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The calculation of deep levels associated with NN pair impurities in GaP

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Abstract

On the basis of the approach of Green's function, the present work establishes a calculation theory for the deep levels associated with NN pair impurities in GaP by use of a set of special points in the Brillouin zone. Moreover, the paper employs four radial functions rather than the plane wave functions as the Lowdin orbitals for 2s2p electrons to construct the symmetrical functions of the GaP: NN system. Applying this theory to A_1 state which is more required to be considered in the applications, the paper obtains a detail scheme of calculating the 16 matrices $E_{ij}(i=1, 2, 3, 4; j=1, 2, 3, 4)$ and therefore the deep levels associated with the closest – neighbour nitrogen pairs in GaP, which can directly calculate out the numerical results of the energy levels if we know the experimental parameters J_0 and J_1 .

Keywords: Pair impurities, Green's function, special points, deep levels. PACS: 71.55. -I; 71.55. Eq; 61.72. -y

1. Introduction

It has been proven that III-V semiconductors associated with substitutional impurities play the remarkable role in manufacturing new semiconductor electric - optical instruments. With respect to the substitutional nitrogen impurities in GaP, beginning from a long times ago many investigators have focused their interests on triplet impurity complexes or a pair impurities such as NN_i ($i = 1, 2, \dots$) pairs in GaP, ^[1 - 8] since all such impurities can generate deep levels within the band gap of III-V semiconductors, change the indirect band gap into direct band gap, and thus improve the properties of optic - electron emission of semiconductor instruments. Nevertheless, the theoretical calculation on deep levels associated with pair impurities in III-V semiconductors such as GaP is rather difficult, therefore, it is significant to improve the theoretical calculation in technique. For this purpose, the present paper is trying to establish a calculation scheme by use of a set of special points in the Brillouin zone.

2. The Calculation Scheme

In consideration of GaP: NN, assuming that all the substitutional NN pair impurities are placed at the anion sites of the perfect crystal, respectively noted with position vectors \vec{d} and \vec{d}' , it will generate one or more localised electron states within the band gap of the crystal. In terms of the approach of Green's function, the "trapped" electron can be described by the following equation

$$|\psi\rangle = G_0(E)V|\psi\rangle \quad (1)$$

Where V is the defect potential arising from the substitutional NN pairs, and $G_0(E)$ represents the Green's function of the perfect crystal defining as

$$G_0(E) = \frac{1}{E - H_0} \quad (2)$$

Where H_0 represents the Hamiltonian of the perfect crystal. In accord with sp^3 hybridization of the bond lengths around NN pair impurities, the defect potential V is given by

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$$V = \sum_i [(|id\rangle V_i \langle id|) + (|id'\rangle V_i \langle id'|)], \quad (3)$$

Where $i = S, P_x, P_y, P_z$; and V_i represents their corresponding defect potential, which is usually determined by experiments; d and d' respectively associate with the NN pair impurities. The NN pair impurities substituting atoms of the anion sites in GaP results in the symmetry of the system lowering to C_{3v} which can provide two symmetrical states respectively noted by A_1 and E (double degeneracy) for the “trapped” electron. Expanding the state vectors (or wave functions) in terms of the basis vectors of the representation of C_{3v} , it is written

$$|\psi_i^\alpha\rangle = \sum_{m, \vec{R}} \langle l, \vec{R}, m, \alpha | \psi \rangle |l, \vec{R}, m, \alpha\rangle, \quad (4)$$

where $|l, \vec{R}, m, \alpha\rangle$ ($m = 1, 2, \dots$) represents the m th basis vector of the l th irreducible representation of C_{3v} , α notes the subdivision of the m th basis vector, \vec{R} represents the R th shell layer away from the NN pair impurities [9]. Therefore, $\langle A_1, \vec{R}, m | \psi \rangle$ and $\langle E, \vec{R}, m, \alpha | \psi \rangle$ ($\alpha = 1, 2$) respectively represent the symmetrical wave functions of A_1 and E states.

If an electron is trapped in A_1 state, substituting the notation \vec{R} with d associates with one of the NN pair, and d' associates with the another, we introduce four parameters $\mu, \beta, \gamma, \delta$, and respectively defining.

$$\beta = V(P, d) \langle A_1, d, 2 | \psi \rangle, \mu = V(S, d) \langle A_1, d, 1 | \psi \rangle, \gamma = V(S, d') \langle A_1, d', 1 | \psi \rangle \text{ and } \delta = V(P, d') \langle A_1, d', 2 | \psi \rangle,$$

This is merely a technique in dealing with problems. The distribution of the symmetrical wave functions is in accord with sp^3 hybridization, so at the positions placed by NN pair impurities, it can approximately accept

$$\langle A_1, d, 1 | \psi \rangle = \langle A_1, d, 2 | \psi \rangle = \langle A_1, d', 1 | \psi \rangle = \langle A_1, d', 2 | \psi \rangle = 0.$$

In consideration of the ortho normalization between all the basis vectors of the representation of C_{3v} from eq. (1) and eq.(4) we acquire a group of equations associated with μ, β, γ and δ as follows:

$$\begin{aligned} &\mu \langle A_1, d, 1 | G_0 | A_1, d, 1 \rangle + \beta \langle A_1, d, 1 | G_0 | A_1, d, 2 \rangle + \gamma \langle A_1, d, 1 | G_0 | A_1, d', 1 \rangle + \\ &\delta \langle A_1, d, 1 | G_0 | A_1, d', 2 \rangle = 0, \\ &\mu \langle A_1, d, 2 | G_0 | A_1, d, 1 \rangle + \beta \langle A_1, d, 2 | G_0 | A_1, d, 2 \rangle + \gamma \langle A_1, d, 2 | G_0 | A_1, d', 1 \rangle + \\ &\delta \langle A_1, d, 2 | G_0 | A_1, d', 2 \rangle = 0, \\ &\mu \langle A_1, d', 1 | G_0 | A_1, d, 1 \rangle + \beta \langle A_1, d', 1 | G_0 | A_1, d, 2 \rangle + \gamma \langle A_1, d', 1 | G_0 | A_1, d', 1 \rangle + \\ &\delta \langle A_1, d', 1 | G_0 | A_1, d', 2 \rangle = 0, \\ &\mu \langle A_1, d', 2 | G_0 | A_1, d, 1 \rangle + \beta \langle A_1, d', 2 | G_0 | A_1, d, 2 \rangle + \gamma \langle A_1, d', 2 | G_0 | A_1, d', 1 \rangle + \\ &\delta \langle A_1, d', 2 | G_0 | A_1, d', 2 \rangle = 0. \end{aligned} \quad (5)$$

The requirement of that there are significant solutions of eq. (5) associated with μ, β, γ and δ would be

$$\det |IG_0(E)| = 0, \quad (6)$$

Where $IG_0(E)$ is a 4×4 matrix consisting of all the coefficients of eq. (5), all the deep levels of A_1 state can be calculated out by eq.(6). Moreover, the wave functions of A_1 state are calculated by eq. (5) and the joint normalization constraint

$$\sum_{\vec{R}, m} \langle (A_1, \vec{R}, m | \psi) \rangle^2 = 1. \quad (7)$$

3. Deep Leves of A_1 State

(1) The symmetrical wave functions

With respect to the zinc- blende lattice, one feasible scheme to construct the symmetrical functions of A_1 state is written ^[9]

$$\begin{aligned} |A_1, d, 1\rangle &= |S_d\rangle, \quad |A_1, d', 1\rangle = |S_{d'}\rangle \\ |A_1, d, 2\rangle &= \frac{1}{\sqrt{3}}(|P_{xd}\rangle + |P_{yd}\rangle + |P_{zd}\rangle) \\ |A_1, d', 2\rangle &= \frac{1}{\sqrt{3}}(|P_{xd'}\rangle + |P_{yd'}\rangle + |P_{zd'}\rangle) \end{aligned} \quad (8)$$

Among these symmetrical states, the Lowdin orbitals for 2s2p electrons can be employed by ^[10]

$$\psi_{2s}(r) = \frac{1}{4\sqrt{2\pi}} \left(\frac{Z}{a'}\right)^{3/2} \left(2 - \frac{Z}{a'}r\right) e^{-Zr/2a'} \quad (9)$$

$$\psi_{2p_x}(r) = \frac{1}{4\sqrt{2\pi}} \left(\frac{Z}{a'}\right)^{5/2} x e^{-Zr/2a'} \quad (10)$$

$$\psi_{2p_y}(r) = \frac{1}{4\sqrt{2\pi}} \left(\frac{Z}{a'}\right)^{5/2} y e^{-Zr/2a'} \quad (11)$$

$$\psi_{2p_z}(r) = \frac{1}{4\sqrt{2\pi}} \left(\frac{Z}{a'}\right)^{5/2} z e^{-Zr/2a'} \quad (12)$$

(2) Calculations of the matrices of E

In the equations from (9) through (12), Z is the number of protons in the nucleus, $a' = \hbar^2 / \mu e'^2$, $e' = e / \sqrt{4\pi\epsilon_0}$. Using eq. (2) and eq (6), those matrices are respectively given by...

$$E_{11} = \sum_{n, \vec{k}} \frac{|\langle A_1, d, 1 | n \vec{k} \rangle|^2}{E - E_0(\vec{k})} \quad (13)$$

$$E_{12} = \sum_{n, \vec{k}} \frac{|\langle A_1, d, 1 | n \vec{k} \rangle \langle n \vec{k} | A_1, d, 2 \rangle|}{E - E_0(\vec{k})} \quad (14)$$

$$E_{44} = \sum_{n, \vec{k}} \frac{|\langle A_1, d', 2 | n \vec{k} \rangle|^2}{E - E_0(\vec{k})}. \quad (15)$$

In the above equations, $E_0(\vec{k})$ represents the energy level of the perfect crystal, and is calculated by

$$E_0(\vec{k}) = E_i - \sum_s J(\vec{R}_s) \exp(-2\pi i \vec{k} \cdot \vec{R}_s) \quad (16)$$

Where E_i is the energy of atom (i), \vec{R}_s represents the position vector of one of the neighbour atoms, and the parameter $J(\vec{R}_s)$ is generally determined by experiments? Moreover, the present calculation scheme will employ the ten special in the Brillouin zone in case of the zinc - blende lattice [11]. Assuming the position of NN pair atoms respectively at

$$\vec{d} = \frac{a}{8}(\bar{1}, \bar{1}, \bar{1}), \vec{d}' = \frac{a}{8}(1, 1, 1)$$

In the Cartesian coordinate system. In accord with the zinc-blende structure of the host crystal, the coordinates of the six nearest - neighbor atoms around the NN pair atoms we consider are respectively [9]:

$$\frac{1}{8}(-1, 3, 3)a, \frac{1}{8}(3, -1, 3)a, \frac{1}{8}(3, 3, -1)a, \frac{1}{8}(1, -3, -3)a, \frac{1}{8}(-3, 1, -3)a \text{ and } \frac{1}{8}(-3, -3, 1)a$$

And here a represents the lattice constant of the zinc-blende structure.

4. Details of the Scheme for Numerical Calculations

In order to calculate out the energy levels, at first, it needs to calculate out the numerical results of the 16 matrices of eq.(6), namely, E_{ij} (i=1,2,3,4; j=1,2,3,4). For example,

$$E_{12} = \sum_{n, \vec{k}, j} \frac{|\langle A_1, d, 1 | n \vec{k} \rangle \langle n \vec{k} | A_1, d, 2 \rangle|}{E - E_0(\vec{k})} e^{i \vec{k} \cdot (\vec{R} - \vec{R}_j)} \tag{17}$$

Where the factor $e^{i \vec{k} \cdot (\vec{R} - \vec{R}_j)}$ is required by the periodicity of the crystal. From eq.(8) Through eq.(12)

$$E_{12} = \frac{1}{32\sqrt{3}\pi} \left[\left(\frac{Z}{a'} \right)^4 (x + y + z) \left(2 - \frac{Z}{a'} r \right) e^{-\frac{Z}{a'} r} \sum_{\vec{k}, j} \frac{1}{E - E_0(\vec{k})} e^{i \vec{k} \cdot (\vec{R} - \vec{R}_j)} \right] \tag{18}$$

$$E_{21} = \frac{1}{32\sqrt{3}\pi} \left[\left(\frac{Z}{a'} \right)^4 (x + y + z) \left(2 - \frac{Z}{a'} r \right) e^{-\frac{Z}{a'} r} \sum_{\vec{k}, j} \frac{1}{E - E_0(\vec{k})} e^{-i \vec{k} \cdot (\vec{R} - \vec{R}_j)} \right] \tag{19}$$

Similarly, it is easy to get the formulas of calculating the other 12 matrices, they are respectively given by:

$$E_{13} = \frac{1}{32\pi} \left[\left(\frac{Z}{a'} \right)^3 \left(2 - \frac{Z}{a'} r \right) \left(2 - \frac{Z}{a'} r' \right) e^{-\frac{Z}{2a'}(r+r')} \sum_{\vec{k}, j} \frac{1}{E - E_0(\vec{k})} e^{i \vec{k} \cdot (\vec{R} - \vec{R}_j)} \right] \tag{20}$$

$$E_{31} = \frac{1}{32\pi} \left[\left(\frac{Z}{a'} \right)^3 \left(2 - \frac{Z}{a'} r \right) \left(2 - \frac{Z}{a'} r' \right) e^{-\frac{Z}{2a'}(r+r')} \sum_{\vec{k}, j} \frac{1}{E - E_0(\vec{k})} e^{-i \vec{k} \cdot (\vec{R} - \vec{R}_j)} \right] \tag{21}$$

$$E_{14} = -\frac{1}{32\sqrt{3}\pi} \left[\left(\frac{Z}{a'} \right)^4 \left(2 - \frac{Z}{a'} r \right) (x' + y' + z') e^{-\frac{Z}{2a'}(r+r')} \sum_{\vec{k}, j} \frac{1}{E - E_0(\vec{k})} e^{i \vec{k} \cdot (\vec{R} - \vec{R}_j)} \right] \tag{22}$$

$$E_{41} = -\frac{1}{32\sqrt{3}\pi} \left[\left(\frac{Z}{a'} \right)^4 \left(2 - \frac{Z}{a'} r \right) (x' + y' + z') e^{-\frac{Z}{2a'}(r+r')} \sum_{\vec{k}, j} \frac{1}{E - E_0(\vec{k})} e^{-i \vec{k} \cdot (\vec{R} - \vec{R}_j)} \right] \tag{23}$$

$$E_{32} = -\frac{1}{32\sqrt{3}\pi} \left[\left(\frac{Z}{a'} \right)^4 \left(2 - \frac{Z}{a'} r' \right) (x + y + z) e^{-\frac{Z}{2a'}(r+r')} \sum_{\vec{k}, j} \frac{1}{E - E_0(\vec{k})} e^{-i \vec{k} \cdot (\vec{R} - \vec{R}_j)} \right] \tag{24}$$

$$E_{23} = -\frac{1}{32\sqrt{3}\pi} \left[\left(\frac{Z}{a'} \right)^4 \left(2 - \frac{Z}{a'} r' \right) (x + y + z) e^{-\frac{Z}{2a'}(r+r')} \sum_{\vec{k}, j} \frac{1}{E - E_0(\vec{k})} e^{i\vec{k} \cdot (\vec{R} - \vec{R}_j)} \right] \quad (25)$$

$$E_{24} = -\frac{1}{96\pi} \left[\left(\frac{Z}{a'} \right)^5 (x + y + z) (x' + y' + z') e^{-\frac{Z}{2a'}(r+r')} \sum_{\vec{k}, j} \frac{1}{E - E_0(\vec{k})} e^{i\vec{k} \cdot (\vec{R} - \vec{R}_j)} \right] \quad (26)$$

$$E_{42} = -\frac{1}{96\pi} \left[\left(\frac{Z}{a'} \right)^5 (x + y + z) (x' + y' + z') e^{-\frac{Z}{2a'}(r+r')} \sum_{\vec{k}, j} \frac{1}{E - E_0(\vec{k})} e^{-i\vec{k} \cdot (\vec{R} - \vec{R}_j)} \right] \quad (27)$$

$$E_{34} = -\frac{1}{32\sqrt{3}\pi} \left[\left(\frac{Z}{a'} \right)^4 \left(2 - \frac{Z}{a'} r' \right) (x' + y' + z') e^{-\frac{Z}{a'} r'} \sum_{\vec{k}, j} \frac{1}{E - E_0(\vec{k})} e^{i\vec{k} \cdot (\vec{R} - \vec{R}_j)} \right] \quad (28)$$

$$E_{43} = -\frac{1}{32\sqrt{3}\pi} \left[\left(\frac{Z}{a'} \right)^4 \left(2 - \frac{Z}{a'} r' \right) (x' + y' + z') e^{-\frac{Z}{a'} r'} \sum_{\vec{k}, j} \frac{1}{E - E_0(\vec{k})} e^{-i\vec{k} \cdot (\vec{R} - \vec{R}_j)} \right] \quad (29)$$

$$E_{11} = \frac{1}{32\pi} \left[\left(\frac{Z}{a'} \right)^3 \left(2 - \frac{Z}{a'} r' \right)^2 e^{-\frac{Z}{a'} r'} \sum_{\vec{k}} \frac{1}{E - E_0(\vec{k})} \right] \quad (30)$$

$$E_{22} = \frac{1}{96\pi} \left[\left(\frac{Z}{a'} \right)^5 (x + y + z)^2 e^{-\frac{Z}{a'} r'} \sum_{\vec{k}} \frac{1}{E - E_0(\vec{k})} \right] \quad (31)$$

$$E_{33} = \frac{1}{32\pi} \left[\left(\frac{Z}{a'} \right)^3 \left(2 - \frac{Z}{a'} r' \right)^2 e^{-\frac{Zr'}{a'}} \sum_{\vec{k}} \frac{1}{E - E_0(\vec{k})} \right] \quad (32)$$

$$E_{44} = \frac{1}{96\pi} \left[\left(\frac{Z}{a'} \right)^5 (x' + y' + z')^2 e^{-\frac{Zr'}{a'}} \sum_{\vec{k}} \frac{1}{E - E_0(\vec{k})} \right] \quad (33)$$

If we know J_0 and J_1 in eq. (16), it is not difficult to calculate out the numerical numbers of E_{ij} ($i=1,2,3,4; j=1,2,3,4$).

Substituting their numerical results into eq. (6), the four energy levels of E will be obtained.

5. Conclusions

In conclusion, the present paper proposed a theoretical scheme of calculating the electronic energies of the imperfect system GaP: NN. Using from eq. (18) through eq. (33) to calculate E_{ij} ($i=1,2,3,4; j=1,2,3,4$), $E_0(\vec{k})$ is given by eq. (16), it should pointed out that the calculations associated with those closest-neighbor atoms must differ Ga atoms at cation sites from P atoms at anion sites, because they have different atomic energies.

Moreover, it is very clear from the calculation scheme that if we want to calculate out the deep levels associated with NN_2 , NN_3 , pairs in GaP, it merely requires to respectively consider the second closest- neighbor pair, the third closest - neighbour pair nitrogen atoms. In fact, if nitrogen atoms are added into GaP semiconductor, some phosphur atoms will be substituted by nitrogen atoms, and then inevitably generates NN_1 , NN_2 , ... pairs of impurities as well as single impurities in the P (phosphur) sites, producing a number of "electron traps". Some experimental results have demonstrated that the closest - neighbor nitrogen pairs generate the deepest levels; the second closest - neighbor nitrogen pairs generate the second deepest levels, and so on [3, 5 - 7].

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