Academician of the Academy of Sciences of the BSSR N. N. Sirota and E. M. Gololobov

1962

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Abstract

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Physical Chemistry

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Atomic Scattering Factors and the Distribution of Electron Density in Aluminum Antimonide at 20 and −100° C

The present work completes the first cycle of investigations of atomic scattering factors and the distribution of electron density in semiconductor compounds with antimony of elements of the third group of D. I. Mendeleev' s periodic system. Below are presented the results of determining the atomic scattering factors of the ions of aluminum antimonide at room temperature (20°) and at −100°; values are given for the calculated electron density, which are compared with data obtained in the study of indium and gallium antimonides. The binary system aluminum–antimony was studied in detail by G. G. Urazov et al. ([1,2]), who established the existence in it of one compound, AlSb, melting with an open maximum. Aluminum antimonide, like indium and gallium antimonides, has the sphalerite lattice. In its semiconductor properties, aluminum antimonide differs from indium and gallium antimonides by a relatively large forbidden-band width ($\Delta E = 1.6$ eV), a comparatively small temperature coefficient of variation of the semiconductor parameters, and also the highest melting temperature among the $A^{III}B^{V}$ antimonides.

The investigation was carried out on aluminum antimonide obtained by fusing stoichiometric components–aluminum and antimony–in a corundum crucible in an evacuated quartz ampoule. Specially purified antimony (99.99%) and specially purified aluminum (99.99%) were used to prepare the compound. X-ray photographs of finely ground powders (5-7 μ) were taken on a URS-50-I apparatus in filtered CuK_{α} radiation, using a Geiger-Müller counter. The methods of recording and analyzing the obtained data were analogous to those described earlier. For photographing at low temperatures, a special holder was made, in which a plate of pressed powder was placed and continuously blown with nitrogen vapor. The temperature was controlled by a copper-constantan thermocouple, the junction of which was attached to the specimen in the immediate vicinity of the irradiated region ([4]).

The lattice constants of aluminum, gallium, and indium antimonides determined by us (in Å) are as follows:

Fig. 1 and Fig. 2

Figure 1: Fig. 1 and Fig. 2

	at 20°	at −100°
AlSb	6.136	6.133
GaSb	6.087	6.082
InSb	6.477	6.473

The obtained values of the lattice constant at room temperature agree well with the literature data ([5]). From the data given, the mean coefficients of linear expansion were calculated:

$$\alpha_{l\,\mathrm{AlSb}} = 4.1 \cdot 10^{-6}; \quad \alpha_{l\,\mathrm{GaSb}} = 5.7 \cdot 10^{-6}; \quad \alpha_{l\,\mathrm{InSb}} = 4.9 \cdot 10^{-6}.$$

From the absolute values of the intensities of reflections on AlSb x-ray diagrams taken at room temperature and at −100°, the values of the squares of the structure amplitudes F^2, referred to the formula unit AlSb, were determined (Fig. 1). From the obtained F^2 data, the atomic scattering

Fig. 1. Variation of F^2 at room temperature (a) and at −100° (b) as a function of

$$\sum_{i=1}^{3} h_i^2 :$$

1 –for reflections with even indices whose sum is divisible by four; 2 –for reflections with odd indices; 3 –for reflections with even indices whose sum is not divisible by four

Fig. 2. Variation of the atomic scattering factors of aluminum and antimony ions at room temperature (a) and at −100° (b) as a function of

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

factors of aluminum and antimony ions were calculated for room temperature and for low temperature (Fig. 2), and their logarithms were also calculated. From the Gaussian distribution of electron density $\rho_1 = Al_3^{-\alpha r^2}$, for the rectilinear segment of the curve $\ln f - \sum_{i=1}^{3} h_i^2$, the values of A and α were determined for aluminum and antimony ions.

At 20°: $A_{\mathrm{Al}} = 62.381$; $\alpha_{\mathrm{Al}} = 11.587$; $A_{\mathrm{Sb}} = 418.443$; $\alpha_{\mathrm{Sb}} = 14.716$.

At −100°: $A_{\mathrm{Al}} = 68.951$; $\alpha_{\mathrm{Al}} = 12.411$; $A_{\mathrm{Sb}} = 466.46$; $\alpha_{\mathrm{Sb}} = 15.871$.

Fig. 3. Electron-density distribution in the unit cell in the (110) plane in the (111) and (113) directions at room temperature (a) and at −100° (b)

Figure 2: Fig. 3. Electron-density distribution in the unit cell in the (110) plane in the (111) and (113) directions at room temperature (a) and at −100° (b)

Fig. 4. Map of the electron-density distribution in the (110) plane of the unit cell of AlSb at 20°

Figure 3: Fig. 4. Map of the electron-density distribution in the (110) plane of the unit cell of AlSb at 20°

By synthesizing three-dimensional Fourier series according to the previously adopted method, the distribution of electron density in the (110) plane of the unit cell was determined. Figure 3 shows the electron-density distributions in the (111) and (113) directions of the (110) plane at 20° (Fig. 3a) and at −100° (Fig. 3b). In Fig. 4 we present a map of the electron density of AlSb at 20°.

Fig. 3. Electron-density distribution in the unit cell in the (110) plane in the (111) and (113) directions at room temperature (a) and at −100° (b)

As can be seen from the graphs presented, in the compound AlSb, as also in the compound GaSb ([6]), near the point 5/8 5/8 5/8, approximately halfway between the antimony and aluminum ions in the (111) direction in the (110) plane, the electron density falls practically to zero, in contrast to InSb ([7]), in which an electron bridge is located in this region. In the compound GaSb an area of increased electron density is observed at the position 6/8 6/8 6/8, and a slight increase in electron density near the point 1/2 1/2 1/2. In the compound AlSb, near the indicated points 6/8 6/8 6/8 and 1/2 1/2 1/2 there is also a region of increased electron density, in absolute magnitude slightly greater than in GaSb. With lowering of the temperature to −100°, these regions of increased electron density appear more distinctly. The general pattern of the change in electron density in the compound AlSb upon going from 20° to −100° is characterized by an increase in the values of electron density near the centers of the ions and by a more distinct manifestation of the details of the electron-density distribution at small density values. In the (113) direction, midway between the aluminum and antimony ions, the electron density is practically equal to zero. At low temperatures the region of reduced electron-density values becomes somewhat broader. A similar picture occurs in the compound GaSb. In contrast to the compounds AlSb and GaSb, in InSb at the center of the distance between the In and Sb ions in the indicated direction an area of somewhat increased electron density is observed; the extent of this area at −100° decreases somewhat, but it also becomes more clearly expressed.

Fig. 4. Map of the electron-density distribution in the (110) plane of the unit cell of AlSb at 20°

At the position 1/8 1/8 1/8 in the (111) direction in the (110) plane, the com-

pound AlSb has an increased value of the electron density, reaching 0.40 el/Å^3; in GaSb at this point the electron density is ···

a value of 0.35 el/Å^3, and in InSb–0.30 el/Å^3. At −100°, the electron density in the indicated "bridge" increases somewhat.

The results obtained make it possible to estimate the radii of the aluminum and antimony ions in the compound AlSb. At the electron-density level 1 el/Å^3, $r_{Al} = 0.6$ Å; $r_{Sb} = 0.93$ Å.

At the electron-density level 0.5 el/Å^3, $r_{Al} = 0.75$ Å; $r_{Sb} = 1.2$ Å.

The conventional character of the concept of ionic radii is evident. However, the values given are of definite interest. Also noteworthy is the appreciable nonsphericity of the antimony ions, if their surface is regarded as a surface of equal densities at low electron densities. The greatest effect of temperature is observed, as we have already noted, in the compound InSb, and the smallest in AlSb. This effect may also be connected with the values of the characteristic temperatures. The characteristic temperatures determined by us in the interval $20 \div -100$°C are as follows: AlSb $\theta = 320$°K, GaSb $\theta = 240$°K, InSb $\theta = 210$°K.

The characteristic temperature of GaSb agrees comparatively well with literature data determined by various methods. For GaSb, from elastic constants, the characteristic temperature was determined to be 233°K ([8]), while the characteristic temperatures for AlSb and InSb have been determined for the first time.

The results obtained in the present investigation may be of interest for understanding the nature of interatomic interaction in semiconductor compounds $A^{III}B^{V}$.

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Received 26 I 1962

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