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CONDENSON STATES DYNAMICS IN THE LAYERED CRYSTALS OF THE INDIUM SELENIDES UNDER ELASTIC DEFORMATIONS

The conditions of self-consistent localized state formation connected with the interaction between an electron and the longitudinal acoustic phonon in the In_4Se_3 and $\beta\text{-InSe}$ crystals have been investigated. In the consequence of studying of the deformation influence on the dispersion law with the low-energy non-parabolicity the evolution of appearance or disappearance of the condenson states have been established. The main characteristics such as binding energy and localization radii of the condenson states are determined.

Keywords: indium selenides, dispersion law with low-energy non-parabolicity, homogeneous deformation, condenson states

1. Introduction

As it is known [1-3], the interaction between an electron and the longitudinal acoustic phonon in the homopolar crystals leads to the formation of self-consistent localized state called as condensons. The dispersion law is crucial in the phenomena of the charge carrier localization. For the first time we have shown that the charge inhomogeneity in the form of the “multicondenson drops” (early it was possible for only the one-dimensional materials) is realized in the layered In_4Se_3 crystal owing to its dispersion law with low-energy non-parabolicity and peak-like density of states of $E^{-1/4}$ type [4,5]. Today, the developed by us condenson state

concept for the In_4Se_3 crystal is used [8,9] for the explanation of its unique high thermoelectric figure of merit [10]. Considering the thermoelectric properties of the In_4Se_3 [8, 9] we experimentally corroborate the existence of the condenson states in this crystal. With results obtained in works [8, 9] it can be concluded that formation of the condenson state can be controlled by cationic (Sn) and anion (Te) substitution too.

It is of interest to investigate the charge carrier localization phenomenon in other InSe layered crystal where accordingly to our simulation [6, 7] its band structure can be considered as initial to the band structure of In_4Se_3 . As it follows from *ab initio* calculations of the energy spectra under pressure [6], the

shape of the top of the valence band of deformed β -InSe resembles the shape of the valence and conduction bands of the In_4Se_3 crystal in the k_x - direction of the Brillouin zone, that it is the result of an increase of negative coefficients of the squared power terms and the possible decrease of the coefficients of the four power terms of the k -vector components. Therefore, from this point of view, it is of interest to study the dynamics of the inhomogeneous states of the condensation type, their appearance or disappearance which connected with intensification or weakening of the low-energy non-parabolicity of the dispersion law owing to deformation induced by the external factors. In the second section of our work, the theory of the condensation state in In_4Se_3 crystal will be present. Investigation of the impact of deformation effects on the low-energy non-parabolicity of the dispersion law

and the condition of the condensation state formation are given in section 3. In section 4, investigation of the condensation states in the β -InSe crystal is shown. We summarize our results in section 5.

2. Theory of condensation states in the 3D – In_4Se_3 layered crystal

A crystal In_4Se_3 , in which it was founded the condensation related thermoelectric properties [8, 9], has the complicated structure composed of one-dimensional chains of In and non-flat warped two-dimensional ion-covalent layers In – Se [11, 12].

The dispersion law with the additional four power terms of the wave vector [4-6, 13], which describes the dispersion dependences in the vicinity of the forbidden energy gap (Fig.1a), has the form:

$$E(\vec{k}) = Ak_x^2 + Bk_y^2 + Ck_z^2 + A_1k_x^4 + B_2k_y^4 + C_3k_z^4 \quad (1)$$

Here quadratic term coefficients A, B, and C have the negative values.

Using equation (1), the especial condensation state in the framework of theory developed by Dejgen and Pekar [1] in this 3D-crystal was theoretically predicted. The condensation state is a kind of a polaron state,

where a conduction electron is localized in the region deformed by itself due to the deformational interaction between the electron and acoustic phonons. As it was shown in the continual and deformation potential approaches [4, 5] the energy functional can be written as

$$E(\Psi) = E_0(\Psi) - \tilde{A} \int |\Psi|^4 d^3\vec{r}, \quad (2)$$

Where

$$E_0(\Psi) = \int \left[A \left(\frac{\partial \Psi}{\partial x} \right)^2 + B \left(\frac{\partial \Psi}{\partial y} \right)^2 + C \left(\frac{\partial \Psi}{\partial z} \right)^2 \right] d^3\vec{r} + \int \left[A_1 \left(\frac{\partial^2 \Psi}{\partial x^2} \right)^2 + B_1 \left(\frac{\partial^2 \Psi}{\partial y^2} \right)^2 + C_1 \left(\frac{\partial^2 \Psi}{\partial z^2} \right)^2 \right] d^3\vec{r} \quad (3)$$

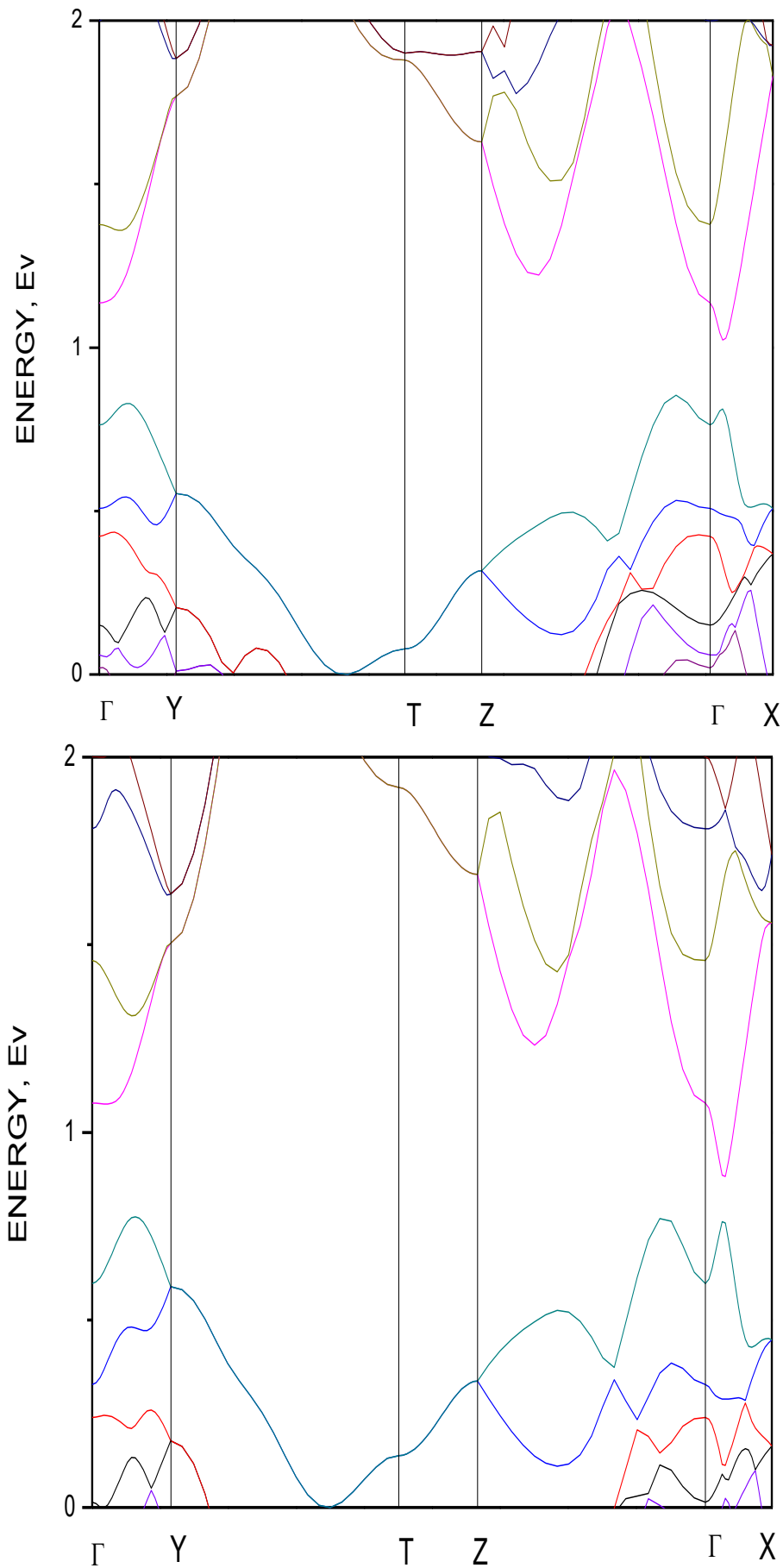


Fig.1. Energy structure fragments in the vicinity of the energy gap for the undeformed In_4Se_3 and for In_4Se_3 under pressure.

determines the kinetic energy of the charge carriers, the parameter \tilde{A} describes the electron-phonon interaction through the

deformation potential [4, 5]. At the checking of the probe function in the form:

$$\Psi(r) = \left(\frac{\mu\sqrt{2}}{(a_1 a_2 a_3)^{1/3}} \right)^{3/2} \exp \left[-\pi\mu^2 \left[\left(\frac{x^2}{a_1} \right)^2 + \left(\frac{y^2}{a_2} \right)^2 + \left(\frac{z^2}{a_3} \right)^2 \right] \right] \quad (4)$$

expression (2) leads to the appearance of the localized condensation states in the In_4Se_3

crystal. Localization radii r_c of these states are determined from the relationship:

$$\pi\mu \left(\frac{x^2}{a_1^2} + \frac{y^2}{a_2^2} + \frac{z^2}{a_3^2} \right)_{min} \quad (5)$$

Here a_1, a_2, a_3 are the lattice parameters, μ_{min} is a dimensionless variational parameter at which $E(\mu)$ has a minimum. The dispersion law coefficients and the electron-phonon interaction parameter insert the main contribution in μ_{min} and $E(\mu)$ correspondingly.

Our investigations of the band structures for the In_4Se_3 crystals indicate on the transformation of both the conduction band and valence band under pressure (Fig.1, b). In this case, in the next paragraph of our work, we will analyze the effect of the transformation of the dispersion law non-parabolicity under elastic deformation on the parameters of the condensation states in the In_4Se_3 crystal.

3. Impact of deformation effects on the low-energy non-parabolicity of the dispersion law and the condition of the condensation state formation in the In_4Se_3 crystal

It is noted that our first investigation of the deformation influence (namely, shear strain) on the dispersion law of the charge carriers in the vicinity of the energy gap for the In_4Se_3 crystal were carried out in [7, 15]. In the framework of the group-theoretical analysis together the Pikus' method of invariants [16] for the model of interacting bands in In_4Se_3 it was shown [7, 15], that the parabolic dispersion law in the $k_z (k_y)$ direction at the presence of the shear strains of ε_{xz} and ε_{xy} type ($\sim k^2$) which are non-diagonal components of the secular matrix $D(\vec{k}, \vec{\varepsilon})$, transformed into dispersion law with the low-energy non-parabolicity, that is favorable for the realization of the condensation states. We also have shown [17] that with taking into consideration of the uniaxial strain the tensor components $\varepsilon_{xx}, \varepsilon_{yy}$ and ε_{zz} can be led to the change of already existed low-energy non-parabolicity of the dispersion law of electrons and holes of the In_4Se_3 crystal:

$$E(\vec{k}, \varepsilon) = E_0 + Ak_x^2 + Bk_y^2 + Ck_z^2 + A_1k_x^4 + B_1k_y^4 + C_1k_z^4 + b_{xx}\varepsilon_{xx} + b_{yy}\varepsilon_{yy} + b_{zz}\varepsilon_{zz} \quad (6)$$

To determine the components of the dispersion law (6) and deformation potential tensor components b_{ij} the calculations of the band structure of both the undeformed and deformed In_4Se_3 crystal was performed by us.

As it is known, the additional potential energy is obtained from the comparison of the energies corresponding to the initial localization of the conduction band minimum and the valence band maximum and their localization after crystal stresses:

$$E(P) = E_0 + \sum_{i,j} b_{ij}^n \varepsilon_{ij} \quad (7)$$

The dispersion law coefficients (6), obtained by means of the approximation method of the dispersion relations in the vicinity of the main extreme of the conduction and valence bands

in the Γ -X, Γ -Y and Γ -Z directions of the Brillouin zone, and calculated deformation potentials in the Tables 1 and 2 are presented.

Table 1

Parameters of the dispersion law (6) for undeformed and deformed In_4Se_3 crystal

Γ -X		Γ -Y		Γ -Z	
$A_v, eV \cdot \text{\AA}^2$	50.896	$B_v, eV \cdot \text{\AA}^2$	15.155	$C_v, eV \cdot \text{\AA}^2$	8.0284
A_c	-109.307	B_c	7.455	C_c	19.039
$A_{1v}, eV \cdot \text{\AA}^4$	-16562.624	$B_{1v}, eV \cdot \text{\AA}^4$	-1040.081	$C_{1v}, eV \cdot \text{\AA}^4$	-212.060
A_{1c}	26143.619	B_{1c}	452.512	C_{1c}	-110.786
ε_{xx}					
$A_v, eV \cdot \text{\AA}^2$	41.737	$B_v, eV \cdot \text{\AA}^2$	13.696	$C_v, eV \cdot \text{\AA}^2$	7.678
A_c	-101.432	B_c	8.985	C_c	19.708
$A_{1v}, eV \cdot \text{\AA}^4$	-14901.927	$B_{1v}, eV \cdot \text{\AA}^4$	-1053.350	$C_{1v}, eV \cdot \text{\AA}^4$	-201.482
A_{1c}	25002.791	B_{1c}	390.281	C_{1c}	-122.319
ε_{yy}					
$A_v, eV \cdot \text{\AA}^2$	37.777	$B_v, eV \cdot \text{\AA}^2$	11.098	$C_v, eV \cdot \text{\AA}^2$	5.242

A_c	-104.734	B_c	5.736	C_c	17.325
$A_{1v}, eV \cdot \text{Å}^4$	-14967.350	$B_{1v}, eV \cdot \text{Å}^4$	-897.879	$C_{1v}, eV \cdot \text{Å}^4$	-172.166
A_{1c}	25912.379	B_{1c}	552.432	C_{1c}	-99.321
ε_{zz}					
$A_v, eV \cdot \text{Å}^2$	66.645	$B_v, eV \cdot \text{Å}^2$	16.305	$C_v, eV \cdot \text{Å}^2$	9.097
A_c	-115.848	B_c	6.038	C_c	18.473
$A_{1v}, eV \cdot \text{Å}^4$	-18634.322	$B_{1v}, eV \cdot \text{Å}^4$	-1028.489	$C_{1v}, eV \cdot \text{Å}^4$	-232.799
A_{1c}	26639.291	B_{1c}	474.299	C_{1c}	-88.287

Table 2

 Deformation potentials for the In₄Se₃ crystal

b_{xx}^v, eV	b_{xx}^c, eV	b_{yy}^v, eV	b_{yy}^c, eV	b_{zz}^v, eV	b_{zz}^c, eV
-0.242	0.190	2.870	0.916	-2.396	-1.585

Table 3

 Condensation parameters for undeformed and deformed In₄Se₃ crystal

	$\varepsilon = 0$	ε_{xx}	ε_{yy}	ε_{zz}
E_b, eV	-0.021	-0.017	-0.021	-0.026
$r_c^0, \text{Å}$	128.0	133.5	128.3	122.8
μ_{\min}	0.040	0.038	0.040	0.042

In a consequence of the performed calculations, it was founded that the coefficients of both quadratic and four power

terms of the k -vector components in the dispersion law (6) for electrons and holes under uniaxial deformations essentially

change. Besides the decrease of the displaced extreme depth for the conduction band in the Γ -X direction under uniaxial stresses along [100] and [010] directions and the enhancement of the extreme depth along [001] take place.

Using obtained coefficients, in the framework of the continuum and deformation potentials approaches on the basis of relationships (2)-(5) and (6) we determined the parameters of condenson states (see Table 3).

4. Investigation of the condenson states in the β -InSe crystal

As it follows from our earlier investigations [6], dispersion law with the four power terms of the k -vector components is not a unique one which characterizes only the In_4Se_3 crystal. Dispersion law with low-energy non-parabolicity and the abnormal anisotropy takes place in the deformed InSe crystal for β and γ - modifications too [6,18-21]. In [5] we performed the calculations of the band

structure of both the undeformed and deformed β -InSe crystal and obtained the analytical dependence of the type (1) which describes the dispersion relations in the vicinity of the energy gap along main Γ -K, Γ - M and Γ -A directions in Brillouin zone of the hexagonal system. It was shown [6] the low-energy non-parabolicity in the β -InSe crystal under hydrostatic pressure becomes more expressively similar to one in the In_4Se_3 crystal. It suggests the similarity of the dispersion laws for charge carriers in the In_4Se_3 and in the deformed γ -InSe and β -InSe crystals. Such dispersion law allows us to produce the specific condenson states due to the electron-phonon interaction in the β -InSe layered crystal.

The dispersion relation in the form (1) for the β -InSe layered crystal is confirmed too by the means of the investigations of the dispersion law in the vicinity of the Brillouin zone center in the framework of the Pikus' method of invariants [16]:

$$E(\vec{k}, \varepsilon) = E_0 + A(k_x^2 + k_y^2) + Bk_z^2 + C(k_x^2 + k_y^2)^2 + Dk_z^4 + a(\varepsilon_{xx} + \varepsilon_{yy}) + b\varepsilon_{zz} \quad (8)$$

The obtained coefficients of the dispersion law and the values for the

parameters of deformational potentials in Tables 4, 5 are presented.

Table 4.

Dispersion law parameters for undeformed and deformed β -InSe crystal [17, 22]

Γ -A		Γ -M	
$B_v, eV \cdot \text{\AA}^2$	-64.696	$A_v, eV \cdot \text{\AA}^2$	-2.322
B_c	61.069	A_c	27.348
$D_v, eV \cdot \text{\AA}^4$	4501.849	$C_v, eV \cdot \text{\AA}^4$	-5.179

D_c	-4515.058	C_c	-262.789
ε_{xx}			
$B_v, eV \cdot \overset{0}{A^2}$	-69.639	$A_v, eV \cdot \overset{0}{A^2}$	-1.898
B_c	66.223	A_c	30.907
$D_v, eV \cdot \overset{0}{A^4}$	5564.173	$C_v, eV \cdot \overset{0}{A^4}$	-17.549
D_c	-5561.285	C_c	-264.913
ε_{zz}			
$B_v, eV \cdot \overset{0}{A^2}$	-62.428	$A_v, eV \cdot \overset{0}{A^2}$	-1.849
B_c	58.930	A_c	39.872
$D_v, eV \cdot \overset{0}{A^4}$	4104.599	$C_v, eV \cdot \overset{0}{A^4}$	-31.758
D_c	-4121.515	C_c	-451.889

Table 5

Deformation potentials for the β -InSe layered crystal

b_{xx}^v, eV	b_{xx}^c, eV	b_{zz}^v, eV	b_{zz}^c, eV
1.087	7.049	-14.298	-3.326

In considered case of the interaction between an electron and the longitudinal acoustic

phonon and using of the dispersion law (8) the energy functional can be written as

$$\begin{aligned}
 E_0[\Psi, u] = & \int \left[A \left(\left(\frac{\partial \Psi}{\partial x} \right)^2 + \left(\frac{\partial \Psi}{\partial y} \right)^2 \right) + B \left(\frac{\partial \Psi}{\partial z} \right)^2 \right] d^3 \vec{r} + \int \left[C \left(\left(\frac{\partial^2 \Psi}{\partial x^2} \right)^2 + \left(\frac{\partial^2 \Psi}{\partial y^2} \right)^2 \right) + D \left(\frac{\partial^2 \Psi}{\partial z^2} \right)^2 \right] d^3 \vec{r} + \\
 & + \int \left[2C \left(\frac{\partial^2 \Psi}{\partial x^2} \right) \left(\frac{\partial^2 \Psi}{\partial y^2} \right) \right] d^3 \vec{r} + \int \sum_{ij} b_{ij} u_{ij} |\Psi|^2 d^3 \vec{r} + \frac{1}{2} \sum_{ijkl} C_{ijkl} \varepsilon_{ij} \varepsilon_{kl} \quad (9)
 \end{aligned}$$

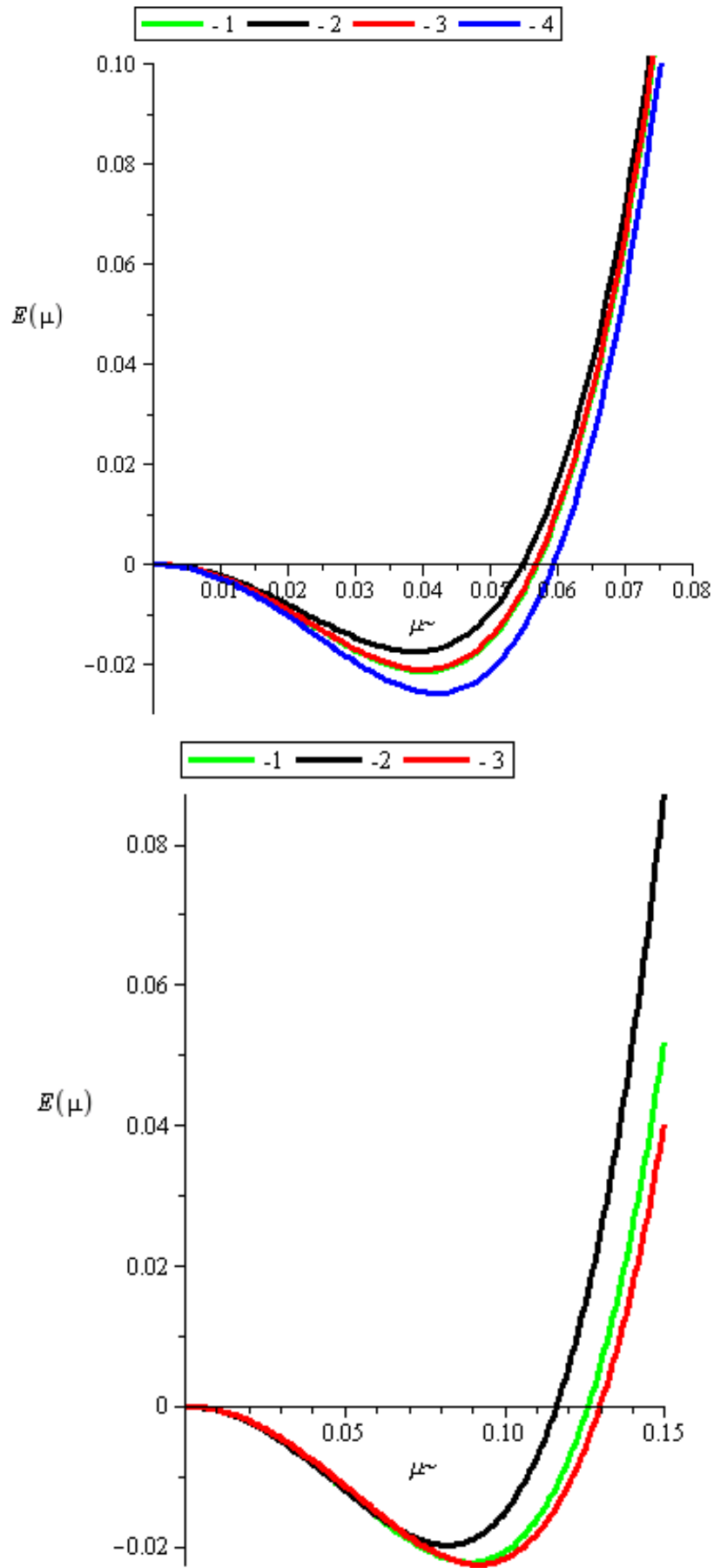


Fig.2. Functional dependences $E(\mu)$ for the undeformed and deformed In_4Se_3 and $\beta\text{-InSe}$ crystals.

Substituting the parameters A , B , C and D of the dispersion law from the Tabl. 4 in the equations (9), we obtain the condensation parameters for the β -InSe crystal (Table 6). Here the integration in (9) is performed over the Brillouin zone for the hexagonal lattice. For this purpose, we adapt the following values of the elastic tensor components: $C_{11} = C_{22} = 73.0$ GPa, $C_{12} = 27.0$ GPa, $C_{13} = 30.0$ GPa, $C_{33} = 36.0$ GPa [23].

As it follows from our evaluations the condensation states (“electron + lattice

deformation”) are not formed at given parameters of the dispersion law (8). However, the localized states of “hole+lattice deformation” type can be realized in the β -InSe crystal (Fig 2b).

The dependences for the localized electron energy for In_4Se_3 crystal (Fig. 2a) and the localized holes energy for InSe (Fig. 2b) versus the variational parameter μ have the forms.

Table 6

Localized states parameters for the holes in undeformed and deformed β -InSe crystal

	$\varepsilon = 0$	ε_{xx}	ε_{zz}
E_b, eV	-0.022	-0.0198	-0.023
$r_c^0, \text{\AA}$	41.21	44.71	40.10
μ_{\min}	0.089	0.082	0.092

Thus, as it follows from Tables 3 and 6, binding energy E_b for the condensons changes in dependence on uniaxial deformations. More stable condensation states in the In_4Se_3 crystal occur in the presence of the stress along the strong bond (at ε_{zz}). On the contrary, the binding energy decrease at the action of the uniaxial stress along the weak bond [100] (normally to the layers) that can be led to the disappearance of the condensation states. In the β -InSe crystal the binding E_b is smaller in the presence of the axial deformations along the Γ -M direction. The radii r_c of the condensation state localization are bigger for In_4Se_3 than for β -InSe crystal.

5. Conclusion

Basing on the first-principles

calculations of the band structures under the pressure effect for the layered crystals of the indium selenides, characterized by unusual dispersion with the low-energy non-parabolicity, one concludes that the existing potential relief in both the conduction and valence bands for the In_4Se_3 and β -InSe crystals can be changed owing to the insignificant stresses when the spectrum transformation is observed. In favor of later there are testified the valuations of the coefficients of the quadratic and four power terms of the wave vector components in the dispersion laws (6) and (8) for the electrons and holes, and also the calculations of the effective masses [17, 22] and the main characteristics (binding energy and localization radii) of the condensation states under elastic deformation.

Thus, our obtained results show that the charge inhomogeneity regions in the form of

the condensation, which takes place in the In_4Se_3 and $\beta\text{-InSe}$ three-dimensional semiconductors can be changed in the presence of the stresses. It explains why in the undeformed $n\text{-InSe}$ hexagonal crystal, where according to our investigations the condensation states are not realized, the high thermoelectric efficiency similar to the In_4Se_3 crystal [24] has been not achieved. However, as it follows from [24], the increase of the dimensionless figure of merit for the heterostructure $\text{InSe}/\text{In}_4\text{Se}_3$ was discovered owing to the essential decrease of

the thermal conductivity. In our opinion this fact can be connected with the charge carriers scattering on the self-consistent localized states. One waits that the lattice mismatch strains can appear in the result of the formation of this heterostructure. It leads to the significant changing of the electron structure and to the occurrence of the favorable conditions for the condensations accordingly. Our studies can be useful for the question solution of the further enhanced thermoelectricity in the indium selenides.

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ДИНАМИКА КОНДЕНСОННЫХ СОСТОЯНИЙ В СЛОИСТЫХ КРИСТАЛЛАХ СЕЛЕНИДА ИНДИЯ ПРИ УПРУГИХ ДЕФОРМАЦИЯХ

Исследованы условия возникновения самосогласованных локализованных состояний, обусловленных взаимодействием электронов с деформацией решетки, в селенидах индия In₄Se₃ и β -InSe и проанализировано влияние на них упругих деформаций. В результате установлена эволюция появления или исчезновения конденсонных состояний и определены их основные характеристики (энергию связи и радиус конденсона).

Ключевые слова: Селениды индия; Закон дисперсии с низкоэнергетической непараболичностью; Упругая деформация; Конденсонные состояния

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ДИНАМІКА КОНДЕНСОННИХ СТАНІВ У ШАРУВАТИХ КРИСТАЛАХ СЕЛЕНІДУ ІНДІЮ ПРИ ПРУЖНИХ ДЕФОРМАЦІЯХ

Досліджено умови виникнення самоузгоджених локалізованих станів, зумовлених взаємодією електронів з деформацією ґратки, в селенідах індію In_4Se_3 і $\beta\text{-InSe}$ та проаналізовано вплив на них пружних деформацій. У результаті встановлена еволюція появи або зникнення конденсонних станів і визначені їхні основні характеристики (енергію зв'язку та радіус конденсона).

Ключові слова: Селеніди індію; Закон дисперсії з низькоенергетичною непараболічністю; Пружна деформація; Конденсонні стани

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