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Effect of strain on the E – k dispersion of GaAs in 1-D using the K.P method.

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Abstract

The Energy – wave vector (E- k) dispersion of Gallium Arsenide (GaAs) and the effect of strain on the dispersion is investigated.
The K.P method is used instead of other methods like; tight binding and pseudopotential methods because this method has an advantage of giving realistic band structure close to the Γ point without being too demanding on computer resource.
The 1 – D, E – k dispersion plots shows significant effect of strain even in the neighborhood of the Γ point.

Keyword: S Strain, K.P method, Energy-wave vector dispersion, Gallium Arsenide.

1. INTRODUTION

Many semiconductor devices depend on GaAs or a compound with GaAs, such as $Al_xGa_{1-x}As$ or $In_xGa_{1-x}As$. Important devices that depend on GaAs technology include quantum well modulators, graded band-gap heterojunction transistors, high electron mobility transistors, vertical cavity lasers, quantum cascade lasers, and broad band light-emitting diodes, LED TVs [1] which are popular and have very good quality, solar cells.

Gallium Arsenide (GaAs) is an important semiconductor material for high-cost, high-efficiency solar cells and is used for single-crystalline thin film solar cells and for multi-junction solar cells.

The K.P. method [2,3,4] can incorporate the effect of strain and the influence of external fields (electric or magnetic). In semiconductors, the lowest conduction band will have contributions from the remote conduction bands as well as from the valence bands depending on the energetic separation of these bands from the lowest band. On the other hand, the valence edge of any semiconductor materials is expected to comprise two or three of the valence bands with comparable contributions. Depending on the accuracy required in the calculation and the energetic separation of the bands in the bulk materials, different number of bands may be included in the calculation. Sometimes it is sufficient to include heavy holes and light holes, sometimes we have to include spin orbit split-off and even have to include the effect of conduction band in the description of the band structures. This method has the advantage of giving realistic band structure close to the Γ point without being too demanding on computer resource.

2. THEORETICAL FORMALISM

For a periodic potential V(r), the electron wave function [2,4] satisfies the single electron Schrödinger

$$H\Psi(r) = [\frac{-\hbar 2}{2m}\nabla^2 + V(r)]\Psi(r) = E(k)\Psi(r) \quad (1)$$

The general solution of Eq. (1) is the Bloch function,

$$\Psi_{nk}(r) = e^{ik.r}u_{nk}(r) \quad (2)$$

When we substitute Eq. (2) into (1), we obtain

$$\frac{p2}{2m} + \frac{\hbar}{m}\,k.p + \frac{\hbar^2k^2}{2m} + v(r))u_{nk}(r) = E_n(k)u_{nk}(r) \quad (3)$$

Using $H_0 = \frac{p2}{2m} + V(r)$, Eq. (3) can be written as,

$$(H_0 + \frac{\hbar}{m}\,k.p + \frac{\hbar^2k^2}{2m})\,u_{nk}(r) = (E_n(k))\,u_{nk}(r) \quad (4)$$

The solution of Eq. (4) at r point (k=0) without spin orbit interaction is known and given by:

$$H_0u_{0k}(r) = [\frac{p^2}{2m} + V(r)]u_{0k}(r) = E_{n0}u_{n0}(r) \quad (5)$$

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In Eq.5, for direct band gap semiconductors, $E_{n0}$are band edge energies and $u_{n0}(r)$ are the corresponding wave functions, the Bloch functions at the band edge. The u_{n0}'s for different n, form a complete orthonormal set and one can express the solutions away from r-point $u_{nr}(r)$ in terms of u_{n0} as

$u_{nk}(r) = \sum_m c_{mn}(k) u_{m0}(r)$ (6)

$H_{nm} = \left(E_{n0} + \frac{\hbar^2 k^2}{2m} \right) \delta_{n,m} + \frac{\hbar}{m}\langle u_{n0}|k.p|u_{m0}\rangle + \frac{\hbar^2}{4m^2c^2}\langle u_{n0} \left| [\nabla V \times \mathbf{p}]\bullet\boldsymbol{\sigma} \right| u_{m0}\rangle$

The second term in the above equation is referred as k•p interaction term. The k•p interaction is obtained with perturbation theory The matrix elements of the equation in the basis,

$\{u_1, u_2, \ldots, u_8\} = \{|S\uparrow\rangle, |X\uparrow\rangle, |Y\uparrow\rangle, |Z\uparrow\rangle, |S\downarrow\rangle, |X\downarrow\rangle, |Y\downarrow\rangle, |Z\downarrow\rangle\}$ (7)

are given by,

$$H = \begin{bmatrix} H_1 + H_{SO} + H_R & \mathcal{C} \\ \mathcal{C}^{\bullet} & H_1 + H^{\bullet}_{SO} + H_R \end{bmatrix} \quad (8)$$

The term H_1 in H in Eq. (8) is given by

$$H_1 = \begin{bmatrix} E_c + \frac{\hbar^2 k^2}{2m} & ik_x p_0 & ik_y p_0 & ik_z p_0 \\ ik_x p_0 & E'_V + \frac{\hbar^2 k^2}{2m} & 0 & 0 \\ ik_y p_0 & 0 & E'_V + \frac{\hbar^2 k^2}{2m} & 0 \\ ik_z p_0 & 0 & 0 & E'_V + \frac{\hbar^2 k^2}{2m} \end{bmatrix}$$

Here, E_c and E_v' are the conduction and valence band edge energies when the spin-orbit interaction is not included [6,7]. The parameter P_o accounts for the mixture of conduction and valence bands at $k \neq 0$ and is obtained from

$P_o = -i(\hbar/m)\langle S|P_Z|Z\rangle = -i(\hbar/m)\langle S|P_Z|X\rangle = -i(\hbar/m)\langle S|P_Z|Y\rangle$ (9)

The parameter P can be expressed in the energy units as, $E_P = \frac{2m}{\hbar^2}P_0^2$

The spin-orbit interaction terms, H_{so} and Γ, in Eq. (8) can be explicitly written in matrix form and are presented in equation Eqs. (10) and (11) respectively,

$$H_{so} = \frac{\Delta}{3}\begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & -i & 0 \\ 0 & i & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \quad (10)$$

$$\Gamma = \frac{\Delta}{3}\begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & i \\ 0 & -1 & i & 0 \end{bmatrix} \quad (11)$$

The remote band interaction Hamiltonian, H_R in the matrix expression Eq. (8) can be written as,

$$H_R = \frac{\hbar^2}{m}\begin{bmatrix} A'k^2 & Bk_y k_z & Bk_x k_z & Bk_x k_y \\ Bk_y k_z & M'(k_y^2 + k_z^2) + L'k_x^2 & N'k_x k_y & N'k_x k_z \\ Bk_x k_z & N'k_x k_y & M'(k_y^2 + k_z^2) + L'k_x^2 & N'k_y k_z \\ Bk_x k_y & N'k_x k_z & N'k_y k_z & M'(k_y^2 + k_z^2) + L'k_x^2 \end{bmatrix} \quad (12)$$

The interaction parameters in expression Eq. (12) are explicitly written in the following expressions

$$A' = \frac{1}{m}\sum_{nj}\frac{\langle S|P_X|n\Gamma 5j|}{E_C - E_{n,\Gamma 5}}$$

$$B = \frac{2}{m}\sum_{nj}\frac{\langle S|P_x|n\Gamma_{5j}\rangle\langle n\Gamma_{5j}|P_x|Z\rangle}{\frac{E_C + E_v}{2} - E_{n\Gamma 5}} \quad (13)$$

$$H_1 = \frac{1}{2m}\sum_{nj}\frac{\left|\langle X|P_X|n\Gamma 5j\rangle\right|^2}{E_v - E_{n,\Gamma 5}}$$

$$H_2 = \frac{1}{2m}\sum_{nj}\frac{\left|\langle X|P_X|n\Gamma 4j\rangle\right|^2}{E_v - E_{n,\Gamma 4}} \quad (14)$$

$$G = \frac{1}{2m}\sum_{nj}\frac{\left|\langle X|P_X|n\Gamma 3j\rangle\right|^2}{E_v - E_{n\Gamma 3}}$$

$$F' = \frac{1}{2m}\sum_{nj}\frac{\left|\langle X|P_X|n\Gamma 1j\rangle\right|^2}{E_v - E_{n,\Gamma 1}}$$

$M = H_1 + H_2$ $N' = F' - G + H_1 - H_2$ $L' = F' + 2G$

$$\mathfrak{Q}_{c\alpha} = \left|\frac{1}{2},\frac{1}{2}\right\rangle = \left|S\downarrow\right\rangle$$

$$\mathfrak{Q}_{c\beta} = \left|\frac{1}{2},\frac{1}{2}\right\rangle = \left|S\uparrow\right\rangle \quad (15)$$

And for the valence band:

$$\mathfrak{Q}_{hh,\alpha} = \left|\frac{3}{2},\frac{3}{2}\right\rangle = \frac{1}{\sqrt{2}}\left|(X+iY)\uparrow\right\rangle \quad \mathfrak{Q}_{hh,\beta} = \left|\frac{3}{2},-\frac{3}{2}\right\rangle = \frac{1}{\sqrt{2}}\left|(X-iY)\downarrow\right\rangle \quad (16)$$

$$\mathfrak{Q}_{hh,\alpha} = \left|\frac{3}{2},\frac{3}{2}\right\rangle = \frac{1}{\sqrt{2}}\left|(X+iY)\uparrow\right\rangle \quad (17)$$

$$\mathfrak{Q}_{hh,\beta} = \left|\frac{3}{2},-\frac{3}{2}\right\rangle = \frac{1}{\sqrt{2}}\left|(X-iY)\downarrow\right\rangle$$

$$\mathfrak{Q}_{so,\alpha} = \left|\frac{1}{2},-\frac{1}{2}\right\rangle = -\frac{1}{\sqrt{3}}\left|(X-iY)\uparrow\right\rangle + \sqrt{\frac{1}{3}}\left|Z\downarrow\right\rangle \quad (18)$$

$$\mathfrak{Q}_{so,\beta} = \left|\frac{1}{2},\frac{1}{2}\right\rangle = \frac{1}{\sqrt{3}}\left|(X+iY)\uparrow\right\rangle + \sqrt{\frac{1}{3}}\left|Z\uparrow\right\rangle$$

With the basis set defined in Eqs. (15)–(18) and using Lowdin's perturbation theory [5,6,7] to include the effect of remote band, the 8×8 k•p Hamiltonian can be written as

$$H = \begin{array}{c} \begin{matrix} \left|S\downarrow\right\rangle & \left|S\uparrow\right\rangle & \left|\frac{3}{2},\frac{-3}{2}\right\rangle & \left|\frac{3}{2},\frac{-1}{2}\right\rangle & \left|\frac{3}{2},\frac{1}{2}\right\rangle & \left|\frac{3}{2},\frac{1}{2}\right\rangle & \left|\frac{1}{2},\frac{-1}{2}\right\rangle & \left|\frac{1}{2},\frac{1}{2}\right\rangle \end{matrix} \\ \begin{bmatrix} A & 0 & T^+ + V^+ & 0 & -\sqrt{3}(T-V) & \sqrt{2}(W-U) & (W-U) & \sqrt{2}(T^+ + V^+) \\ 0 & A & \sqrt{2}(W-U) & -\sqrt{3}(T^+ + U^+) & 0 & T-U & -\sqrt{2}(T-V) & W^+ + U \\ T+V & \sqrt{2}(W^+ - U) & -P+Q & -S^+ & R & 0 & \left(\frac{3}{2}\right)^{\frac{1}{2}} S & -\sqrt{2}Q \\ 0 & -\sqrt{3}(T^+ + V^+) & -S & -P-Q & 0 & R & -\sqrt{2}R & \left(\frac{1}{2}\right)^{\frac{1}{2}} S \\ -\sqrt{3}(T^+ - V^+) & 0 & R^+ & 0 & -P-Q & S^+ & (\frac{1}{2})^{\frac{1}{2}} S^+ & \sqrt{2}R^+ \\ \sqrt{2}(W^+ - U) & T^+ - V^+ & 0 & R^+ & S & -P+Q & \sqrt{2}Q & \left(\frac{3}{2}\right)^{\frac{1}{2}} S^+ \\ W^+ & -\sqrt{2}(T^+ - U^+) & \left(\frac{3}{2}\right)^{\frac{1}{2}} S^+ & -\sqrt{2}R^+ & \left(\frac{1}{2}\right)^{\frac{1}{2}} S & \sqrt{2}Q & Z & 0 \\ \sqrt{2}(T+V) & W+U & -\sqrt{2}Q & \left(\frac{1}{2}\right)^{\frac{1}{2}} S^+ & \sqrt{2}R & \left(\frac{3}{2}\right)^{\frac{1}{2}} S & 0 & Z \end{bmatrix} \end{array}$$

Where the parameters,

$$A = E_C + \left(A' + \frac{\hbar^2}{2m}\right)k^2 \qquad W = i\frac{1}{\sqrt{3}}Bk_x k_y$$

$$T = \frac{1}{\sqrt{6}}Bk_z\left(k_x + ik_y\right) \qquad W^+ = -i\frac{1}{\sqrt{3}}Bk_x k_y$$

$$T^+ = \frac{1}{\sqrt{6}}Bk_z\left(k_x - ik_y\right) \qquad P = -E_v + \gamma_1\frac{\hbar^2 k^2}{2m}$$

$$V = \frac{1}{\sqrt{6}}P_0\left(k_x - ik_y\right) \qquad Q = \gamma_3\frac{\hbar^2}{2m}\left(k_x^2 + k_y^2 - 2k_z^2\right)$$

$$V^+ = \frac{1}{\sqrt{6}}P_0\left(k_x + ik_y\right) \qquad R = -\frac{\sqrt{3}}{2}\left[\gamma_2\frac{\hbar^2}{m}\left(k_x^2 - k_y^2\right) - 2i\gamma_3 k_x k_y\right]$$

$$U = \frac{1}{\sqrt{3}}P_0 k_z \qquad R^+ = -\frac{\sqrt{3}}{2}\left[\gamma_2\frac{\hbar^2}{m}\left(k_x^2 - k_y^2\right) + 2i\gamma_3 k_x k_y\right]$$

$$S = \sqrt{3}\gamma_3\frac{\hbar^2}{m}k_z\left(k_x - ik_y\right) \qquad Z = E_V - \Delta - \gamma_1\frac{\hbar^2}{2m}k^2$$

$$S^+ = \sqrt{3}\gamma_3\frac{\hbar^2}{m}k_z\left(k_x + ik_y\right) \qquad E_V = E_V' + \frac{\Delta}{3}$$

This study is within the scope of 1-D in the Z direction

$k_x = k_y = 0$ (that is E-k dispersion in a well)

$$A = E_C + \left(A' + \frac{\hbar^2}{2m}\right)k_z^2$$

$$T = \frac{1}{\sqrt{6}}Bk_z\left(k_x + ik_y\right) \to 0$$

$$T^+ = \frac{1}{\sqrt{6}}Bk_z\left(k_x - ik_y\right) \to 0$$

$$V = \frac{1}{\sqrt{6}} P_0 \left(k_x - ik_y\right) \to 0$$

$$V^+ = \frac{1}{\sqrt{6}} P_0 \left(k_x - ik_y\right) \to 0$$

$$U = \frac{1}{\sqrt{3}} P_0 k_z ; \; E_p = \frac{2m}{\hbar^2} p_0^2$$

$$\therefore P_0 = \frac{\hbar E_p^{1/2}}{(2m)^{1/2}}$$

Hence

$$U = \frac{1}{\sqrt{3}} \frac{\hbar E_p^{1/2}}{(2m)^{1/2}} k_2$$

$$W = i\frac{1}{\sqrt{3}} B k_x k_y \to 0$$

$$W^+ = -i\frac{1}{\sqrt{3}} B k_x k_y \to 0$$

$$P = -E_v + \gamma_1 \frac{\hbar^2 k^2}{2m}$$

$$Q = \gamma_2 \frac{\hbar^2}{m} k_x^2$$

$$R = -\frac{\sqrt{3}}{2}\left[\gamma_2 \frac{\hbar^2}{m}\left(k_x^2 - k_y^2\right) - 2i\gamma_3 k_x k_y\right] \to 0$$

$$R^+ = -\frac{\sqrt{3}}{2}\left[\gamma_2 \frac{\hbar^2}{m}\left(k_x^2 - k_y^2\right) - 2i\gamma_3 k_x k_y\right] \to 0$$

$$S = \sqrt{3\gamma_3} \; \frac{\hbar^2}{m} k_z \left(k_x - ik_y\right) \to 0$$

$$S^+ = \sqrt{3\gamma_3} \; \frac{\hbar^2}{m} k_z \left(k_x + ik_y\right) \to 0$$

$$Z = E_V - \Delta - \gamma_1 \frac{\hbar^2}{2m} k^2$$

$$E_V = E_V' + \frac{\Delta}{3}$$

The resulting 8 x 8 Hamiltonian matrix in 1-D is given by the matrix

$$\begin{pmatrix}
A & 0 & 0 & 0 & 0 & -u\sqrt{2} & -u & 0 \\
0 & A & -u\sqrt{2} & 0 & 0 & 0 & 0 & u \\
0 & -u\sqrt{2} & -P+Q & 0 & 0 & 0 & 0 & \sqrt{2Q} \\
0 & 0 & 0 & -P-Q & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & -P-Q & 0 & 0 & 0 \\
-u\sqrt{2} & 0 & 0 & 0 & 0 & -P+Q & \sqrt{2Q} & 0 \\
-u & 0 & 0 & 0 & 0 & \sqrt{2Q} & Z & 0 \\
0 & u & -\sqrt{2Q} & 0 & 0 & 0 & 0 & Z
\end{pmatrix} \tag{19}$$

From the Eigen-value Equation $H\Psi = E\Psi$, Eq.(19) becomes

$$\begin{pmatrix}
A-E & 0 & 0 & 0 & 0 & -u\sqrt{2} & -u & 0 \\
0 & A-E & -u\sqrt{2} & 0 & 0 & 0 & 0 & u \\
0 & -u\sqrt{2} & -P+Q-E & 0 & 0 & 0 & 0 & \sqrt{2Q} \\
0 & 0 & 0 & -P-Q-E & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & -P-Q-E & 0 & 0 & 0 \\
-u\sqrt{2} & 0 & 0 & 0 & 0 & -P+Q-E & \sqrt{2Q} & 0 \\
-u & 0 & 0 & 0 & 0 & \sqrt{2Q} & Z-E & 0 \\
0 & u & -\sqrt{2Q} & 0 & 0 & 0 & 0 & Z-E
\end{pmatrix} \tag{20}$$

From Eq.(20) we have

$$A - E - \sqrt{2}u - u = 0 \tag{21}$$

$$A - E - \sqrt{2}u + u = 0 \tag{22}$$

$$-\sqrt{2}u - P + Q - E - \sqrt{2}Q = 0 \tag{23}$$

$$-P - Q - E = 0 \tag{24}$$

$$-P - Q - E = 0 \tag{25}$$

$$-\sqrt{2}u - P + Q + \sqrt{2}Q - E = 0 \tag{26}$$

$$-u+\sqrt{2Q}\ +Z-E=0 \tag{27}$$

$$u-\sqrt{2Q}\ +Z-E=0 \tag{28}$$

The equations represented from Eqs.(21)–(28) gives the 1-DE-k dispersion without strain. For Gallium Arsenide (GaAs) the equations takes the form

$$E=-5.29\ +\ 5.70\times10^{-19}k_z^2\ -5.65\times10^{-9}k_z$$
$$E=-5.29\ +\ 5.70\times10^{-19}k_z^2\ -9.69\times10^{-9}k_z$$
$$E=-6.81\ -4.81\times10^{-37}k_z^2\ -3.30\times10^{-9}k_z$$
$$E=-6.81\ -2.61\times10^{-37}k_z^2$$
$$E=-6.81\ -2.61\times10^{-37}k_z^2$$
$$E=-6.81\ -1.54\times10^{-36}k_z^2\ -3.30\times10^{-9}k_z$$
$$E=-7.15\ -1.17\times10^{-36}k_z^2\ -2.34\times10^{-9}k_z$$
$$E=-7.15\ -1.05\times10^{-37}k_z^2\ +2.34\times10^{-9}k_z$$

The above equations give the E-k dispersion [8,9] of GaAs without strain shown in Figure 1.

3. EFFECT OF STRAIN ON THE E-k DISPERSION

Effects such as strain, non-square quantum wells, symmetry forbidden transitions and electric and magnetic field can be addressed within the K.P method. The lattice mismatched epitaxial growth of semiconductors heterostructures [10,11,12] causes elastic strain in the system. In the strained materials the elastic strain causes a shift in elastic sites. The shift in lattice sites causes a change in crystalline potential in comparison to the unstrained crystal. This change in potential causes the change in energy band parameters such as band gap, the degeneracy of heavy and light holes at the r point in valence band and effective mass of electron and holes.
The strain Hamiltonian [13,14] in the basis defined inEqs. (15)–(18) is given as

$$H_s=\begin{bmatrix} a_c\varepsilon_h & 0 & -v^+ & 0 & -\sqrt{3}v & \sqrt{2}u & u & \sqrt{2}v^+ \\ 0 & a_c\varepsilon_h & \sqrt{2}u & \sqrt{3}v^+ & 0 & v & -\sqrt{2}v & -u \\ -v & \sqrt{2}u & -p+q & -s^+ & r & 0 & \sqrt{\frac{3}{2}}s & -\sqrt{2}q \\ 0 & \sqrt{3}v & -s & -p-q & 0 & r & -\sqrt{2}r & \frac{s}{\sqrt{2}} \\ \sqrt{3}v^+ & 0 & r^+ & 0 & -p-q & s^+ & \frac{s^+}{\sqrt{2}} & \sqrt{2}r^+ \\ \sqrt{2}u & v^+ & 0 & r^+ & s & -p+q & \sqrt{2}q & \sqrt{\frac{3}{2}}s^+ \\ u & -\sqrt{2}v^+ & \sqrt{\frac{3}{2}}s^+ & -\sqrt{2}r^+ & \frac{s}{\sqrt{2}} & \sqrt{2}q & -p & 0 \\ -\sqrt{2}v & -u & -\sqrt{2}q & \frac{s^+}{\sqrt{2}} & \sqrt{2}r & \sqrt{\frac{3}{2}}s & 0 & -p \end{bmatrix} \tag{29}$$

4. RESULTS AND DISCUSSION

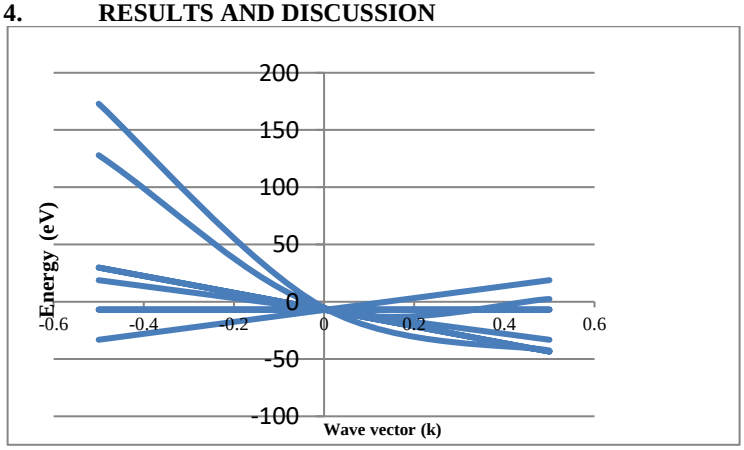

Figure 1: The E-k dispersion of GaAs without strain in 1- D.

The 1-D does not provide the necessary parameters to account for the band gap but it indicates that GaAs is a direct band gap material since all the E-k curves pass through k=0. Figure 1 show the E – k dispersion without strain.
The K.P model adapted to 1-D was sufficient to get an E-k dispersion in a quantum well of GaAs.
Strain effects is clearly seen in Figures 2 to 6.

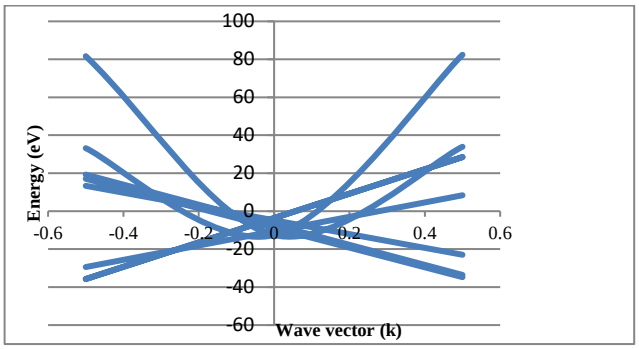

Figure 2: The E-k dispersion of GaAs with 3.5% strain in 1- D.

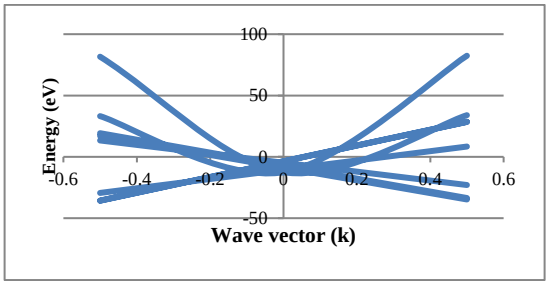

Figure 3: The E-k dispersion of GaAs with 5% strain in 1- D.

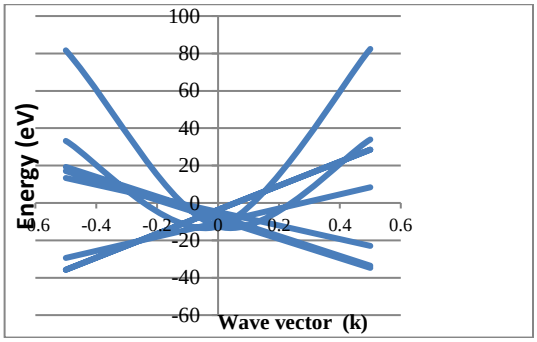

Figure 4: The E-k dispersion of GaAs with 8% strain in 1- D.

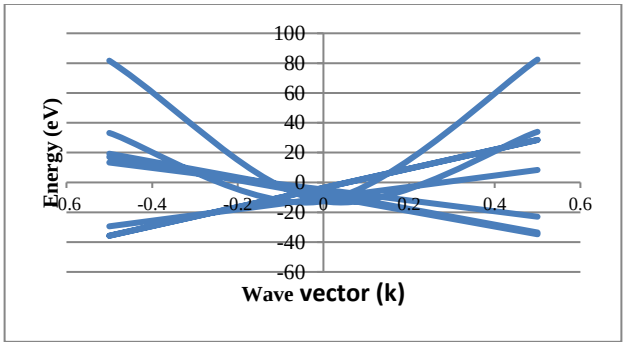

Figure 5: The E-k dispersion of GaAs with 11% strain in 1- D.

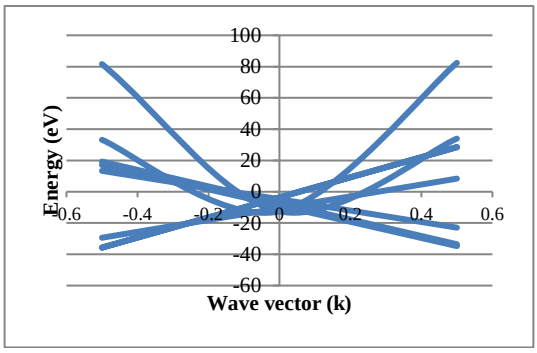

Figure 6: The E-k dispersion of GaAs with 26% strain in 1- D.

4. CONCLUSION

Based on the calculations, the 1-D does not provide the necessary parameters to account for the band gap but it indicates that GaAs is a direct band gap material since all the E-k curves pass through k=0.
The K.P model adapted to 1-D was sufficient to get an E-k dispersion in a quantum well of GaAs.

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