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Electron-phonon interaction in ternary mixed crystals of zinc compounds

J. H. HOU*

College of Physics and Information Engineering, Shanxi Normal University, Linfen 041004, China

The electron-phonon interaction in ternary mixed crystal of zinc compounds is studied. The electron-phonon interaction Hamiltonian including the unit-cell volume variation in ternary mixed crystals is obtained by using the modified random element isodisplacement model and Born-Huang method. The polaronic self-trapping energy and renormalized effective mass of $ZnSe_xTe_{1-x}$, ZnS_xSe_{1-x} and ZnS_xTe_{1-x} compounds are numerically calculated. It is confirmed theoretically that the nonlinear variation of the self-trapping energy and effective mass with the composition is essential and the unit-cell volume effects cannot be neglected except the week e-p coupling. The deducting dimension of the mixed crystal strengthening the nonlinearity and volume effects.

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1. Introduction

Due to the parameters, such as the band-gap energy and the optical-phonon frequency, can be controlled by the composition ratio x. The mixed crystals are very important materials for many electronics and photo electronic devices. Then the lattice dynamics of ternary mixed crystals (TMCs) has been maintained interests in the past decades [1-7].

As was known, the electron-phonon (e-p) interaction is also very important in determining the electronic and optical properties of TMC systems. The characteristics of phonon mode in TMCs are different from those in binary crystals [1]. There are two branches of phonon frequency for either longitudinal optical (LO) or transverse optical (TO) modes in TMCs. The electron-phonon coupling of the two branches of LO modes has been investigated and the corresponding e-p interaction Hamiltonian has also been derived [8-10].

It has been confirmed that the obvious nonlinearity of the polaronic energy and effective mass varying with the composition ratio of the TMCs have been found in the previous work [9-11]. The unit-cell volume effects cannot also be neglected except for the weak e-p coupling TMCs.

In this paper, we provide a comparision of the electron–optical-phonon interaction in three dimensional (3D), two dimensional (2D) and one dimensional (1D) mixed crystals, and the effect of unit-cell volume variation will be taken into account. The Fröhlich-like Hamiltonians for the e-p interaction are obtained with the effect of the unit-cell volume variation. The compositional dependence results of the polaronic self-trapping energies and normalized effective masses in zinc TMC systems are numerically performed.

2. 3D, 2D and 1D e-p interaction Hamiltonians

The e-p interaction in $A_xB_{1-x}C$ type of 3D TMC compounds had been considered based on modified random-element-isodisplacement (MREI) model and Born and Huang theory [11-13]. Two branches of LO phonon modes coupling with electrons were recognized in the TMC system, whose frequencies were determined as

$$\omega_1^2 = \frac{-\left(b'_{22}+b'_{11}\right)+\sqrt{\left(b'_{22}-b'_{11}\right)^2+4b'_{12}b'_{21}}}{2}, \tag{1a}$$

$$\omega_2^2 = \frac{-\left(b'_{22}+b'_{11}\right)-\sqrt{\left(b'_{22}-b'_{11}\right)^2+4b'_{12}b'_{21}}}{2}. \tag{1b}$$

The above dynamical coefficients $b'_{ij} \quad \left(i, j=1,2,3\right)$ and related parameters had been listed in Refs. [14] and [15].

A Fröhlich-like Hamiltonian for the electron coupling with the two branches of LO-phonon modes in the 3D TMC system had been derived in ref. [10]

$$H_I = \sum_{n,\vec{k}} G^*_{n\vec{k}} e^{-i\vec{k}\cdot\vec{r}} a^\dagger_{n\vec{k}} + h.c., \tag{2}$$

where

$$\left|G_{n\bar{q}k_z}\right|^2 = \frac{e^2}{Vk^2}\left(\frac{\hbar}{2\omega_{nL}}\right) \cdot \left(\frac{1}{T_{11}+2B_nT_{12}+B_n^2T_{22}}\right)\left(\frac{b_{31}+B_nb_{32}}{\varepsilon_0+b_{33}}\right)^2. \tag{2a}$$

The n = 1 and 2 corresponding respectively the higher and lower frequency of the LO-phonon branches. The parameters Bs are represented as following

$$B_1 = -\frac{T_{12}b'_{21} + T_{11}\left(b'_{11} + \omega_{1L}^2\right)}{T_{11}b'_{12} + T_{12}\left(b'_{22} + \omega_{1L}^2\right)}\ , \qquad (3a)$$

$$B_2 = -\frac{T_{12}b'_{21} + T_{11}\left(b'_{11} + \omega_{2L}^2\right)}{T_{11}b'_{12} + T_{12}\left(b'_{22} + \omega_{2L}^2\right)}\ . \qquad (3b)$$

here the matrix elements T_{ij} can be found in ref. [16].

The e-p system Hamiltonian in 3D TMCs can finally be obtained as

$$H = \frac{p^2}{2m} + \sum_{n,\vec{k}} \hbar\omega_{nL} a_{n\vec{k}}^{\dagger} a_{n\vec{k}} + \sum_{n,\vec{k}} G_{n\vec{k}}^{*} e^{-i\vec{k}\cdot\vec{r}} a_{n\vec{k}}^{\dagger} + h.c.\cdot \qquad (4)$$

To derive the 2D e-p interaction Hamiltonian in TMCs, one can divide the phonon wave-vector into *xy*- and *z*- components, i.e. $\vec{k} \equiv (\vec{q}, k_z)$ [16]. Then the Fröhlich-like Hamiltonian of e-p interaction in TMCs is rewritten as

$$H_I = \sum_{n,\vec{q}.k_z} G_{n\vec{q}k_z}^{*} e^{-i\vec{q}\cdot\vec{\rho}} a_{nqk_z}^{\dagger} + h.c.\ , \qquad (5)$$

where

$$\left|G_{n\vec{q}k_z}\right|^2 = \frac{e^2}{V\left(q^2 + k_z^2\right)}\left(\frac{\hbar}{2\omega_{nL}}\right) \qquad (5a)$$

$$\cdot\left(\frac{1}{T_{11} + 2B_n T_{12} + B_n^2 T_{22}}\right)\left(\frac{b_{31} + B_n b_{32}}{\varepsilon_0 + b_{33}}\right)^2 .$$

The $\vec{\rho}$ in above equation express the electron's position-vector in *xy*-plane.

Summing $\left|G_{n\vec{q}k_z}\right|^2$ over k_z independently to equation (5), the 2D e-p coupling function can be obtained as

$$\left|M_n(\vec{q})\right|^2 = \sum_{k_z} \left|G_{n\vec{q}k_z}\right|^2 = \frac{\left|g_n\right|^2}{2Sq}\ , \qquad (6)$$

where

$$g_n^{*} = \frac{ie}{\varepsilon_0 + b_{33}}\left(\frac{\hbar}{2\omega_{nL}}\right)^{1/2} \qquad (6a)$$

$$\cdot\left(\frac{1}{T_{11} + 2B_n T_{12} + B_n^2 T_{22}}\right)^{1/2} \left(b_{31} + B_n b_{32}\right).$$

The 2D e-p system Hamiltonian can then be written as

$$H = \frac{p^2}{2m} + \sum_{n\vec{q}} \hbar\omega_{nL} a_{n\vec{q}}^{\dagger} a_{n\vec{q}} + \sum_{n\vec{q}} M_n^{*}(\vec{q}) e^{-i\vec{q}\cdot\vec{\rho}} a_{n\vec{q}}^{\dagger} + h.c.\cdot \qquad (7)$$

Similarly, the 1D e-p coupling function can be derived by summing $\left|G_{n\vec{q}k_z}\right|^2$ over q independently

$$\left|I_n(\vec{q})\right|^2 = \sum_{\vec{q}} \left|G_{n\vec{q}k_z}\right|^2 = \frac{\left|g_n\right|^2}{4\pi L}\ , \qquad (8)$$

The Hamiltonian of a 1D e-p system can finally be written as

$$H = \frac{p^2}{2m} + \sum_{nk_z} \hbar\omega_{nL} a_{nk_z}^{\dagger} a_{nk_z} + \sum_{nk_z} I_n^{*}(k_z) e^{-ik_z\cdot z} a_{nk_z}^{\dagger} + h.c.\cdot \qquad (9)$$

3. 3D, 2D and 1D polaronic energy

The intermediate coupling polaronic energy in a 3D TMC system can be generally calculated by the LLP variational method [17], for instance, the polaronic energy can be given as [10]

$$E = \frac{p^2}{2m^{*}} - E_{tr}\ . \qquad (10)$$

where the E_{tr} express the self-trapping energy and can be derived as:

$$E_{tr} = \alpha_{1L}\hbar\omega_{1L} + \alpha_{2L}\hbar\omega_{2L}\ , \qquad (11a)$$

the renormalized effective mass m^{*} is given as

$$m^{*} = \left[1 + \left(\alpha_{1L} + \alpha_{2L}\right)/6\right] m\ . \qquad (11b)$$

In following, we extend the LLP variational method to calculate the polaronic energy in the 2D TMC systems.

Carrying out two unitary transformations and performing the suitable variational treatments, the 2D intermediate coupling polaronic energy in TMC system can be obtained as

$$E(p) = \frac{p^2}{2m}\left(1 - \eta^2\right) - \sum_{n\vec{q}} \frac{\left|M_n(\vec{q})\right|^2}{\frac{\hbar^2 q^2}{2m} + \hbar\omega_{nL} - (1-\eta)\frac{\hbar\vec{q}\cdot\vec{p}}{m}}\ , \qquad (12)$$

in single phonon approximation. The η in above can be obtained as

$$\eta = \sum_n \frac{\pi\alpha_{nL}}{8} \Bigg/ \left(1 + \sum_n \frac{\pi\alpha_{nL}}{8}\right), \qquad (13)$$

and the dimensionless e-p coupling constant α_{nL} is defined as

$$\alpha_{nL} = \frac{\left|g_n\right|^2}{4\pi\hbar^2\omega_{nL}^2}\left(\frac{2m\omega_{nL}}{\hbar}\right)^{1/2}. \qquad (14)$$

The electron band-mass is represented by a linear interpolation as:

$$m = x m_A + (1-x) m_B\ , \qquad (15)$$

where the electron band-masses of materials AC and BC are expressed by m_A and m_B, respectively.

The polaronic energy in 2D TMC system can finally be written as

$$E(p) = \frac{p^2}{2m}\left(1 + \sum_n \frac{\pi\alpha_{nL}}{8}\right)^{-1} - \sum_n \frac{\pi}{2}\alpha_{nL}\hbar\omega_{nL} + O(p^4)\ ,$$

i.e.

$$E = -E_{tr} + \frac{p^2}{2m^*}\cdot \qquad (16)$$

where the self-trapping energy and the re-normalized effective mass of polaron in 2D TMC system are given by the following equations:

$$E_{tr} = \frac{\pi}{2}\alpha_{1L}\hbar\omega_{1L} + \frac{\pi}{2}\alpha_{2L}\hbar\omega_{2L}, \qquad (17a)$$

$$m^* = \left[1+\pi\left(\alpha_{1L}+\alpha_{2L}\right)/8\right]m. \qquad (17b)$$

In accordance with the same treatment, the self-trapping energy and the re-normalized effective mass of the polaron in 1D TMC system are given by the following equations:

$$E_{tr} = \frac{\pi}{4}\alpha_{1L}\hbar\omega_{1L} + \frac{\pi}{4}\alpha_{2L}\hbar\omega_{2L}\ , \qquad (18a)$$

$$m^* = \left[1+\left(\alpha_1+\alpha_2\right)/8\right]m\ . \qquad (18b)$$

4. Numerical results and discussions

The variational computations for the polaronic self-trapping energies and re-normalized effective masses in 3D TMC systems of $ZnSe_xTe_{1-x}$, ZnS_xSe_{1-x} and ZnS_xTe_{1-x} are numerical performed by using Eqs.(11*a*) and (11*b*). The volume variations of the two-ion unit-cell are included in the calculations. It can be obviously found the self-trapping energies and re-normalized effective masses varying nonlinearly with the composition ratio *x* of the TMCs in Fig. 1. Except for the TMCs formed by small mismatch binary compounds, such as ZnS_xSe_{1-x} system, the volume effect can not be ignored.

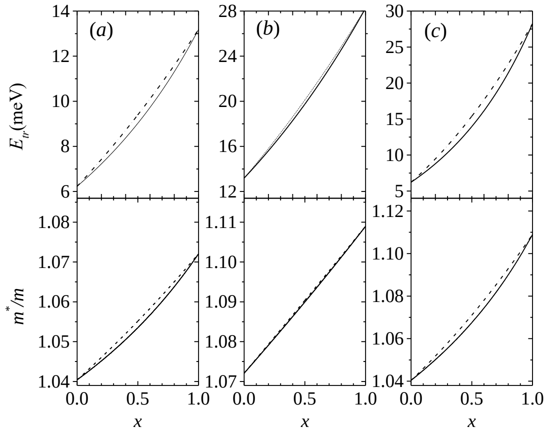

Fig. 1. Self-trapping energies (in units of meV) and renormalzied coefficients m^*/m of 3D polarons with (solid) and without (dashed) involving unit-cell volume effect as functions of x for TMCs: (a) $ZnSe_xTe_{1-x}$, (b) ZnS_xSe_{1-x}, (c) ZnS_xTe_{1-x}

The 2D and 1D results of the polaronic self-trapping energies and re-normalized effective masses varying with the composition ratio *x* are illustrated in Figs. 2 and 3 respectively by using the Eqs.(17) and (18). It can be found the the larger flexures of the curves corresponding self-trapping energies and re-normalized effective masses of the polarons varying with the composition ratio *x* in 2D TMC respectively in Fig. 2. It is due to the deducting dimension of the TMCs strengthing the e-p interaction and lattice mismatch of two binary materials. The results are consistent with common sense expectations. So that the more obviously nonlinearity of self-trapping energies and re-normalized effective masses varying with the composition ratio *x* can be inferred in case of 1D TMCs. The expected curves are shown in Fig. 3. The unit-cell volume variation on the compositional dependence of the polaron effects cannot be neglected generally, for instance of $ZnSe_xTe_{1-x}$ and ZnS_xTe_{1-x}.

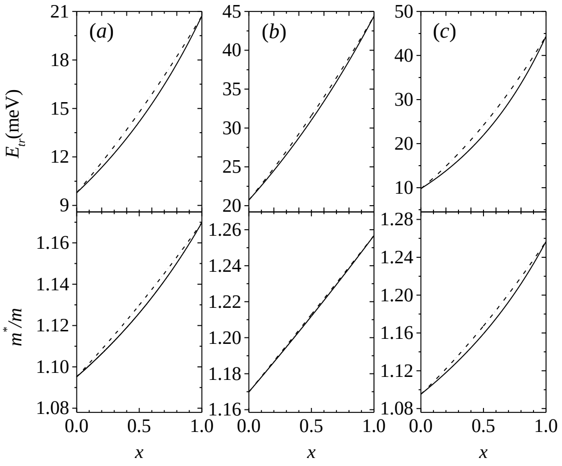

Fig. 2. Self-trapping energies (in units of meV) and renormalzied coefficients m^*/m of 2D polarons with (solid) and without (dashed) involving unit-cell volume effect as functions of x for TMCs: (a) $ZnSe_xTe_{1-x}$, (b) ZnS_xSe_{1-x}, (c) ZnS_xTe_{1-x}

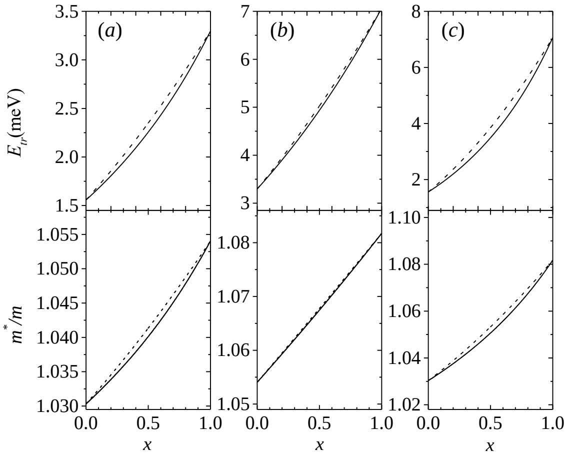

Fig. 3. Self-trapping energies (in units of meV) and renormalzied coefficients m^*/m of 1D polarons with (solid) and without (dashed) involving unit-cell volume effect as functions of x for TMCs: (a) $ZnSe_xTe_{1-x}$, (b)ZnS_xSe_{1-x}, (c) ZnS_xTe_{1-x}

5. Conclusion

The computed results of the polaronic self-trapping energies and renormalized effective masses for 3D, 2D and 1D zinc TMC compounds are numerically performed. It is verified that the polaronic self-trapping energies and renormalized effective masses varying nonlinearly with the composition *x* in both 3D, 2D and 1D zinc TMCs. The effect of the uint-cell volume variation on polaron effects as funcitions of composition ratio cannot be neglected generally, except for the zinc TMC compounds with very small lattice mismatch and very weak e-p coupling.

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*Corresponding author: jhhou@126.com