Valence Band Deformation Potentials in Semiconductors

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Strain alters the shape of the valence band structure, affecting the effective mass and mobility. We present a method for calculating the valence band deformation potentials by determining the deformation potential operator D_{ij} and calculating the matrix elements of the strain Hamiltonian H_ε based on $\mathbf{k}\cdot\mathbf{p}$ perturbation theory coupled with deformation potential theory. H_ε, itself is obtained via the Pikus-Bir transformation. In particular the pseudopotential is used and the transformation of the atomic basis vector is fixed by means of the measured deformation potentials of GaSb. The following ansatz for the strained atomic basis vector is used

$$\tau' = \tau + \begin{pmatrix} \xi^{(xx)}\varepsilon_{xx} & \xi^{(xy)}\varepsilon_{xy} & \xi^{(xz)}\varepsilon_{xz} \\ \xi^{(yx)}\varepsilon_{yx} & \xi^{(yy)}\varepsilon_{yy} & \xi^{(yz)}\varepsilon_{yz} \\ \xi^{(zx)}\varepsilon_{zx} & \xi^{(zy)}\varepsilon_{zy} & \xi^{(zz)}\varepsilon_{xz} \end{pmatrix} \tau \tag{1}$$

where $\xi^{(ij)} = \xi^{(ij)}_{hh}\delta_{m',\pm\frac{3}{2}}\delta_{m,\pm\frac{3}{2}} + \xi^{(ij)}_{lh}\delta_{m',\pm\frac{1}{2}}\delta_{m,\pm\frac{1}{2}} + \xi^{(ij)}_{12}\delta_{m',\pm\frac{3}{2}}\delta_{m,\pm\frac{1}{2}} + \xi^{(ij)}_{13}\delta_{m',\pm\frac{3}{2}}\delta_{m,\mp\frac{1}{2}}$, with m and m' labelling the magnetic quantum number. It was possible to show that the potential part of the deformation potential operator satisfies a Fredholm intergal equation of the second kind. Our calculation yields

$$D_{ij} = \frac{\hbar^2}{m}\partial_i\partial_j + \sum_G \left(\frac{V_G^S S_G^A}{1 - 4\pi\frac{S_G^S}{\Omega}} - i\frac{V_G^A S_G^S}{1 - 4\pi i\frac{S_G^A}{\Omega}} \right) (\tau_i G_j - \xi_\chi^{(ij)} G_i \tau_j) e^{i\mathbf{G}\mathbf{x}} \tag{2}$$

where $S_G^S = \cos(\mathbf{G}\cdot\tau)$ and $S_G^A = \sin(\mathbf{G}\cdot\tau)$. The basis functions for the heavy hole (HH) and light hole (LH) states are approximated by a superposition of spherical harmonic functions [1]. We fix the coefficients $\xi^{(ij)}_{hh}$, $\xi^{(ij)}_{lh}$, $\xi^{(ij)}_{12}$ and $\xi^{(ij)}_{13}$ via the deformation potentials for GaSb [2], $a_v = -8.3$ eV, $b_v = -1.8$ eV, $d_v = -4.6$ eV, with the pseudopotential form factors $V_3^S = -0.22$, $V_8^S = 0$, $V_{11}^S = 0.05$, $V_3^A = 0.06$, $V_4^A = 0.05$, $V_{11}^A = 0.01$ and the lattice constant $a_0 = 6.09\text{Å}$. They consist of a kinetic and a potential contribution, $a_v = a_v^{kin} + a_v^{pot}$, $b_v = b_v^{kin} + b_v^{pot}$, $d_v = d_v^{kin} + d_v^{pot}$. The calculated kinetic contributions for GaSb are $a_v^{kin} = -12.09$ eV, $b_v^{kin} = -4.8$ eV, $d_v^{kin} = -8.3$ eV. $\xi^{(ij)}_{hh}$ and $\xi^{(ij)}_{lh}$ have only real entries:

$$\xi_{hh} \sim \begin{pmatrix} 6.43 & 1 & 1 \\ 1 & 6.43 & 1 \\ 1 & 1 & 1.62 \end{pmatrix}, \quad \xi_{lh} \sim \begin{pmatrix} 3 & 1 & 1 \\ 1 & 3 & 1 \\ 1 & 1 & 8.58 \end{pmatrix}. \tag{3}$$

Contrary to (3), $\xi^{(ij)}_{12}$ and $\xi^{(ij)}_{13}$ have four complex entries, respectively,

$$\xi_{13} \sim \begin{pmatrix} 0.98 - 0.56i & 0.59 - 0.04i & 1 \\ 0.59 + 0.04i & 0.98 + 0.56i & 1 \\ 1 & 1 & 1 \end{pmatrix}, \quad \xi_{12} \sim \begin{pmatrix} 1 & 1 & -0.25 - 0.67i \\ 1 & 1 & -0.25 + 0.67i \\ -0.33 + 0.92i & 1 & -0.33 - 0.92i \end{pmatrix}. \tag{4}$$

Having determined the transformation of the atomic basis vector, theoretical values for the valence band deformation potentials have been calculated for the semiconductors: Si, Ge, GaP, GaAs, InSb, InP, InAs and AlSb. The obtained results are in satisfactory-to-excellent agreement with experimental data as well as calculated values from previous works [2], [3], and [4]. The method presented here does not make use of the internal strain parameter, which was introduced by Kleinman [5] in order to specify the position of the atom in the strained lattice. The measurement of the internal strain parameter is rather difficult and only few experimental data are available, not all in agreement with each other [6]. Thus our calculation features a new method to avoid such problems. Once the transformation of the atom position is fixed it can be applied to all semiconductors of diamond and zincblende structures. Table 1 contains the values of the lattice constants and the form factors [7] taken for our calculation. The obtained results for a_v, b_v and d_v as well as experimental and theoretical values from other works are given in Table 2.

References

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	a_0	V_3^S	V_8^S	V_{11}^S	V_3^A	V_4^A	V_{11}^A
Si	5.43	-0.21	0.04	0.08	0	0	0
Ge	5.64	-0.23	0.01	0.06	0	0	0
GaP	5.45	-0.22	0.03	0.07	0.12	0.07	0.02
GaAs	5.65	-0.23	0.01	0.06	0.07	0.05	0.01
InSb	6.47	-0.2	0	0.04	0.06	0.05	0.01
InP	5.86	-0.23	0.01	0.06	0.07	0.05	0.01
InAs	6.05	-0.22	0	0.05	0.08	0.05	0.03
AlSb	6.13	-0.21	0.02	0.06	0.06	0.04	0.02

Table 1: Pseudopotential form factors in Ry. Column one contains the lattice constants in $\AA$.

	a_v	b_v	d_v	a_v^{Exp}	b_v^{Exp}	d_v^{Exp}
Si	-8.51	-2.36	-4.96	-10^b	-2.2^a	-5.1^a
Ge	-8.19	-2.27	-4.65	-12.7^a	-2.6^a	-4.7^a
				-8.6^b	-2.2^b	
GaP	-8.32	-2.1	-4.74	-9.3^b	-1.8^a	-4.6^a
GaAs	-8.12	-1.91	-4.58	-9.77^a	-1.7^a	-4.55^a
				-8.14^c	-2^b	
InSb	-8.64	-1.93	-4.81	-7.7^a	-2.05^a	-4.8^a
				-10.3^b		-5^b
InP	-8.18	-1.85	-4.54	-6.35^a	-2.02^a	-4.2^a
				-8.6^b	-1.8^b	-4.9^b
InAs	-8.29	-1.82	-4.62	-6^a	-1.8^a	-3.6^a
				-6.5^b		-4.5^b
AlSb	-8.67	-1.92	-4.77	-5.9^a	-1.35^a	-4.3^a
				-9.9^b	-1.5^b	-4.7^b

Table 2: Theoretical values of the deformation potentials a_v, b_v and d_v in eV. Experimental and calculated values from previous works are given in the last three columns. ^{a} Reference [2], ^{b} Reference [3], ^{c} Reference [4].