GaAs Band structure calculation using $k \cdot p$-theory including strain

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December 15, 2015

Abstract

The $k \cdot p$-method is here briefly described. The derivation of the Hamiltonian including spin-orbit coupling is sketched. Its applied to the band structure of Zincblende GaAs for small k. The model includes the conduction band and three valence bands. Perturbation from other bands are included using Löwdin perturbation theory. Influence from strain is included and analyzed. How perturbations split degenerate energy levels is presented.

1 Introduction

In this report, the $k \cdot p$-method for calculating band structures is presented. Its starting point is Bloch's theorem, where wavefunctions are decomposed into plane waves with wavevector k and crystal-periodic functions. The Bloch wave produces an effective Hamiltonian for the periodic function. The effective Hamiltonian includes a $k \cdot p$ term which can be treated with perturbation theory. In practice, one has to restrict the amount of bands taken into account. We use 8 bands: 3 p-orbitals forming the valence band and an s-orbital forming the conduction band. Each state has two spin states.

Spin comes into the calculation through the spin-orbit effect. The movement of electrons and holes produces magnetic fields that is taken into account. It has the effect of mixing the p-orbitals together.

While only 8 bands enter the calculation explicitly, the effect of other bands can be included through Löwdin perturbation theory. The effect is then reduced to a few parameters which can be experimentally determined.

We use this method on GaAs with Zincblende structure including strain to calculate the band structure close to the Γ-point.

2 Theory

For more details on theory, consult [1]. The band structure is found in principle by solving the Schrödinger equation

$$\left[\frac{p^2}{2m_0} + V(x)\right]\phi(x) = E\phi(x) \tag{1}$$

and then plotting E(k) in various directions. In order to solve equation 1 approximations are needed. The $k \cdot p$-method is a semi-empirical method. The band structure is extrapolated for a measured set of parameters using degenerate perturbation theory. The first step in the $k \cdot p$-method is to substitute a Bloch wave $\phi(x) = e^{ikx}u(x)$ into equation 1. With simple algebra this results in

$$\left[\frac{p^2}{2m_0} + V(x) + \frac{\hbar}{m_0}k \cdot p + \frac{h^2k^2}{2m_0}\right]u(x) = Eu(x) \tag{2}$$

Suppose a solution at $k = 0$ is known. Then we can treat the term $H_{per} = \frac{\hbar}{m_0}k \cdot p + \frac{h^2k^2}{2m_0}$ as a perturbation if k is small enough. The $k \cdot p$ operator induces transitions between bands, although the matrix element is hard to compute theoretically. The model can be made more accurate if spin-orbit coupling is included. The spin-orbit effect comes from the magnetic fields generated by the moving charges. The field interacts with the spin of the electrons, modifying energies. The spin-orbit Hamiltonian can be written $H_{\text{so}} = \frac{\hbar^2}{4m^2c^2}(\Delta V \times p)$ provided that it's operating on ϕ. If H_{so} operates on the periodic function $u(x)$, the additional term $\frac{\hbar^2}{4m^2c^2}(\Delta V \times k)$ appears. This last term is negligible compared to the first, because k is small.

For computations, one has to restrict the amount of bands included in the model. The 8-band model is considered in this paper. In this model, three valence bands and the conductance band are taken into account, with two spin states for each. The effect of other bands can be included using Löwdin's perturbations theory. The three valence band are p-orbitals while the conductance band is an s-orbital. Furthermore, the spherical component of the band wavefunctions are given by deformed spherical harmonics. Using symmetry its possible to deduce which matrix element is zero and which has to be measured.

For convenience, a basis of the p-orbitals is chosen where they are real functions. In this basis they are labeled as $|s\uparrow>, |x\uparrow>, |y\uparrow>, |z\uparrow>$ with states of the opposite spin following. With this specification, the 8-band Hamiltonian is written as

$$H = \begin{bmatrix} G & \Gamma \\ -\Gamma^* & G^* \end{bmatrix} \tag{3}$$

where $G = G_1 + G_2 + G_3 + G_{so}$ and Γ are defined as follows,

$$G_1 = \begin{bmatrix} E_c & iPk_x & iPk_y & iPk_z \\ -iPk_x & E_{v'} & 0 & 0 \\ -iPk_y & 0 & E_{v'} & 0 \\ -iPk_z & 0 & 0 & E_{v'} \end{bmatrix}$$

$$G_2 = \begin{bmatrix} A'k^2 & 0 & 0 & 0 \\ 0 & L'k_x^2 + M(k_y^2 + k_z^2) & N'k_xk_y & N'k_xk_z \\ 0 & N'k_xk_y & L'k_y^2 + M(k_x^2 + k_z^2) & N'k_xk_y \\ 0 & N'k_xk_z & N'k_yk_z & L'k_z^2 + M(k_x^2 + k_y^2) \end{bmatrix}$$

$$G_{so} = -\frac{\Delta}{3}\begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & i & 0 \\ 0 & -i & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \qquad \Gamma = -\frac{\Delta}{3}\begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & i \\ 0 & 1 & -i & 0 \end{bmatrix}.$$

G_1 consists of the unperturbed energies and the transitions generated by the p-operator. G_2 is the result of Löwdin's perturbation theory, which includes the effect of higher bands. G_{so} and Γ is the spin-orbit effect.

Strain in the crystal will modify the Hamiltonian. The strain is described by a strain tensor e_{ij}, which encodes how the crystal is deformed. The Hamiltonian corresponding to such a strain tensor is given in [2] as

$$G_{strain} = \begin{bmatrix} a_c(e_{xx} + e_{yy} + e_{zz}) & -iP\Sigma_j e_{xj}k_j & -iP\Sigma_j e_{yj}k_j & -iP\Sigma_j e_{zj}k_j \\ iP\Sigma_j e_{xj}k_j & le_{xx} + m(e_{yy} + e_{zz}) & ne_{xy} & ne_{xz} \\ iP\Sigma_j e_{yj}k_j & ne_{xy} & le_{yy} + m(e_{xx} + e_{zz}) & ne_{yz} \\ iP\Sigma_j e_{zj}k_j & ne_{xz} & ne_{yz} & le_{zz} + m(e_{xx} + e_{yy}) \end{bmatrix},$$

where a_c, n, l and m are material constants.

Most parameters in the model cannot be theoretically calculated. They need to be empirically determined. P is the optical matrix element, coming from the $k \cdot p$ term. Δ represents the strength of the spin-orbit interaction. Table 1 summarizes the values used, which are taken from [2].

3 Results

Figure 1 shows the calculated band structure of GaAs when varying k. We can identify four bands from the solid lines. These are the conduction band, the light and heavy hole bands and the split-off band. The light and heavy holes are degenerate at $k = 0$ but split for non-zero k.

The effect of 2% biaxial strain in the (001) strain is included in the dashed lines. The most significant effect of strain is the splitting of the light and heavy holes and the reduction of the band gap. At non-zero k, the effect of strain is different for k_z compared to k_x and k_y.

Varying both k_x and k_y lets us plot an energy surface. For the light hole band, this surface is plotted in figure 2. The strain produces the indents on the sides. A constant energy cross-section of this figure would not look like a circle, as it would for a free particle. They are instead warped.

Table 1

Constant	GaAs
E_g (eV)	1.424
Δ (eV)	0.341
m_e^*	0.0665
A'(eVnm^2)	−0.0047
L'(eVnm^2)	0.0057
M(eVnm^2)	−0.0048
N'(eVnm^2)	0.0043
l (eV)	-0.73
m (eV)	4.37
n (eV)	-7.88
P	0.0053
C_{12}/C_{11}	0.46

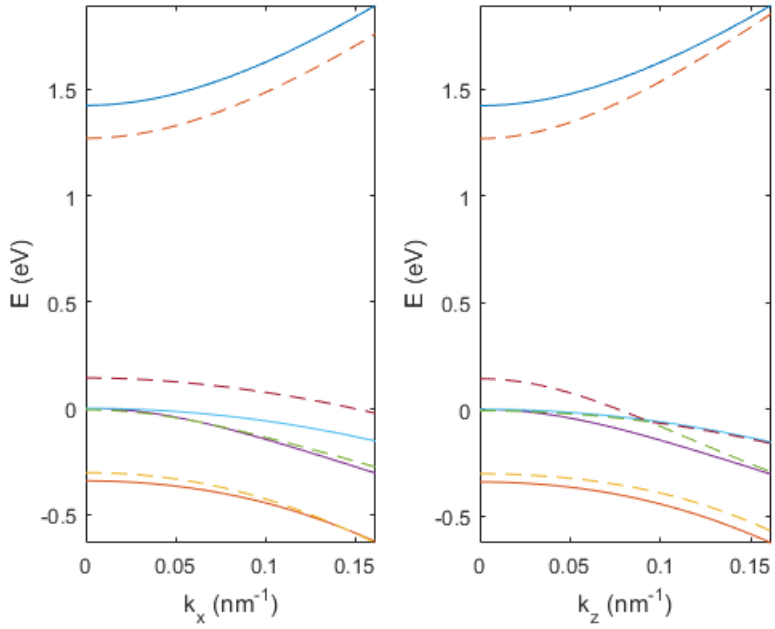

Figure 1: Band structure as a function of the wavevector. Solid lines are unstrained. Dashed lines include 2% biaxial strain in the (001) plane.

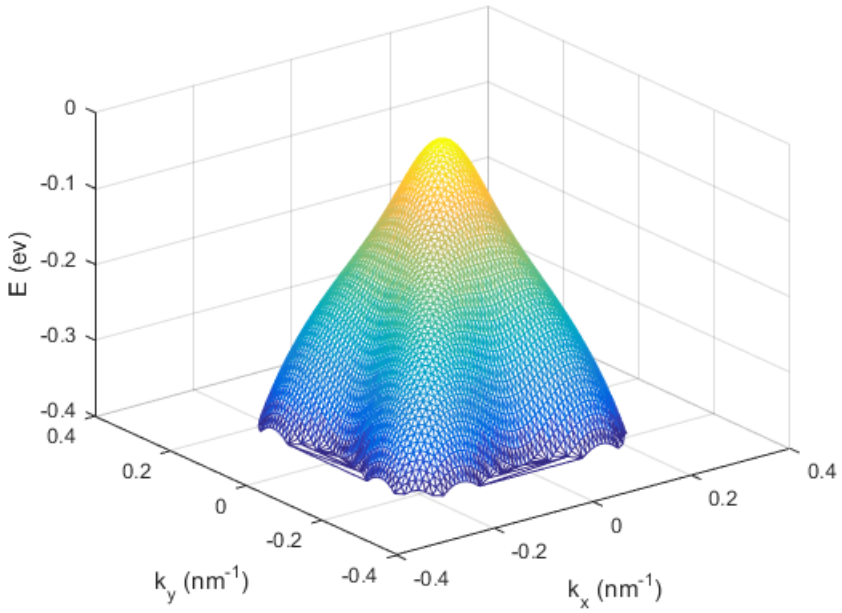

Figure 2: The energy of the light hole band as a function of k_x and k_y. 2% biaxial strain in the (001) plane.

4 Discussion

The unperturbed state consisted of a doubly degenerate conduction band and a valence band of six-fold degeneracy. Adding a spin-orbit term produced a split-off band from the valence band. Going to non-zero k further splits the valence band into the light and heavy hole bands. Lastly, the biaxial strain splits the light and heavy holes already at $k = 0$. This may be of interest in applications, as it influences the properties of the material. An example is for lasers, where compressive strain can increase the performance [2]. Strain can be built into the material by growing it with mismatched lattice constants [3].

References

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[3] E. A. Caridi, J. B. Stark, *Strain tensor elements for misfit-strained [hhk]-oriented cubic crystals, Applied Physics Letters, Volume 60, Issue 12, March 23, 1992, pp.1441-1443*