points for gallium ions deviate appreciably from the straight lines and thus determine the difference between the interionic distribution of electron density and a Gaussian-type distribution.

From the obtained values f_{Sb} and f_{Ga} the electron density was calculated ([3]). In the calculation the edge of the unit cell was divided into 60 equal parts. Figure 3 gives curves of the distribution of electron density in the direction [111] in the plane (110) (Fig. 3a) and in the direction [113] in the same plane (Fig. 3b).

According to the data obtained, the values of the ionic radii of gallium and antimony ions can be determined. At an electron-density level equal to

1 electron per cubic angstrom, the ionic radius of gallium is approximately 0.5 Å, and that of antimony 0.8 Å. At an electron-density level of 0.5 el/Å^3 the ionic radius of gallium is 0.75 Å, and that of antimony 0.8 Å. These values of the ionic radii can be compared with the number of electrons contained in the volume of an ion of the given radius and, consequently, with the number of electrons located between the ions. At the same time, the data obtained testify to the conventional character both of the concept of ionic radii themselves and of ideas about close-packed structures.

Attention is drawn to the character of the electron-density distribution between the antimony and gallium ions in the [111] direction (Fig. 3a). Let us note a noteworthy fact: in the regions located near half the distance ($^5/_8\ ^5/_8\ ^5/_8$) between the gallium and antimony ions in the [111] direction and in the [113] direction in the (110) plane, the electron density practically falls to zero. Between the nearest gallium and antimony ions, the electron density near the point $^1/_8\ ^1/_8\ ^1/_8$ decreases to 0.36 el/Å^3, forming a "bridge" of electron density.

Fig. 1. **a** –change of F^2 as a function of $\sum_{i=1}^{3} h_i^2$: **1** –for reflections with even indices, the sum of which is divisible by four; **2** –for reflections with odd indices; **3** –for reflections with even indices, the sum of which is not divisible by four. **b** –change of the atomic scattering factors of antimony (1) and gallium (2) ions as a function of $\sum_{i=1}^{3} h_i^2$

Fig. 2. Change of the logarithm of the atomic scattering factors of antimony (1) and gallium (2) ions as a function of $\sum_{i=1}^{3} h_i^2$

Fig. 2

Figure 2: Fig. 2

Fig. 3. Electron-density distribution in the unit cell in the (110) plane: a—in the [111] direction and b—in the [113] direction

Figure 3: Fig. 3. Electron-density distribution in the unit cell in the (110) plane: a—in the [111] direction and b—in the [113] direction

In the [111] direction between Sb and Ga, near the point $^3/_4$ $^3/_4$ $^3/_4$, a region of somewhat increased electron density is observed (from 0.12 to 0.16 el/Å^3). Near the point $^1/_2$ $^1/_2$ $^1/_2$ a region of a certain increase in electron density, from 0.08 to 0.12 el/Å^3, is also observed.

Figure 4 gives a map of the electron-density distribution in the (110) plane of the GaSb unit cell. In analyzing the character of this distribution, certain features should be noted. On the map one can clearly see the above-mentioned "bridges" of increased electron density between the nearest Sb and Ga ions, with an electron density of 0.36 el/Å^3.

(the lower part of Fig. 4). Between the gallium ions located in the upper part of the figure and the antimony and gallium ions in the lower part of the figure, a band of reduced electron density is revealed, in which, however, certain differences in the distribution of electrons can be noted.

Fig. 3. Electron-density distribution in the unit cell in the (110) plane: *a*—in the [111] direction and *b*—in the [113] direction

Fig. 4. Map of the electron-density distribution in the (110) plane of the GaSb unit cell

The atomic scattering factors of gallium and antimony ions determined in the present work, and the revealed picture of the electron-density distribution in the lattice of the semiconductor compound GaSb, may be useful in discussing the features of the nature of interatomic interaction and the physical properties of this compound.

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Fig. 4. Map of the electron-density distribution in the (110) plane of the GaSb unit cell

Figure 4: Fig. 4. Map of the electron-density distribution in the (110) plane of the GaSb unit cell

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