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Band-edge deformation potentials in a tight-binding framework

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We calculate, within the tight-binding approximation, hydrostatic and uniaxial deformation potentials for seven III-V compounds (GaAs, InAs, GaSb, AlSb, InSb, InP, and GaP). These deformation potentials are expressed in terms of (i) the usual tight-binding parameters describing the unstrained bulk, (ii) an analytical law for the dependence of these parameters upon distance, and (iii) (for the uniaxial [111] deformation potential only) the internal displacements. We show that it is possible to derive a "universal variation law" that provides deformation potentials in reasonable agreement with available experimental data.

The interest in semiconductor strained-layer structures [such as (In,Ga)As-GaAs] is connected with their potential for high-speed and optoelectronic device applications.[1] A tight-binding description of unstrained heterostructures has recently provided theoretical values for band offsets that agree fairly well with experimental data (0.527 eV for GaAs/AlAs, 0.379 eV for CdTe/HgTe, and 0.452 eV for GaSb/AlSb).[2] The main reason for this agreement is that realistic electronic bulk band structures and dielectric constants are used in this calculation. To apply this technique to strained structures it would be very useful to accurately describe the effect of strain within the tight-binding approximation. In this paper we report a very simple method that takes into account the effect of strain on the tight-binding parameters.

To obtain a good description of both valence and conduction bands of an unstrained bulk semiconductor, one can use Vogl's parametrization,[3] which makes use of an sp^3s^* basis set. We shall consider here only the effect of elastic strain which, in heterostructures, corresponds to layer thickness L smaller than some strain-dependent critical thickness.[4,5] The strain modifies the band structure.[6,7] Let us focus our interest on the effect of the strain on the states near the band gap. Without strain or spin-orbit coupling the valence-band edge at $\mathbf{k}=\mathbf{0}$ in a zinc-blende-type material is a sixfold degenerate multiplet. The spin-orbit interaction lifts this degeneracy into a fourfold $p_{3/2}$ multiplet ($J=\frac{3}{2}$, $m_J=\pm\frac{3}{2},\pm\frac{1}{2}$) and a $p_{1/2}$ multiplet ($J=\frac{1}{2}$, $m_J=\pm\frac{1}{2}$) as shown in Fig. 1. The application of a uniaxial stress splits the $p_{3/2}$ multiplet and also, because of the hydrostatic pressure component of the strain, shifts the "center of gravity" of the $p_{3/2}$ multiplet and the $p_{1/2}$ band relative to the conduction band as illustrated schematically in Fig. 1. The modifications of the band edges are related to deformation potentials. If we call E_c the bottom of the conduction band, and E_{v1}, E_{v2}, and E_{v3} the tops of the three upper valence bands, we obtain the following.[7]

(1) For hydrostatic strain,

$$a=\frac{\delta E_g}{\delta P}B, \tag{1}$$

where δE_g is the variation of the band-gap width due to a stress variation δP and B is the bulk modulus of the compound.

(2) For a uniaxial strain in the [100] direction,

$$\begin{aligned}
\Delta(E_c-E_{v2}) &= -\tfrac{1}{3}\Delta_0+\delta E_H+\tfrac{1}{2}\delta E_{100}\,,\\
\Delta(E_c-E_{v1}) &= \tfrac{1}{6}\Delta_0+\delta E_H-\tfrac{1}{4}\delta E_{100}\\
&\quad -\tfrac{1}{2}(\Delta_0^2+\Delta_0\delta E_{100}+\tfrac{9}{4}\delta E_{100}^2)^{1/2}\,,\\
\Delta(E_c-E_{v3}) &= \tfrac{1}{6}\Delta_0+\delta E_H-\tfrac{1}{4}\delta E_{100}\\
&\quad +\tfrac{1}{2}(\Delta_0^2+\Delta_0\delta E_{100}+\tfrac{9}{4}\delta E_{100}^2)^{1/2}\,,
\end{aligned} \tag{2}$$

where Δ_0 is the spin-orbit splitting at the top of the valence band for the unstrained bulk, δE_H is the shift of

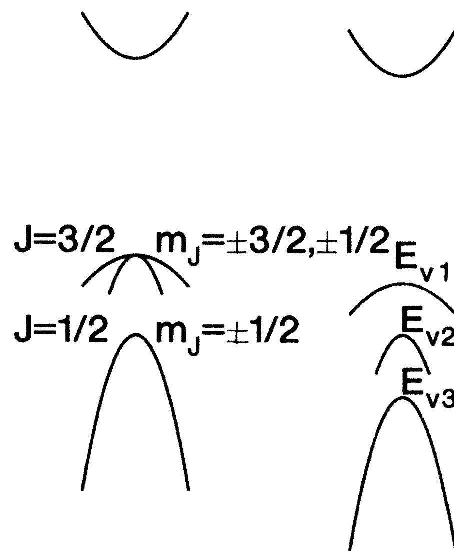

FIG. 1. The left-hand side shows the valence bands ($J=\frac{3}{2}$, $m_J=\pm\frac{3}{2},\pm\frac{1}{2}$, and $J=\frac{1}{2}$, $m_J=\pm\frac{1}{2}$ in spherical notation) and lowest conduction band in an unstressed zinc-blende compound near $\mathbf{k}=\mathbf{0}$. The right-hand side shows the effect of compressive stress on the bands.

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the gap due to the hydrostatic component of the strain. The linear splitting of the $p_{3/2}$ multiplet, δE_{100}, is related to the uniaxial deformation potential b as follows:

$$\delta E_{100} = 2b(\epsilon_{xx} - \epsilon_{zz}) , \quad (3)$$

where ϵ_{xx} and ϵ_{zz} are the strain components.

(3) For a uniaxial strain in the [111] direction, the changes in energy difference between the conduction and valence bands are also given by Eq. (2), where δE_{100} is replaced by δE_{111} equal to $2\sqrt{3}d\epsilon_{xy}$.

Equations (1)-(3) give a definition of the a, b, and d deformation potentials in terms of the band-edge modifications. In the present work these band-edge modifications are calculated and we deduce theoretical values of a, b, and d from a tight-binding calculation applied to the band structure of strained materials. The effect of strain on a perfect crystal is double.

(i) *A modification of atomic arrangement.* In the case of an elastic strain, we can assume[8,9] that the actual positions of the atoms will be close to those found from macroscopic arguments.[10] This assumption is used for hydrostatic or [100] uniaxial strain. On the other hand, in the case of [111] uniaxial strain, we also have to consider internal displacements.[11] In the absence of internal displacement, one of the four nearest neighbors of an atom will be much nearer—or further—from the central atom than the other neighbors. Generally, the internal displacement shifts one sublattice of the compound in such a way that the central atom is closer to the center of its four neighbors (for details see Ref. 11).

(ii) *From a tight-binding point of view,* this atomic rearrangement induces a modification of the off-diagonal interactions. These interactions depend on the distance R between two atoms. The most commonly used dependence is given by Harrison's law[12] in R^{-2} which has been used by different authors[13,14] in an sp^3s^* parametrization. This law provides a good general trend, but it has been shown in Ref. 15 that a more-refined fit can be useful. In linear-muffin-tin-orbital tight binding, the band-structure parameters decrease faster than R^{-2}.[16] Moreover, bulk tight-binding second-neighbor parametrizations show that the next-nearest-neighbor interactions are smaller than those deduced from nearest neighbors with a R^{-2} variation.[17] Thus, as band-structure parameters result from a fit, we decide here to express the tight-binding matrix elements $H_{\alpha\beta}$ (where H is the Hamiltonian, and α and β are atomic orbitals) as

$$H_{\alpha\beta} = H_{\alpha\beta}^{(0)}(R_0/R)^{n_{\alpha\beta}} , \quad (4)$$

where the $n_{\alpha\beta}$ are adjustable parameters chosen to obtain, for all the III-V compounds studied, a good variation of the band gap with *hydrostatic pressure only* (in fact, only n_{ss}, $n_{pp\sigma}$, and $n_{pp\pi}$, in the Slater and Koster notation,[18] have an incidence on a deformation potential, thus the other $n_{\alpha\beta}$ have been taken to equal 2.0, according to Harrison's law). We use orbit-dependent parameters because, as s states are more localized near the atom than p states, n_{ss} will probably be larger than n_{pp}. To perform this fit we have used experimental data given in Ref. 19, and we obtain $n_{ss} = 3.76$, $n_{pp\sigma} = 1.98$, and $n_{pp\pi} = 2.16$. The calculated deformation potentials are given in Table I. In this calculation, the spin-orbit coupling has been taken into account. So we have used a set of band parameters that provides good band edges (as in Ref. 3), and also good spin-orbit splittings at the top of valence band.[20] These parameters are given in Table II. In fact, inclusion of spin-orbit couplings does not strongly modify the values of the deformation potentials. In the absence of experimental values for the internal strain parameters, we have used an internal displacement parameter ξ equal to unity for all the compounds. This value is close to the results given elsewhere.[21] A smaller value of ξ would slightly decrease the d deformation potential. The agreement with experimental data is quite reasonable. A better agreement with experimental deformation potentials would be possible with an independent fit for each material. Some authors[14] have also used a variation of the atomic levels with nearest-neighbor positions. This dependence corresponds to a crystal-field effect due to a lowering of the symmetry.[22] We have realized an independent fit for GaAs, and have obtained exponents $n_{\alpha\beta}$ corresponding to those obtained in Ref. 15. However, our purpose here is to provide a variation law valid for all III-V compounds. We can compare the results obtained with this new "universal law" with GaAs and InP conduction-band deformation potentials a_c recently measured.[23] Experiment gives $a_c = -9.3$ and -7.0 eV, respectively, for GaAs and InP. These values agree very well with our results of $a_c = -9.6$ and -7.6 eV. For comparison, a recent *a priori* calculation by Cardona and Christensen[24] provides $a_c = -8.8$ eV for GaAs, and $a_c = -5.9$ eV for InP.

We can note that in the model just described, *there is*

TABLE I. Experimental (upper line) and theoretical (lower line) deformation potentials. The experimental values are taken from Ref. 19. The calculated values correspond to $n_{ss} = -3.76$, $n_{pp\sigma} = -1.98$, $n_{pp\pi} = -2.16$, and to an internal strain parameter $\xi = 1$.

	GaAs	InAs	GaSb	AlSb	InSb	InP	GaP
a	−9.2	−6.0	−8.3	−5.9	−7.7	−6.35, −6.60	−9.3, −9.9
	−8.34	−6.86	−8.22	−7.53	−7.04	−6.45	−9.73
b	−2.0	−1.8	−2.0	−1.35	−2.0	−2.0, −1.55	−1.8, −1.5
	−2.79	−2.33	−2.30	−2.10	−2.00	−2.11	−2.79
d	−4.5	−3.6	−4.7	−4.3	−4.8, −5.0	−5.0, −4.2	−4.5
	−4.77	−3.83	−3.98	−3.61	−3.35	−3.54	−4.75

TABLE II. Empirical matrix elements of the sp^3s^* Hamiltonian in eV. The notations are those used in Ref. 3. The first value is obtained neglecting spin-orbit coupling. The second value corresponds to spin-orbit splitting given in Ref. 20.

	GaAs		InAs		GaSb		AlSb
$E(s,a)$	−8.3431	−8.3431	−9.5381	−9.5381	−7.3207	−7.3207	−6.1714
$E(p,a)$	1.0414	0.9252	0.9099	0.7733	0.8554	0.5982	0.9807
$E(s^*,a)$	7.5412	7.4249	7.4099	7.2730	6.6354	6.3715	6.7607
$E(s,c)$	−2.6569	−2.6569	−2.7219	−2.7219	−3.8993	−3.8993	−2.0716
$E(p,c)$	3.6685	3.5523	3.7201	3.5834	2.9146	2.6575	3.0163
$E(s^*,c)$	6.7397	6.6235	6.7401	6.6095	5.9846	5.7287	6.1543
$V(s,s)$	−6.4513	−6.4513	−5.6052	−5.6052	−6.1567	−6.1567	−5.6448
$V(x,x)$	1.9546	1.9546	1.8398	1.8398	1.5789	1.5790	1.7199
$V(x,y)$	5.0779	5.0178	4.4693	4.3977	4.1285	3.9959	3.6648
$V(sa,pc)$	4.4800	4.4607	3.0354	3.0205	4.9601	4.9078	4.9121
$V(sc,pa)$	5.7839	5.7413	5.4389	5.3894	4.6675	4.5880	4.2137
$V(s^*a,pc)$	4.4378	4.3083	3.3744	3.2191	4.9895	4.6951	4.3662
$V(s^*c,pa)$	4.8083	4.6473	3.9097	3.7234	4.2180	3.8791	3.0739
λ_a	0.0	0.1338	0.0	0.1385	0.0	0.3202	0.0
λ_c	0.0	0.0553	0.0	0.1290	0.0	0.0573	0.0

	InSb		InP		GaP	
$E(s,a)$	−8.0157	−8.0157	−8.5274	−8.5274	−8.1124	−8.1124
$E(p,a)$	0.6738	0.4033	0.8735	0.8285	1.1250	1.0952
$E(s^*,a)$	6.4471	6.1766	8.2579	8.2129	8.5150	8.4796
$E(s,c)$	−3.4643	−3.4643	−1.4826	−1.4826	−2.1976	−2.1976
$E(p,c)$	2.9162	2.6456	4.0465	4.0015	4.1140	4.0851
$E(s^*,c)$	5.9423	5.6717	7.0726	7.0726	7.1850	7.1563
$V(s,s)$	−5.5193	−5.5193	−5.3615	−5.3615	−7.4909	−7.4909
$V(x,x)$	1.4018	1.4018	1.8801	1.8801	2.1516	2.1516
$V(x,y)$	3.8761	3.7351	4.2324	4.2084	5.1369	5.1213
$V(sa,pc)$	3.7881	3.7455	2.2266	2.2227	4.2771	4.2724
$V(sc,pa)$	4.5900	4.5017	5.5825	5.5642	6.3190	6.3075
$V(s^*a,pc)$	3.5641	3.2591	3.4607	3.4081	4.6541	4.6184
$V(s^*c,pa)$	3.4073	3.0371	4.4848	4.4187	5.0950	5.0534
λ_a	0.0	0.3064	0.0	0.0244	0.0	0.0222
λ_c	0.0	0.1234	0.0	0.1426	0.0	0.0578

no fit of the b and d deformation potentials. These deformation potentials, corresponding to shear deformations, are not dependent on $n_{\alpha\beta}$. A good description of b and d then directly follows from the tight-binding description of unstrained compounds. It is possible to get better values of these deformation potentials by introducing some dependence of diagonal interactions $H_{\alpha\alpha}$ with distance,[14] taking into account the crystal-field effect. Then some "crystal-field parameters" have to be introduced which now allow a fit of b and d. However, b and d are not known experimentally with an excellent accuracy, so that the improvement of their values is of the order of the experimental precision and does not justify the increase in complexity of the theoretical description.

In conclusion, we have pointed out that strain effects on semiconductor band structures can be well described in a tight-binding framework. The deformation potentials are obtained by introduction of simple strain-dependent modifications of tight-binding parameters. We have derived a variation law for these modifications that can be used for several compounds. This can be useful for the study of strained systems (we have just obtained in this way very encouraging results for strained quantum wells, which will be the purpose of a forthcoming paper).

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[1]G. C. Osbourn, Phys. Rev. B **27**, 5126 (1983).
[2]C. Priester, G. Allan, and M. Lannoo (unpublished).
[3]P. Vogl, H. P. Hjalmarson, and J. D. Dow, J. Chem. Solids **44**, 365 (1983).
[4]T. G. Andersson, Z. G. Chen, V. D. Kulakovskii, A. Uddin, and J. T. Vallin, Appl. Phys. Lett. **51**, 752 (1987).
[5]J. W. Matthews and A. E. Blakeslee, J. Cryst. Growth **27**, 118 (1974).

[6]E. O. Kane, Phys. Rev. **178**, 1368 (1969).

[7]F. H. Pollak and M. Cardona, Phys. Rev. **172**, 816 (1968).

[8]C. G. Van de Walle and R. M. Martin, Phys. Rev. B **34**, 5621 (1987).

[9]O. H. Nielsen and R. M. Martin, Phys. Rev. B **32**, 3792 (1985).

[10]C. Kittel, *Introduction to Solid State Physics,* 3rd ed. (Wiley, New York, 1967), Chap. 4.

[11]W. Harrison, *Electronic Structure and the Properties of Solids* (Freeman, San Francisco, 1980), Chap. 8.

[12]W. A. Harrison, Phys. Rev. B **24**, 5835 (1981); see Ref. 11, Chap. 6.

[13]A. Blacha, H. Presting, and M. Cardona, Phys. Status Solidi B **126**, 11 (1984).

[14]L. Brey and C. Tejedor, Phys. Rev. Lett. **39**, 1022 (1987); L. Brey, C. Tejedor, and J. A. Verges, Phys. Rev. B **29**, 6840 (1984).

[15]Shang Yuan Ren, J. D. Dow, and D. J. Wolford, Phys. Rev. B **25**, 7661 (1982).

[16]O. K. Andersen, O. Jepsen, and D. Glötzel, in *Highlights of Condensed-Matter Theory,* edited by F. Bassani, F. Fumi, and H. P. Tosi (North-Holland, Amsterdam, 1985), p. 100.

[17]E. Kauffer, P. Pecheur, and M. Gerl, J. Phys. C **9**, 2319 (1976).

[18]H. A. Bethe, Ann. Phys. (Leipzig) **3**, 133 (1929).

[19]*Landolt-Börnstein: Numerical Data and Functional Relationships in Science and Technology,* edited by O. Madelung (Springer-Verlag, Berlin, 1982).

[20]D. J. Chadi, Phys. Rev. B **16**, 790 (1977).

[21]L. Brey, N. E. Christensen, and M. Cardona, Phys. Rev. B **36**, 2638 (1987).

[22]J. C. Slater and G. F. Koster, Phys. Rev. **94**, 1498 (1954).

[23]D. D. Nolte, W. Walukiewicz, and E. E. Haller, Phys. Rev. Lett. **59**, 501 (1987).

[24]M. Cardona and N. E. Christensen, Phys. Rev. B **35**, 6182 (1987).