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Fig. 1

Figure 1: Fig. 1

Fig. 2

Figure 2: Fig. 2

Abstract

Full Text

Physical Chemistry

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DISTRIBUTION OF ELECTRON DENSITY IN INDIUM ANTIMONIDE

Among the semiconducting compounds $A^{III}B^{V}$ of groups III–V of the periodic system of D. I. Mendeleev with the sphalerite crystal lattice, the compound InSb is distinguished by the highest mobility of charge carriers—electrons and holes—and by a comparatively small width of the forbidden band. Therefore an X-ray investigation of the distribution of electrons between the ions of this compound is of considerable interest for elucidating the picture and the features of the chemical interatomic interaction that determines its physical properties.

In the present work the changes in the atomic scattering factors of indium and antimony ions in the compound InSb under study have been determined and

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. *b*—change of the atomic scattering factors of antimony ions (1) and indium ions (2) as a function of $\sum_{i=1}^{3} h_i^2$

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

maps of the electron-density distribution in various planes of the lattice. The main results of the study are presented below. As the object of study we used single-crystal samples of the compound InSb, obtained by fusing spectrally pure components in quartz ampoules and subjected to zone refining. The lattice

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Fig. 3. Map of the electron-density distribution in the (110) plane of the InSb elementary cell

Figure 3: Fig. 3. Map of the electron-density distribution in the (110) plane of the InSb elementary cell

Fig. 4. Electron-density distribution in the elementary cell in the (110) plane. a—in the [111] direction, b—in the [113] direction

Figure 4: Fig. 4. Electron-density distribution in the elementary cell in the (110) plane. a—in the [111] direction, b—in the [113] direction

constant determined by us at room temperature was 6.474 Å, which agrees with the data of work ([1]).

The method of the work was, in its main features, analogous to that used previously ([2-5]). X-ray patterns were recorded on a URS-50-I recording X-ray apparatus with an ionization counter. InSb powder, elutriated in toluene, with a particle size not exceeding 5 μ, was used. The powder was pressed into flat cuvettes made of organic glass with a layer thickness of 1.5 mm. The intensity of the reflections was determined from the areas of the peaks of the curves recorded on an ÉPP-09 potentiometer. Dispersion corrections were introduced in the calculations.

Fig. 3. Map of the electron-density distribution in the (110) plane of the elementary cell of InSb

Fig. 4. Electron-density distribution in the elementary cell in the (110) plane. *a*—in the [111] direction, *b*—in the [113] direction

On the basis of the experimental data, the absolute values of the reflection intensities I_{hkl} were determined; from these the squares of the structure amplitudes were calculated for lines with even indices, the sum of which is divisible by four (F_1^2), and for lines with odd indices (F_2^2) (Fig. 1*a*). From these data the values of the atomic scattering factors of antimony ions f_1 and indium ions f_2 were calculated.

The logarithms of the scattering factors of antimony ions for $\sum_{i=1}^{3} h_i^2 > 8$ and the atomic scattering factors of indium ions for $\sum_{i=1}^{3} h_i^2 > 11$ fall on straight lines (see Fig. 2). The straight-line portions of the logarithmic curves of the atomic scattering factors for antimony ions are characterized by the value $f_{\mathrm{Sb}}(0) = 44.46$ and by the tangent of the angle of slope $\mathrm{tg}_{\mathrm{Sb}}\,\varphi = 0.02$; correspondingly, for indium ions $f_{\mathrm{In}}(0) = 39.65$ and $\mathrm{tg}_{\mathrm{In}}\,\varphi = 0.019$.

Thus, the presence of linear portions of the f-curves indicates the possibility of describing part of the electron-density distribution with

using distribution functions of the Gaussian type $\rho_1 = Ae^{-ar^2}$. In this case $A_{\mathrm{Sb}} = 323.084$, $A_{\mathrm{In}} = 317.414$, $\alpha_{\mathrm{Sb}} = 11.780$, $\alpha_{\mathrm{In}} = 12.396$.

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The results of calculations of the electron-density distribution in the (110) plane of the unit cell are presented by us in the form of a map in Fig. 3.

Figure 4 shows the electron-density distribution between the In–Sb ions in the [111] direction (Fig. 4a) and [113] direction (Fig. 4b) in the (110) plane.

The map of the distribution of electron densities in the (110) plane indicates the presence of an increased electron density between the indium and antimony ions between 000 and $\frac{1}{4}\ \frac{1}{4}\ \frac{1}{4}$ and between the points $\frac{1}{4}\ \frac{1}{4}\ \frac{1}{4}$ and 111 in the [111] direction, and also between the points $\frac{1}{4}\ \frac{1}{4}\ \frac{1}{4}$ and 001 in the [113] direction.

From the data on the distribution of electron densities, certain estimates can be made of the ionic radii of indium and antimony ions. At the electron-density level of 0.5 el/Å^3, the ionic radius of antimony is 1.00 Å, and the ionic radius of indium is 1.05 Å. At the electron-density level of 0.25 el/Å^3, the ionic radius of antimony is 1.40 Å and that of indium is 1.40 Å. The obtained values of the ionic radii may be of considerable interest for the crystal chemistry of $A^{III}B^{V}$ compounds.

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