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OF CRYSTALS WITH CHALCOPYRITE LATTICE

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To cite this version:
Ju. Polygalov, A. Poplavnoi, A. Ratner. ANION SHIFT INFLUENCE ON BAND STRUCTURE
OF CRYSTALS WITH CHALCOPYRITE LATTICE. Journal de Physique Colloques, 1975, 36 (C3),
pp.C3-129-C3-135. <10.1051/jphyscol:1975324>. <jpa-00216294>

HAL Id: jpa-00216294
https://hal.archives-ouvertes.fr/jpa-00216294
Submitted on 1 Jan 1975

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ANION SHIFT INFLUENCE ON BAND STRUCTURE OF CRYSTALS WITH CHALCOPYRITE LATTICE

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Abstract. — In this paper we calculate the energy band structure of ZnSiAs$_2$, ZnSnAs$_2$, AgGaS$_2$, AgGaSe$_2$, AgGaTe$_2$ with and no account of anion displacements by the pseudopotential method. It is shown that account of the anion displacements leads to considerable changes in the energy band structure. In the approximation of rigid ions the constants of optical strain were calculated for the valency band top and for the bottom of conductivity band of crystals under consideration.

Results of a wide investigation of the band structure of ternary A$^{III}$B$^{IV}$C$_2$ and A$^{II}$B$^{III}$C$_2$ semiconductors with chalcopyrite lattice were given in studies [1, 2] and several reviews (e. g. [3] to [5]). The most interesting results on fine structure of band edges and some additional band extrema were obtained lately by the modulation spectroscopy method [4, 5]. This investigations turned out to be in a rather good agreement with theoretical calculations made by the pseudopotential method [3, 6, 7].

At the same time the precise investigations of the chalcopyrite crystal structure showed a number of peculiarities which distinguish this lattice from that of sphalerite. The differences are as follows (for the sake of brevity we shall speak of the compounds A$^{III}$B$^{IV}$C$_2$): 1) the substitution of atoms of groups III by those of groups II and IV of the Mendeleev periodic system, 2) the lattice compression in the direction of a tetragonal crystal axis, 3) the difference on the bond length of A$^{III}$-CV and B$^{IV}$-CV [2, 8 to 11]. On account of point, 3) the anion displacement from the lattice points of the face-centred sublattice takes place which is described by the parameter $x_f = 0.25 + \delta$.

The structure difference leads to the appearance of some disturbing terms in the band theory equation of the undisturbed structure A$^{II}$B$^{IV}$C$_2$. The compatibility relations for $T_2^4$ and $D_4^2$ group representations [12] enable us to determine a possible symmetry of these terms. They can be transformed by the representations $\Gamma_1$ and $\Gamma_{12}$ (the line $x^2 + y^2 - 2z^2$),

$$X_4 \left(0 \frac{2\pi}{a}, W_1 \left(\frac{2\pi}{a} \frac{0}{a} \frac{0}{a} \frac{0}{a} \right) \oplus W_1 \left(0 \frac{2\pi}{a} \frac{0}{a} \frac{a}{a} \right)\right)$$

of the group $T_2^4$. In the approximation when the crystal potential is built up as a superposition of spherically symmetrical atomic potentials it is not difficult to determine the symmetry of disturbing terms due to 1) to 3). Because of point 1) disturbing terms of $\Gamma_1$ and $\Gamma_{12}$ symmetry arise 2) gives the disturbance with the symmetry $\Gamma_1$, $\Gamma_2$, $X_4$ and $W_1$.

In the theoretical calculations of the energy band structure of A$^{III}$B$^{IV}$C$_2$ [3] and A$^{II}$B$^{III}$C$_2$ crystals [6, 7] the parameter $x_f$ was supposed to be equal to 0.25 due to the lack of reliable measurements. However, as the measurements [8 to 11] showed the parameter $\delta$ is not small in many cases. E. g., for CdSiP$_2$ the parameter $\delta = 0.052$ [10], and the difference between the Cd-P and Si-P bond lengths is $\sim 16\%$. These differences can effect on the spectrum structure, and for this reason while calculating one should take into account the real atom arrangement in a unit cell (Table I).
In accordance with the symmetry classification of disturbing terms it is reasonable to divide the chalcopyrite reciprocal lattice vectors into three groups:

1) the sphalerite reciprocal lattice vectors \( b_n, \) 
2) the vectors \( b_n(X) \) corresponding the vector \( (0, 2\pi / a) \) in the sphalerite star \( X, \) 
3) the vectors \( b_n(W) \) associated with the vectors \( (2\pi / a, 0, 0), (0, 2\pi / a, 0) \) of the star \( W. \)

Making use of 3 integers \( n, m, l \) these can be written down:

\[
b_n(I) = \frac{2\pi}{a} \left( n, m, \frac{l}{2} \right),
\]

\[
b_n(X) = \frac{2\pi}{a} \left( n, m, \frac{l}{2} \right), \quad \gamma = \frac{c}{a};
\]

\[
b_n(W) = \frac{2\pi}{a} \left( n, m, \frac{l}{2} \right), \quad l \text{ is odd, } n, m \text{ are even and odd respectively.}
\]

The Fourier coefficients of the crystal potential in the chalcopyrite lattice on the vectors (1) can be written in the form

\[
V(b_n, I) = 2 \left[ V_{ill}(b_n) + V_{iv}(b_n) + V_{il}(b_n) \exp \left[ -i \frac{\pi}{2} (n + m + l) \right] \right] \cos 2\pi n\delta + \cos 2\pi m\delta,
\]

\[
V(b_n, X) = \pm 2 V_{ii}(b_n) \cos 2\pi n\delta - \cos 2\pi m\delta \exp[i\pi(n + m + l)],
\]

\[
V(b_n, W) = \Delta V_n(b_n) \left\{ 2 \exp \left[ i\pi \left( m + \frac{1}{2} \right) \right] \exp \left[ i\pi \left( n + \frac{1}{2} \right) \right] \right\} +
\]

\[
+ 2 V_{ii}(b_n) (-1)^{(n + m + l/2)} \sin 2\pi m\delta \pm i \sin 2\pi n\delta \exp \left[ i\pi \frac{1}{2} (n + m + l/2) \right].
\]

Here \( V_{ii}(b_n), V_{iv}(b_n), V_{il}(b_n) \) are Fourier coefficients of the atomic potentials normalized on the chalcopyrite unit cell volume

\[
\Delta V_n(b_n) = \frac{1}{2} \left[ V_{ii}(b_n) - V_{iv}(b_n) \right],
\]

in (3) the sign \(+ + \) refers to the case when \( n \) and \( m \) are even and the sign \(- - \) to the case when \( n, m \) are odd; in (4) \(+ + \) refers to the case when \( n \) is odd and \( m \) is even, the sign \(- - \) refers to the opposite case. If in (2) to (4) we set \( \delta = 0, \) then \( V(b_n, X) \) will vanish.

The disturbance due to point 3) is localized on the anion sublattice and the Fourier coefficients produces nonvanishing on the vectors \( b_n(X) \) which are proportional to atomic formfactors \( V_{ii}(b_n) \) (the corresponding disturbing potential transforms by representation \( X_4(0, 2\pi / a, 0) \) of sphalerite). Besides, the term proportional to \( V_{ii}(b_n) \) is added to the Fourier coefficients on vectors \( b_n(W). \)

Consequently it is necessary to know the atomic formfactors \( V_{ii}(b_n) \) on much greater number of the chalcopyrite reciprocal lattice vectors than in case of calculation with \( x_f = 0.25 [3, 6, 7]. \) This imposes more severe requirements on the pseudopotential choice for cation sublattice atoms.

In this paper we calculate the energy band structure and study the spectrum dependence on the parameter \( x_f \) for two \( A^{III}B^{IV}C_{6}^{II} \) ZnSiAs\(_2\), ZnSnAs\(_2\) compounds and for three \( A^{III}B^{IV}C_{6}^{II} \) AgGaS\(_2\), AgGaSe\(_2\), AgGaTe\(_2\) compounds. The crystal potential of these compounds was constructed as a sum of spherically symmetrical atomic potentials through the lattice. The formfactors for different simple and binary diamond-type semiconductors were determined in a number of works from the experimental data [14, 15].

Since ternary compounds are the closest crystallographic analogs of the semiconductors \( A^{IV}, A^{III}B^{IV}, A^{III}B^{IV} \) in calculation of their crystal potential we used the atomic formfactors determined in [14 to 18].

The recalculation of the formfactors in terms of the chalcopyrite reciprocal lattice vectors and their renormalization was carried out according to the
The atomic formfactors of pseudopotentials in ZnSiAs₂, ZnSnAs₂, AgGaS₂, AgGaSe₂, AgGaTe₂.

The values are given in $R_p$.

<table>
<thead>
<tr>
<th>Sphalerite star</th>
<th>$b_n$</th>
<th>$V_{zn}$</th>
<th>$V_{si}$</th>
<th>$V_{as}$</th>
<th>$V_{zn}$</th>
<th>$V_{ag}$</th>
<th>$V_{ga}$</th>
<th>$V_{s}$</th>
<th>$V_{gs}$</th>
<th>$V_{se}$</th>
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<tr>
<td>$T$</td>
<td></td>
<td></td>
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<tr>
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<td>-0.021</td>
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<td>0.003</td>
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<td>-0.022</td>
<td>-0.011</td>
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<td>0.007</td>
<td>0.006</td>
<td>0.008</td>
<td>0.012</td>
<td>0.011</td>
<td>0.000</td>
<td>0.004</td>
<td>0.000</td>
<td>0.001</td>
<td></td>
</tr>
<tr>
<td>(304)</td>
<td>0.009</td>
<td>0.009</td>
<td>0.006</td>
<td>0.002</td>
<td>0.004</td>
<td>0.009</td>
<td>0.006</td>
<td>0.007</td>
<td>0.004</td>
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<tr>
<td>$X$</td>
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<tr>
<td>(130)</td>
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</table>

The crystal lattice parameters

<table>
<thead>
<tr>
<th>Compounds</th>
<th>$a$, Å</th>
<th>$2c$, Å</th>
<th>$c/a$</th>
<th>$\gamma$ (in the units of $\text{Å}_{\text{f}}$)</th>
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</thead>
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<tr>
<td>ZnSAs₂</td>
<td>5.606</td>
<td>10.890</td>
<td>1.94</td>
<td>0.269</td>
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<tr>
<td>ZnSnAs₂</td>
<td>5.852</td>
<td>11.703</td>
<td>2.00</td>
<td>0.231</td>
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<tr>
<td>AgGaS₂</td>
<td>5.74₃</td>
<td>10.2ₙ₆</td>
<td>1.7ₙ</td>
<td>0.2ₙ₁</td>
</tr>
<tr>
<td>AgGaSe₂</td>
<td>5.9ₙ₇₃</td>
<td>10.ₙ₈₉</td>
<td>1.ₙ₂</td>
<td>0.2ₙ₅</td>
</tr>
<tr>
<td>AgGaTe₂</td>
<td>6.2ₙ₈₃</td>
<td>1₁ₙ₄₉</td>
<td>1ₙ₃</td>
<td>0.2ₙ₀</td>
</tr>
</tbody>
</table>

The atom formfactors were taken from the following substances: for zink and arsenic in ZnSiAs₂ and ZnSnAs₂ from ZnSe and GaAs [14, 15], for tin in ZnSnAs₂ from $\alpha$-Sn [14, 15]. Silicon formfactors in ZnSiAs₂ were taken from paper [20], where they have been determined from experimental data for different silicon polytypes. In this paper the empirical formfactors $V_{si}(\Gamma)$ were determined for a great number of the vector lengths $\Gamma$ (about 70 values) and in a considerably wide range of values of $\Gamma$. Therefore, while calculating $V_{si}(\Gamma)$ the usage of graphic interpolation becomes possible. Ga formfactors were taken from GaP for AgGaS₂ and from GaAs for AgGaSe₂ and AgGaTe₂. The pseudopotentials of S, Se, and Te for AgGaS₂, AgGaSe₂, AgGaTe₂ were determined from the compounds SnS₂, SnSe₂ [17]; ZnTe [18], respectively. The pseudopotential of Ag was taken from [16]. Since in [16] the formfactors were determined for the value $|\Gamma| < 2 K_F$ we carried out the extrapolation according to [7] in the longer.

The atom formfactors determined by the above method are given in table II.

The calculation of the energy band structure was carried out at the symmetrical points $\Gamma$, $T$, and $N$ of the Brillouin zone, and about 170 plane waves were taken into account in expanding of the pseudo-wave function. In calculations the parameters of crystalline lattices [1, 2, 11] given in table III were used.

To study the energy band structure dependence on the value of the anion shift the calculations at different values of $\delta$ were performed. In figure 1 the width of forbidden band the value of crystalline splitting and some most important energy levels in ZnSiAs₂ and ZnSnAs₂ as functions of $\delta$ are represented. In the figure 1 the levels belonging to the valency band are labelled by «v» and those to the conduction band by «c». The zero of energy scale is chosen at the valency band top $E_{v}(\Gamma_4)$ at the experimental values of $\delta$.

The energy spectrum dependence upon $|\delta|$ for AgGaS₂, AgGaSe₂, AgGaTe₂ in many respects is similar to the one which is observed for ZnSnAs₂, as all these semiconductors have a direct energy gap.

In all semiconductors under consideration the value $\delta$ changes with the growth of the parameter $|\delta|$. In ZnSnAs₂, AgGaS₂, AgGaSe₂, AgGaTe₂ this is due to the rise of the levels $r_4$ and $r_5$ at valency band top. The level $r_4$ turns out to rise slower than that of $r_5$. The bottom of the conductivity band ($\Gamma_4$) practically does not change in these crystals as $\delta$ changes. This can be easily explained by the fact that the level $r_4(c)$ is placed at considerable distance from both the valency and conductivity band levels, and it weakly interacts with these after switching on the disturbing terms of 1), 2) and 3).

The $\delta$ dependence of the energy band edges in ZnSiAs₂ turns out to be somewhat different (see Fig. 1). This is the result of the differences in the nature of the conductivity band bottom in ZnSiAs₂ (crystal with pseudo-direct energy gap [4]) and...
The dependence of the most important parameters of the energy structure of ZnSiAs$_2$, ZnSnAs$_2$ versus the value of anion shift.

For the same reason the value $E_g$ in ZnSiAs$_2$ increases and in ZnSnAs$_2$, AgGaS$_2$, AgGaSe$_2$, AgGaTe$_2$ it decreases with the growth of $|\delta|$.

The dependence of the additional maxima of the valency band top at the points $T$ and $N$ of the Brillouin zone upon the value of anion displacement is of interest. The additional maximum at the point $T$ grows in all the semiconductors under consideration and, in particular, in ZnSiAs$_2$ at the experimental value of $\delta$, and the maximum $T_3 \oplus T_4$ turns out to be competing with the valency band top. The additional maximum at the point $N$ in ZnSiAs$_2$ essentially does not change with $\delta$, but it slowly grows in ZnSiAs$_2$ (Fig. 1). In AgGaS$_2$ with increasing of $\delta$ to the experimental value 0.041 the level $N_4$ rises on 0.20 eV, while the level $T_4$ rises on 0.50 eV. In AgGaSe$_2$ the level $N_4$ varies very weakly (within 0.01 eV) and in AgGaTe$_2$ it falls with $\delta$ at approximately the same rate at which this level grows in AgGaS$_2$. The calculated energy band structure of ZnSiAs$_2$, ZnSnAs$_2$, AgGaS$_2$ at the experimental values of $\delta$ is illustrated in figures 2, 3, 4 respectively. Since no reliable experimental values of $\delta(x_f)$ for AgGaSe$_2$ and AgGaTe$_2$ are known, figures 5 and 6 give the calculated energy structures for these crystals at $\delta = 0$ ($x_f = 0.25$).

It is interesting to note that in all the crystals except AgGaTe$_2$ at both $\delta = 0$ and $\delta \neq 0$ (in the range of the experimental values of this value [8 to 11]) the valency band top is placed in the centre of the Brillouin zone (level $\Gamma_4$). In AgGaTe$_2$ at $\delta = 0$ the top of the valency band is at the point $N$ and the additional maximum at $\Gamma$. The levels $T_4$ and $\Gamma_4$ at the point $\Gamma$ rise and the level at $N$ falls with $\delta$ so that at $\delta \approx 0.027$ they coincide. At further growth of $\delta$ the level $T_4$ turns out to be upper and becomes, an additional maximum. Thus, in AgGaTe$_2$ the anion displacement can produce the rearrangement of the valency band top structure.
The possibility of rearrangement of the valency band top in $A'B^{III}C^{VI}$ due to the anion displacement is of great interest. The calculations of the band structure for several crystals we carried out with $x_f = 0.25$ showed the valency band top in these semiconductors to have a complicated structure. In $CuGaS_2$, $Se_2$, $Te_2$, $AgInS_2$, $AgGaS_2$, $Se_2$, with calculated value $E_g \approx 2$ eV the valency band top turns out to be at the point $\Gamma$ and the nearest additional maximum at the point N. In $CuInS_2$, $Se_2$, $Te_2$, $AgInS_2$, $Se_2$, $Te_2$, $AgGaTe_2$ where the calculated value $E_g$ at the point $\Gamma$ is of $\sim 1$ eV.

The valency band top is at the point N. In the compounds where the valency band top is at N the edge of the fundamental absorption is to be non-direct. Besides, the value of $E_g$ obtained from electrical and photoelectrical properties and from electroreflection experiment are to be different. This conclusion, however, is not confirmed by experimental data [5]. In addition, as was noted in [5] the calculated values $E_g$ for $A'B^{III}C^{VI}$ are consistently higher than the experimental data to explain these discrepancies of theory and experiment.

A supposition is made in [5], that the band structure of the $A'B^{III}C^{VI}$ crystals is very sensitive to the d-electrons of noble metals. Small value of the spin-orbit splitting in these compounds as compared with that of their analogs is also explained by the influence of d-electrons on the valency band top [5]. Our results enable to put forward another possible explanation of the above discrepancies: the rearrangement of the valency band top and the decrease of $E_g$ are effected by displacements of anions from the lattice points of the face-centred cubic sublattice.

The anion shifts which do not vary the crystal lattice symmetry correspond to the optical vibrations with symmetry $f_1$ of group $D_{3d}^{12}$ [21]. The intra-valley scattering of charge carriers at the zeroth order in the wave vector $K$ takes place on this mode. The intravalley scattering on the optical phonons with symmetry different from that of $f_1$ occurs in higher orders in $K$ [21]. Since the mode of symmetry $f_1$ is nonpolar the relaxation time can
be evaluated by the deformation potential method [22]. The optical deformation potential for the oscillation \( \Gamma \), can be written as \( D \cdot \xi \), where \( \xi \) is a relative displacement of an anion atom, \( D \) is the shift value of the corresponding energy level per unit displacement. The calculation carried out by the authors allows to estimate the constant \( D \) in the rigid ion model. The results of these estimations are listed in table IV.

Up to now no experimental data on the contribution of the nonpolar optical scattering to the relaxation times of charge carriers in \( A^I B^{IIV} C^{VI}_2 \) and \( A^I B^{II} C^{VI}_2 \) are available. Therefore, we can compare our estimations of the constant \( D \) with the data available for germanium of n- and p-type [22].

The value of \( D \) for n-Ge obtained from various experimental data is in the range (4-9) \( 10^8 \) eV/cm; in p-Ge that is one order higher. Hence, one can conclude that the scattering of the nonpolar optical oscillation in n-ZnSnAs\(_2\) and n-A\(^I\)B\(^II\)C\(^VI\)_2 is two orders of magnitude lower than in n-Ge, and in n-ZnSiAs\(_2\), one order of magnitude lower. Scattering

**TABLE IV**

<table>
<thead>
<tr>
<th>Compounds</th>
<th>ZnSiAs(_2)</th>
<th>ZnSnAs(_2)</th>
<th>AgGaS(_2)</th>
<th>AgGaSe(_2)</th>
<th>AgGaTe(_2)</th>
</tr>
</thead>
<tbody>
<tr>
<td>( D ) (conductivity band)</td>
<td>0.3 + 0.5</td>
<td>0.05</td>
<td>0.5</td>
<td>0.9</td>
<td>0.6</td>
</tr>
<tr>
<td>( D ) (valency band)</td>
<td>1 + 2</td>
<td>2 + 4</td>
<td>4</td>
<td>2 + 3</td>
<td>1 + 2</td>
</tr>
</tbody>
</table>
in p-ZnSiAs₂, p-ZnSnAs₂, p-A'BIC₂Y is one order weaker than in p-Ge. The smaller value of the deformation potential constant for nonpolar optical scattering in A'BIC₂Y and A'B'IC₂/Y₂ is due to the fact that in the vibrations of symmetry Γ', the atoms of one sublattice take part, while in A'V semiconductors the atoms of both sublattices take part in the optical vibrations.

References