Phase Transitions in Compound Semi-Conductors of elements of group IV and VI

Shyam Kishor Thakur[1], Rajendra Prasad[2] and Kunjesh Kumar[3]

[1]Deptt. Of Physics Town Senior Secondary School, Hajipur, Vaishali

[2]Associate Professor, PG Deptt. Of Physics, LS College, Muzaffarpur

[3]Assistant Professor (Guest Faculty), Deptt. Of Electronics, LS College, Muzaffarpur

Abstract : A correlation b/w the structural and superconductor transition temperature is observed for the compound semiconductors of the elements of group IV and VI. The first-order phase transition to the semiconductor state is due to the inter band transitions and Coulomb and electron-phonon interaction. Owing to Bose-Einstein condensation of the optical phonons, a first-order phase transition is produced and becomes closer to the second-order phase transition. We've presented the self-consistent solution for a first-order phase transition.

I. Introduction

Phase transition of first and second order in polar semiconductors have been extensively studied by many workers. A survey of the literature reveals that the compound semiconductors of the elements of group IV and VI are the type A_4 B_6. L.V. Keldysh and Yu. V Kopaev, setting the hamiltonian for the compound semiconductor of the type A_4 B_6, found that these types of semiconductors suffer first-order phase transition[1]. Yu. V Kopaev found that for electron/phonon interaction the phonon system in isotropic semimetals is also subject to instability[2]. In literature, there exists a large number of experimental data evidencing that the symmetry of the electronic states in the extremal points in the empty and field bands that are closest to each other are described by spinar representation, without taking spin into account[3]. In this paper, we've extended the work of Yu. V Kopaev and Keldysh, who used the Hamiltonian, which doesn't contain a term corresponding to interband transitions. We've investigated the model of the type considered in (1) but with allowance for interband transitions.

II. Theory

We divide the Hamiltonian $\hat{H}$ of the system investigated by us into three parts, $\hat{H}_0^e$, $\hat{H}_0^p$ and $\hat{H}_{\text{int}}$, where $\hat{H}_0^e$ is the Hamiltonian of the electrons that do not interact with one another and are in the periodic field of the lattice, $\hat{H}_0^p$ is the Hamiltonian of the free phonons, and $\hat{H}_{\text{int}}$ is the Hamiltonian describing the electron-electron and electron phonon interactions.

Now, leaving out the spin indices, we obtain the form of the Hamiltonian $\hat{H}_0^e$ in the representation of Luttinger and Kohn[4]. As will be shown subsequently, this representation is convenient in that, on the one hand, it has an explicitly separated interband-transition term that is bilinear in the electron creation and annihilation operators, and on the other hand the interaction Hamiltonian can be written in simplest form. The complete and orthonormal system of basis functions of this representation is

$$\psi_{nq} = \psi_{nqv} e^{iqr} \equiv u_{nq}(r) \exp\{-i(q-k_0)r\} \quad \text{..... (1)}$$

where

$$\psi_{nko} = u_{nko}(r) e^{ik_0 r} \quad \text{..... (2)}$$

is the exact solution of the Schrodinger equation in a specified periodic potential of the lattice, known for a fixed value of the wave index k_0 in all the bands. Here n is the number of the band, and q is an arbitrary vector of the Brillouin zone, reckoned from the end of the vector k_0. Wave functions of the type (1)

correspond to creation and annihilation operators a_{nq}^{*} and a_{nq}. In the basis (1), the Schrodinger equation in a given periodic potential corresponds to the Hamiltonian

$$\sum_{qn}\left\{\frac{\hbar^2}{2m_o}q^2+\varepsilon_n\left(k_o\right)\right\}a_{nq}^{+}a_{nq}+\sum_{qnn'}\frac{\hbar}{m_o}P_{nn'}qa_{n'q}^{+}a_{nq} \qquad \text{..... (3)}$$

where m_o is the mass of the free electron, $\varepsilon_n\left(q_o\right)$ is the energy of a state with wave function (2), and the vector $P_{n'n}$ is defined by the equation

$$P_{n'n}=-i\hbar\int d^3r\psi_{n'ko}\left(r\right)\nabla_r\psi_{nko}\left(r\right) \qquad \text{..... (4)}$$

Closed system of equations for the order parameters Δ_e and Δ_{ph} :

$$\Delta_e\left(p\right)=\frac{1}{2\left(2\pi\right)^3}\int d^3qV\left(q-p\right)\left[\frac{\hbar}{m_o}P'q+\Delta_e\left(q\right)+\Delta_{ph}\left(q\right)\right]$$

$$\times\left[\varepsilon^2\left(q\right)+\left|\frac{\hbar}{m_o}P'q+\Delta_e\left(q\right)+\Delta_{ph}\left(q\right)\right|^2\right]^{-1/2}$$

$$\Delta_{ph}\left(p\right)=\frac{2}{2\left(2\pi\right)^3}g\left(p\right)\int d^3q\frac{g\left(q\right)}{\omega_0}\left[\mathrm{Re}\,\Delta_e\left(q\right)+\Delta_{ph}\left(q\right)\right]$$

$$\times\left[\varepsilon^2\left(q\right)+\left|\frac{\hbar}{m_o}P'q+\Delta_e\left(q\right)+\Delta_{ph}\left(q\right)\right|^2\right]^{-1/2} \qquad \text{..... (5)}$$

We have used here the fact that, in as much as the sublattice displacement $\left\langle b_0+b_0^{+}\right\rangle$ is a real number, the electron-phonon coupling constant g(p) is also a real number under our choice of the phases of the electronic wave functions in (5).

We now obtain a self-consistent solution for a first-order phase transition on giving a self-consistent solution of equation (5).

The self-consistency equation for ε is given by

$$\varepsilon=\frac{2\alpha P^{*}}{c^2\rho\left(2\pi\right)^3\left|P\right|}\int d^3q\frac{\hbar}{m_0}Pq\left(\alpha\varepsilon-1\right)\left[\varepsilon^2\left(q\right)+\left|\frac{\hbar}{m_0}Pq\left(1-\alpha\varepsilon\right)\right|^2+\Delta_{ph}^2\right] \qquad \text{..... (6)}$$

III. Discussion of Results

Following to the instability of the electron-phonon system relative to pairing of the electrons and holes from different bands and owing to Bose condensation of the optical phonons, a first-order phase transition is produced and becomes closer to a second-order transition to a degree that depends on the interband interaction of the type $\hbar P.qa_1^{*}a_2/m_0$. The transition is accompanied by a deformation (dilatation) of the lattice along the direction singled out by the vector P. These results were obtained for a one-ellipsoid model. In real A_4B_6 structures there are four equivalent directions. One can expect, however, that since these directions cannot be mutually orthogonal, and the coupling constant with the optical phonons is maximal, from symmetry considerations (Sec. 3), for sublattice displacements in the directions of equivalent axes, the phase transition will occur only in one group of electronic extrema. The point is that, owing to the nonorthogonality of the axes, the deformation and the sublattice shift affect the electronic states that oriented along the three other axes, and the sublattice shift is energywise most favored in one of the directions of the vector of the star, because of the size of the gap depends exponentially on the constant for the coupling with the optical phonons, a coupling that is anisotropic with respect to the polarization of the oscilllations. Owing to the presence of a rhombohedral distortion, the points L and T of the Brilouin zone

become nonequivalent, and the shift of the extrema, due to this distortion, is different for different bands. It may turn out that the maximum of the valence band at the point T will lie lower than the minimum of the conduction band at the point L, i.e., a semimetal is produced. There are indications that the spectrum has a semimetalic character in the rhombohedral phase of SnTe.

Timerov and One of us[7] have shown, for a model with interband transitions similar to the one considered here, that the electron-hole pairing at unequal electron and hole densities can lead to an increase in the super-conducting transition temperature. It is known that it is precisely in A_4B_6 semiconductors with inverted bands that superconductivity appears after doping. In accordance with the considered model, a correlation between the temperatures of the superconducting and structural transitions has been experimentally established.

Thus, these semiconductors behave, from the point of view of super conductivity, like compounds of transition metals with β-W structure, in which there is a low temperature tetragonal restructuring of the lattice, as against the rhombohedral one in the A_4B_6 semiconductors.

The reasons for the rather high superconducting transition temperatures in A_4B_6 compounds may be, besides the usually considered softening of the optical phonon mode, also the restructuring of the electronic spectrum and the smallness of the interband Coulomb interaction of the electrons at large ($\sim \hbar q_F$) momentum transfers. The latter is due to the strong non-orthomality of the factors uk(r) at different k in the exact Bloch wave functions, owing to the interband transition term $\hbar P.qa_1^* a_2 / m_0$.

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