

## Acoustic deformation potentials and heterostructure band offsets in semiconductors

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It is argued that the absolute hydrostatic deformation potentials recently calculated for tetrahedral semiconductors with the linear muffin-tin-orbital method must be screened by the dielectric response of the material before using them to calculate electron-phonon interaction. This screening can be estimated by using the midpoint of an average dielectric gap evaluated at special (Baldereschi) points of the band structure. This dielectric midgap energy (DME) is related to the charge-neutrality point introduced by Tejedor and Flores, and also by Tersoff, to evaluate band offsets in heterojunctions and Schottky-barrier heights. We tabulate band offsets obtained with this method for several heterojunctions and compare them with other experimental and theoretical results. The DME's are tabulated and compared with those of Tersoff's charge-neutrality points.

### I. INTRODUCTION

The matrix elements for the interaction between carriers and acoustic phonons at band extrema of semiconductors can be evaluated from the deformation potentials for uniform strain (dependence of band extrema on strain).<sup>1</sup> While this is straightforward for the shear (traceless) components of the strain, problems arise when handling the hydrostatic components which accompany *longitudinal* phonons.<sup>2</sup> The corresponding deformation potentials are defined, for an infinite solid, to an arbitrary constant which represents the variation of the arbitrarily chosen zero of energy with hydrostatic stress. This arbitrariness should, of course, disappear when dealing with the finite solids found in nature. It should, therefore, be possible to define absolute deformation potentials for a uniform hydrostatic strain with respect to a fixed energy, e.g., the energy at infinity or at a point sufficiently far from the sample. Such deformation potentials would correspond, for the bottom of the conduction band, to the variation of the electron affinity with strain and for the top of the valence band to that of the ionization potential (photoelectric threshold). They should, therefore, be affected by surface properties rather than being a bulk property. Their evaluation as surface dependent quantities represents a formidable theoretical problem. The deformation potentials required to evaluate the electron-phonon interaction for phonons of wavelength much smaller than the sample size should be, however, bulk quantities independent of surface details.

In a recent paper,<sup>2</sup> Vergés *et al.* suggested that the linear muffin-tin-orbital (LMTO) method<sup>3</sup> provides a natural way of overcoming this problem. In this method, the solid is broken up into atomiclike spheres and all potentials are referred to the reference level which is chosen so that the Hartree potential of a single atomic sphere is zero at infinity. The solid can be terminated at any sphere

while leaving the electronic charge distribution in this sphere equal to that it would have in the bulk. An attempt was made to evaluate in this manner the electron-phonon interaction constants relevant to longitudinal acoustic phonons.<sup>2</sup> In doing so, the problem of screening by the dielectric function of the solid was overlooked: unscreened hydrostatic deformation potentials were used.

While the perturbations produced by the shear components of phonons are only insignificantly screened, strong screening should take place for the hydrostatic strain of long-wavelength longitudinal phonons. The present paper addresses this problem. Using the one-dimensional Penn model for the dielectric function,<sup>4</sup> it is shown that the average of the hydrostatic deformation potentials of the valence and conduction states which form the Penn gap must be screened by the full dielectric function [we call the average of the conduction and valence energies at the Penn gap the dielectric midpoint energy (DME)]. Thus the deformation potential of the DME,  $a_D$ , must be partly compensated by the screening response  $a_D[1 - \epsilon^{-1}(q)]$ . This screening response must be subtracted from all deformation potentials calculated in Ref. 2 in order to obtain the appropriate electron-LA-phonon coupling constants.

In this paper, results obtained by this technique for the electron-phonon coupling constants of group-IV elements and III-V and II-VI compound semiconductors are tabulated and compared with the few experimental and some theoretical data available. The calculations are performed with the LMTO method at the first Baldereschi special point.<sup>5</sup> The relevance of the *screened* deformation potentials to the problem of the dependence of the lattice constant of semiconductors on doping with either donors or acceptors is also discussed.

The concept of a midgap energy has been recently introduced by Tejedor, Flores, and Louis<sup>6,7</sup> and by Tersoff<sup>8-10</sup> in connection with the lining up of the band struc-

tures across semiconductor-semiconductor (heterojunction) and semiconductor-metal interfaces (Schottky barriers). This midgap point has also been referred to as the charge-neutrality point.<sup>7-9</sup> We suggest that this midgap point is basically the same as the DME discussed here for the screening of the electron-LA-phonon interaction. We in fact use the DME's calculated with the LMTO method for the first Baldereschi special points to evaluate valence-band offsets in several lattice matched heterojunctions and compare them with other available experimental and theoretical results. In doing so, we discuss the value of the dielectric constant to be used for the screening, an average of that of both constituents somewhat reduced from that for  $q=0$  because of the abruptness of the junctions. We also present a tabulation of DME's with respect to the top of the valence band obtained with the LMTO special point method and compare it with calculations of the charge neutrality point performed by Tersoff.

## II. THE DIELECTRIC MIDPOINT ENERGY (DME)

As discussed in Refs. 1, 2, and 11, the LA phonon produces a perturbation on electronic band edges equivalent to a sinusoidal potential. This perturbation is different for each band edge. For long-wavelength phonons, this perturbation can be easily obtained by multiplying the strain associated with the phonon by a deformation potential which gives the change of the band edge energy-per-unit strain. It is helpful to decompose the local strain into irreducible symmetry components. For a cubic crystal they are the hydrostatic strain (multiple of the unit matrix), and two traceless strains which correspond to shear deformation along the  $\langle 100 \rangle$  and  $\langle 111 \rangle$  axes. The former will be strongly screened by the dielectric response of the crystal while the screening of the latter should be insignificant. Here we discuss the screening of the hydrostatic component, which was neglected in Ref. 2. We shall argue that there is a band energy, obtained as an average of the upper valence band and the lowest conduction band, whose deformation potential must be divided by the zero-frequency intrinsic dielectric response function  $\epsilon(q)$ . This energy will be called the dielectric midpoint energy (DME or  $E_D$ ), and its hydrostatic deformation potential  $dE_D/d\ln V$  ( $V$  is the volume) will be called  $a_D$ . For the wave vectors  $q$  involved in standard transport processes,  $\epsilon(q)$  will be practically equal to its value  $\epsilon$  for  $q=0$ . Large concentrations of free carriers will modify  $\epsilon(q)$  by adding to it their Lindhard polarizability.<sup>12,13</sup> We shall not consider this case here since our discussion can be trivially extended to deal with it. The unscreened deformation potential of all band extrema must be corrected by addition of the screening potential which acts on the DME.

The screening of an external electrostatic potential, acting equally on all band states, is rather trivial: it is performed simply by dividing the potential by  $\epsilon(q)$ . In the case of the perturbations generated by the hydrostatic strain which accompanies an LA phonon, the situation is not so simple since this perturbation is different for each band edge. Thus the notion of singling out some energy

(the DME) which can be screened by division by  $\epsilon(q)$  naturally arises. We give here a heuristic derivation of the DME used in this work. A more rigorous derivation is given in the Appendix.

Let us first discuss briefly the nature of the intrinsic dielectric response of zinc-blende-type semiconductors for  $\omega \approx 0$  (the acoustic phonons of interest here have frequencies much smaller than any characteristic frequency of the dielectric response) and  $q \approx 0$ . This response is generated by direct virtual transitions from the filled electronic states to the empty conduction states plus a small correction for the lattice polarizability (phonon contribution) in the case of ionic materials. We shall neglect this ionic contribution for the time being.

The simplest model for the dielectric response of semiconductors is the isotropic Penn model.<sup>4</sup> In this model, the valence band is described in a Jones zone which is symmetrized in  $k$  space by making it spherical. An average isotropic gap is then introduced between this band and the conduction bands, produced by the crystal potential. Thus the model is basically one-dimensional and the transitions around the "Penn gap" dominate the dielectric response. These concepts, in spite of their highly simplified nature, have been successfully applied to interpret many features related to the dielectric response of semiconductors.<sup>13,14</sup> The main feature we want to use now is the existence of a group of filled states clustered around a given valence-band energy  $E_V$  and a corresponding group of conduction states ( $E_C$ ) which mainly produce the dielectric response. Let us consider the unscreened perturbation induced by an LA phonon on these states, i.e., their hydrostatic deformation potentials. The valence electrons will polarize so as to partially screen this perturbation. One may, at first glance, think that this will take place by setting up an electrostatic potential whose effect will be to replace the hydrostatic deformation potential of the valence band  $a_V$  by  $a_V/\epsilon(q)$ , regardless of the value of the deformation potential of the conduction band. This is of course wrong, since filled valence states and empty conduction states must contribute symmetrically to the dielectric response. (An empty state is a hole. Electrons and holes must be treated on the same footing.) Hence we infer that the dielectric screening represented by division by  $\epsilon(q)$  must be applied to the average of  $a_V$  and  $a_C$ , i.e., to the deformation potential of a fictitious midgap state situated halfway between the conduction and valence states. The question of how to determine this state will be considered next.

The dielectric function  $\epsilon(\omega, q)$  can be calculated by performing a straightforward Brillouin-zone integration of energies and matrix elements for interband transitions.<sup>15</sup> An analysis of this integration (see, for instance, Fig. 6 of Ref. 16) suggests that the main contribution to  $\epsilon$  is for transitions from the two top valence bands (spin degenerate in Ge and Si but not in the zinc-blende structure) and the bottom two conduction bands (with the same degeneracy properties). Thus we shall consider only these bands here. The Brillouin-zone integration can be replaced by a sampling over a small number of so-called Baldereschi special points.<sup>5</sup> For the sake of simplicity, we shall use here the first Baldereschi point (and implicitly

the other 23 generated from it by the operations of the  $O_h$  point groups):

$$\mathbf{k}_B = (2\pi/a_0)(0.622, 0.295, 0). \quad (1)$$

We have calculated the energies of the two top valence bands and the two bottom conduction bands at  $k_B$  for a number of group-IV elements and, III-V and II-VI com-

pound semiconductors with the LMTO method.<sup>3,17</sup> The results are given in Table I for the lattice constants at zero pressure and temperature. For completeness, we have added to this table the energies of these bands at the  $\Gamma$ ,  $X$ , and  $L$  points of the Brillouin zone, points which are also of importance to the dielectric response.<sup>14,15</sup> The table also contains the deformation potentials  $a$  (i.e., the

TABLE I. Energies (in eV) of (a) the top of the valence band and (b) the bottom of the conduction band calculated with the fully relativistic LMTO method at the  $\Gamma$ ,  $X$ ,  $L$ , and  $B$  points. At the  $B$  (first Baldereschi) point, the average values of the inversion asymmetry split spin doublet are listed. The corresponding volume deformation potentials are also given.

	(a)				Deformation potentials $a$			
	$\Gamma_8$	Valence bands $X_7$	$L_{4,5}$	$B$	$\Gamma_8$	$X_7$	$L_{4,5}$	$B$
C	3.73	-2.73	0.91	-0.70	-15.42	-8.77	-12.59	-11.02
Si	-0.85	-3.76	-2.02	-2.99	-7.95	-5.06	-6.97	-5.62
Ge	-0.79	-4.03	-2.18	-3.19	-8.09	-4.28	-6.45	-5.15
$\alpha$ -Sn	-1.39	-4.26	-2.59	-3.53	-7.34	-3.60	-5.68	-4.46
AlP	-1.78	-3.95	-2.53	-3.26	-7.67	-5.39	-7.02	-5.98
AlAs	-1.51	-3.84	-2.35	-3.18	-6.46	-4.13	-5.71	-4.73
AlSb	-1.65	-3.96	-2.57	-3.43	-7.35	-4.41	-6.21	-5.02
GaP	-1.59	-4.32	-2.68	-3.51	-8.07	-4.43	-6.57	-5.34
GaAs	-1.07	-3.85	-2.19	-3.08	-8.77	-4.92	-7.15	-5.89
GaSb	-1.46	-4.18	-2.62	-3.56	-7.95	-4.10	-6.21	-4.97
InP	-2.08	-4.39	-2.99	-3.68	-6.91	-3.77	-5.59	-4.63
InAs	-1.94	-4.56	-2.94	-3.72	-7.83	-4.18	-6.29	-5.20
InSb	-1.95	-4.41	-2.94	-3.79	-7.31	-3.67	-5.72	-4.60
ZnSe	-2.80	-5.08	-3.67	-4.33	-8.62	-4.79	-7.09	-6.11
ZnTe	-2.28	-4.64	-3.22	-4.05	-9.49	-4.79	-7.51	-6.13
CdTe	-2.94	-4.94	-3.71	-4.41	-8.16	-4.45	-6.61	-5.60
HgTe	-2.45	-5.04	-3.43	-4.25	-10.45	-4.69	-8.02	-6.79

  

	(b)				Deformation potentials $a$			
	$\Gamma_6$	Conduction bands $X_6$	$L_6$	$B$	$\Gamma_6$	$X_6$	$L_6$	$B$
C	17.67	8.54	12.14	10.96	-39.71	-17.69	-39.92	-20.41
Si	2.15	-0.25	0.51	1.74	-20.97	-5.73	-11.49	-8.17
Ge	-1.11	-0.23	-0.85	1.66	-17.20	-6.55	-10.99	-8.71
$\alpha$ -Sn	-2.53 <sup>a</sup>	-0.91	-1.81	0.50	-15.28 <sup>a</sup>	-5.84	-9.18	-8.00
AlP	-1.38	-0.32	0.92	1.96	-16.81	-5.31	-11.51	-8.06
AlAs	+0.49	-0.30	-0.54	2.00	-13.83	-4.59	-9.96	-7.15
AlSb	-0.59	-0.73	-0.69	0.95	-15.78	-5.02	-9.91	-7.59
GaP	-0.03	-0.05	-0.11	1.78	-15.90	-5.82	-11.14	-9.11
GaAs	-0.94	+0.20	-0.35	2.04	-15.93	-6.59	-11.49	-10.06
GaSb	-2.01	-0.85	-1.47	0.75	-16.35	-6.51	-9.80	-9.08
InP	-1.58	-0.42	-0.76	1.26	-12.37	-5.23	-9.38	-9.92
InAs	-2.60	-0.85	-1.34	1.08	-14.49	-5.90	-10.18	-10.45
InSb	-2.72	-0.93	-1.82	0.30	-13.12	-6.51	-8.75	-9.39
ZnSe	-1.91	-0.02	-0.53	1.61	-13.26	-6.28	-10.59	-12.85
ZnTe	-1.68	-0.31	-0.44	0.93	-14.74	-6.54	-3.56	-11.21
CdTe	-2.73	-0.68	-1.56	0.18	-10.88	-5.88	-9.06	-11.10
HgTe	-3.66	-0.81	-2.18	-0.33	-12.88	-9.27	-10.24	-12.35

<sup>a</sup>This  $\Gamma_6$  state is now below the top of the valence and in agreement with experiment, see Groves and Paul (Ref. 64). In other cases in which this happens in the tables (e.g., Ge), it is an artifact of the LDA.

volume derivatives) of all the energies mentioned above. The LMTO calculations were fully relativistic, thus including spin-orbit interaction. In the ionic materials (III-V and II-VI compounds), the gap states at  $\mathbf{k}_B$  are split by spin-orbit (s.o.) interaction, the splittings being in all cases less than 0.3 eV. We have listed in Table I the average of the split bands since we feel that these are the values which should be used to determine the  $E_D$ . For the  $\Gamma$ ,  $X$ , and  $L$  points, the top of the valence bands are s.o. split. We list the true top without spin-orbit averaging.

The LMTO calculations just mentioned were performed with the local-density approximation (LDA) to the exchange-correlation potential. This approximation is known to lead to large errors ( $\sim 100\%$ ) in the gaps for direct excitations from the valence to the conduction bands.<sup>18,19</sup> These errors can be removed, in an "ad hoc" manner, by introducing additional potentials at the atomic cores.<sup>17</sup> We have not followed this procedure here since we do not know what its effect on the Baldereschi point states is. The energies listed in Table I are uncorrected LDA results.

The effect of LDA inaccuracies on the DME will be examined next. We list in Table II the values of the average dielectric gap or Penn gap calculated from the data of Table I at  $k_B(E_B)$ . We also list in this table the experimental values of the average dielectric gap  $E_g$  (page 42 of Ref. 20) and the strongest structure in the imaginary part of the dielectric function, usually labeled  $E_2$  (page 169 of Ref. 20) for the materials considered here. We note that the calculated  $E_B$ 's represent rather well the experimental  $E_g$ 's and  $E_2$ 's (deviations less than 10%). The absolute

errors due to the LDA are thus less than for the fundamental (lowest) gap at  $\Gamma$ . The relative errors are of course even smaller, actually insignificant within the semiquantitative nature of the present treatment.

We have also listed in Table I the hydrostatic deformation potentials of the various states under consideration, also calculated with the LMTO method. We should keep in mind that the residual LDA-induced errors seem to be rather small for these deformation potentials.<sup>2,17</sup>

We have listed in Table II the position of the DME with respect to the top of the valence band ( $E_D - E_V$ ) and the corresponding value for the charge neutrality points ( $E_T - E_V$ ) calculated by Tersoff.<sup>10</sup> We find an excellent agreement between these two quantities. This agreement is even more remarkable when one considers that  $E_T$  in Ref. 10 was obtained from first principles band structures after applying a rigid shift between valence and conduction bands so as to correct for the LDA error in the lowest gap (the so-called "scissors" operator). No such shift has been applied here. We have not investigated the source of this paradox.

### III. SCREENED ELECTRON LA-PHONON INTERACTION

As already mentioned, the screening potential which accompanies the LA-phonon perturbation corresponding to an unscreened hydrostatic deformation potential  $a$  (listed in Table I for several extrema) is obtained from the deformation potential of the DMP  $a_D$  with the expression:

TABLE II. Representative values  $E_B$ ,  $E_g$ , and  $E_2$  (in eV), for the Penn gap of several group-IV elemental and III-V and II-VI compound semiconductors.  $E_B$  has been calculated from the top valence and the bottom conduction bands at the Baldereschi point  $\mathbf{k}_B$ .  $E_g$ , from the tabulation in Ref. 20, represents the average gap obtained from  $\epsilon(0)$  with the Penn model.  $E_2$  is the energy of the major structure in  $\epsilon_2(\omega)$  (also from Ref. 20). We also have listed in this table the lattice constant of these materials, the dielectric midpoint energy  $E_D$  obtained from the Baldereschi point data, its difference to the top of the valence band ( $E_D - E_V$ ), and the corresponding difference for Tersoff's charge neutrality level  $E_T - E_V$  (from Ref. 10).  $a_0$  is the lattice constant in  $\text{\AA}$ .

	$E_B$	$E_g$	$E_2$	$E_D - E_V$	$E_T - E_V$	$E_D$	$a_0$
C	11.66	13.5	12.5	1.40		+ 5.13	3.57
Si	4.73	4.77	4.40	0.23	0.36	-0.625	5.43
Ge	4.85	4.31	4.3	0.03	0.18	-0.765	5.65
$\alpha$ -Sn	4.03	3.06	3.75	-0.12		-1.515	6.47
AlP	5.22	5.67		1.13	1.27	-0.65	5.47
AlAs	5.18	5.14	4.7	0.92	1.05	-0.59	5.66
AlSb	4.38	4.14	4.25	0.41	0.45	-1.24	6.13
GaP	5.29	5.75	5.27	0.73	0.81	-0.865	5.44
GaAs	5.12	5.20	4.85	0.55	0.50	-0.520	5.65
GaSb	4.31	4.12	4.1	0.06	0.07	-1.405	6.10
InP	4.94	5.16	4.8	0.87	0.76	-1.210	5.86
InAs	4.80	4.58	4.5	0.62	0.50	-1.32	6.05
InSb	4.09	3.73	4.08	0.20	0.01	-1.745	6.47
ZnSe	5.94	7.05	6.4	1.44	1.70	-1.36	5.65
ZnTe	4.98	5.74	5.3	0.73	0.84	-1.56	6.10
CdTe	4.59	5.79	5.0	0.83	0.85	-2.115	6.48
HgTe	3.92	5.0	5.0	0.16	0.34	-2.29	6.48

$$\Delta a_D = a_D [\epsilon^{-1}(\omega, q) - 1]. \quad (2)$$

For acoustic phonons  $\omega \approx 0$ . For intraband phonon scattering, we can also take  $q \approx 0$  and use the static,  $q$ -independent dielectric constant  $\epsilon$ . In Ge and Si,  $\epsilon$  is purely of electronic origin and thus the Penn gap or the first Baldereschi gap is its main source. The analysis of Sec. II applies to this electronic  $\epsilon$ . In ionic (III-V, II-VI) materials, there is a small contribution below  $\omega_{TO}$  (transverse optic frequency) which can be easily estimated from  $\omega_{TO}$  and  $\omega_{LO}$  (longitudinal optic frequency) with the Lyddane-Sachs-Teller relation.<sup>21</sup> It is not clear whether the DME analysis given in Sec. II also applies to the ionic contribution to  $\epsilon$ . Nevertheless, its effect in Eq. (2) is rather small since it amounts typically to  $\approx 10\%$  of  $\epsilon$  and Eq. (2) is dominated by the  $-1$  inside the brackets. We shall therefore neglect the ionic contribution of  $\epsilon$  and use for  $\epsilon$  only the ir, purely electronic contribution, sometimes called  $\epsilon_{ir}$  or  $\epsilon_\infty$ .

This dielectric constant is listed in Table III (from Ref. 22, p. 114) for the materials of interest here. We also list in this table the screening deformation potential  $\Delta a_D$  obtained with Eq. (1) from the data of Tables I ( $a_D$ ) and III ( $\epsilon$ ), the screened value of  $a_D$  ( $\bar{a}_D = a_D + \Delta a_D$ ), screened values are represented by a bar over the corresponding un-

screened ones), and the screened deformation potentials of the top valence extrema ( $\Gamma_8$ ) and that of the lowest conduction valleys ( $\Gamma_6$ ,  $\Delta_6$ , or  $L_6$  as indicated). We also list in this table values obtained recently by Tersoff<sup>23</sup> ( $a_V^c$ ) by matching his charge neutrality points and Van de Walle *et al.*<sup>24</sup> ( $a_V^e$ ) by calculating superlattices consisting of the same material stressed and unstressed. Since Tersoff's calculation implies infinite screening ( $\epsilon = \infty$ ), we have listed under  $a_V^d$  the values which result from adding  $\Delta a_D$  to  $\bar{a}_V^b$  and thus should be closer to the correctly screened  $\bar{a}_V$ 's.

We note that all theoretically predicted values of  $\bar{a}_V$  are small and rather similar in magnitude. The corrected values from the Tersoff data ( $\bar{a}_V^d$ ) fall between our calculations and those of Van de Walle *et al.* ( $\bar{a}_V^e$ ). The sign reversals which appear now and then between different calculations should not be taken too seriously: the absolute values are very small when compared with unscreened deformation potentials. Hence, even if the signs are different, the differences between the various estimates are small. If we add to these  $\bar{a}_V$ 's the deformation potential of a direct gap at  $\Gamma$ , we obtain in the cases in which the lowest conduction-band minimum is at  $\Gamma$  (all the materials under consideration with the exception of Ge, Si, AIP, AlAs, AlSb, GaP) the deformation potential of the lowest

TABLE III. Infrared dielectric constant  $\epsilon$  and various hydrostatic deformation potentials for the materials under consideration.  $\bar{a}_V$  and  $\bar{a}_c$  represent the screened deformation potentials of the highest valence and the lowest conduction states,  $\bar{a}_D$  that of the dielectric midgap point.  $\Delta a_D$  represents the effect of screening on the deformation potentials. All deformation potentials (in eV) were obtained as described in the text, unless otherwise indicated. In the cases of conduction-band minima along  $\langle 100 \rangle$  (Si, AIP, AlAs, AlSb, GaP, C) we took the deformation potentials to be those at  $X_6$  since these points are either the minima or very close to them.

	$\epsilon^a$	$\Delta a_D$	$\bar{a}_D$	$\bar{a}_V^b$	$\bar{a}_V^c$	$\bar{a}_V^d$	$\bar{a}_V^e$	$\bar{a}_C$
C	5.7	13.0	-2.8	-2.4				-4.7
Si	12	6.3	-0.5	-1.6	-0.4	-1.0	+0.8	+0.6
Ge	16	6.5	-0.4	-1.6	+0.65	+0.2	+1.8	-4.5
$\alpha$ -Sn	20	5.9	-0.3	-1.5				
AIP	8	6.1	-0.9	-1.5				+0.8
AlAs	9.1	5.3	-0.6	-1.2	+0.4	-0.2		+0.7
AlSb	10.2	5.7	-0.6	-1.2				+0.7
GaP	9.1	6.6	-0.6	-1.5				+0.8
GaAs	10.9	7.1	-0.7	-1.6	+0.65	-0.1	+0.7	-8.8
GaSb	14.4	6.5	-0.5	-1.4				-9.8
InP	9.6	6.5	-0.7	-0.4				-5.9
InAs	12.3	7.2	-0.6	-0.6				-7.3
InSb	15.7	6.5	-0.5	-0.8				-6.6
ZnSe	5.9	7.9	-1.6	-0.7				-7.4
ZnTe	7.3	7.5	-1.2	-2.0				-7.3
CdTe	7.2	7.2	-1.1	-1.0				-3.7
HgTe	9.3	8.5	-1.1	-2.0				

<sup>a</sup>From Ref. 22.

<sup>b</sup>Present calculations. Note that Cardona and Christensen (Ref. 65) have found that the calculated unscreened  $a_V$  for diamond is larger than the experimental one. The screened one given here is smaller but leads to better agreement with experiment.

<sup>c</sup>Theoretical, from Ref. 23.

<sup>d</sup>Theoretical, from Ref. 23 after adding  $\bar{a}_D$ .

<sup>e</sup>Theoretical, from Ref. 24.

$\Gamma$  conduction-band valley  $\bar{a}_c$ . Since the deformation potential of this gap is large ( $\sim -9$  eV), the differences just mentioned are not too important in giving the value of  $\bar{a}_c$ . We note that in Ref. 24,  $\bar{a}_c = -7.6$  eV is given for GaAs, which compares well with our result ( $\bar{a}_c = -8.8$  eV). The differences in  $\bar{a}_V$  reflect themselves more strongly in the values of  $\bar{a}_c$  for Ge ( $L_1$  band): in Ref. 24,  $\bar{a}_c = -1.0$  eV is found, as compared with our value of  $\bar{a}_c = -4.5$  eV. For Si ( $\Delta_1$  band), we find  $\bar{a}_c = +0.6$  while  $+3.1$  is found in Ref. 24. We should point out that a calculation of  $\bar{a}_V$  which was implied to include screening has been performed by Wiley<sup>25</sup> for a few group IV and III-V materials. It yields values of  $\bar{a}_V$  around  $+2.5$  eV. However, this calculation uses the vacuum level as reference and the empirical dependence of the ionization energy on lattice constant as a basis. Its connection with the  $\bar{a}_V$ 's required for the electron-phonon interaction problem is not obvious.

#### IV. COMPARISON WITH EXPERIMENT

We shall now compare the calculated values of  $\bar{a}_c$  given in Table III with experimental data. The most precise data should be found for the cases in which the conduction band minimum is at  $\Gamma$  since then no shear deformation potentials contribute to the scattering by LA phonons. Still, polar optical phonon and impurity scattering must be removed from experimental electron transport data in order to obtain the  $\bar{a}_c$ 's, hence the accuracy in the experimental determination of  $\bar{a}_c$  is not expected to be too large. This fact has been best illustrated by Zawadski<sup>26</sup> who has given a plot of the variation of the reported values of  $\bar{a}_c$  versus calendar year for InSb. They fluctuate between 4 and 30 eV, averaging around 12 eV, a value which comes close to the calculated unscreened one ( $-13.1$  eV) and thus must be too high. Two values are reported in the literature which are close to the calculated one for InSb ( $-6.6$  eV). They were found by rather reliable methods:  $|\bar{a}_c| = (4.5 \pm 0.5)$  eV was obtained by measuring the attenuation of an acoustic wave traveling through doped InSb in a magnetic field,<sup>27</sup>  $|\bar{a}_c| = 8.2$  eV was obtained from thermoelectric power in the phonon drag region.<sup>28</sup> Hot electron transport data<sup>29</sup> have yielded  $|\bar{a}_c| = 6.9 \pm 0.4$  eV, in excellent agreement with our calculations. We feel that other existing experimental determinations are more indirect and thus more subject to error than the ones just given, which bracket our calculated value of 6.6 eV. In the case of GaAs, there is by now also a considerable amount of data, especially since the discovery of the modulation doping technique<sup>30</sup> which enables one to dope GaAs by placing the impurities in an adjacent AlAs layer, thus partly avoiding impurity scattering. Analysis of low temperature mobility data for such AlAs-GaAs multiple heterojunctions yields  $|\bar{a}_c| = 13.5$  eV,<sup>31</sup> a result which has been criticized in Ref. 32 as disagreeing with data for *single* heterojunctions which yield  $|\bar{a}_c| = 7$  eV. Analysis of bulk mobility data in high-purity bulk GaAs also give the value  $|\bar{a}_c| = 7.0$  eV, in acceptable agreement with our value of 8.8 eV. We point out that 8.6 eV has also been given by Rode.<sup>33</sup> His values, however, are simply meant to be the pressure coef-

ficient of the gap and thus not very relevant to the problem at hand except for the nontrivial fact, proven here, that the  $\Gamma_{15}$  valence state, after screening, is affected very little by the hydrostatic strain of the LA phonon ( $\bar{a}_V \approx 0$ ). We should also point out that Vinter<sup>34</sup> has recently reinterpreted the data of Ref. 30 by using more accurate wave functions for the quantized electrons. He finds  $|\bar{a}_c| = 12$  instead of 13.5 eV, as found in Ref. 31. We feel that our value of 8.8 eV is also sufficiently close to 12 eV, although the discrepancy between 12 eV and the value found for bulk GaAs (7 eV) cannot be accepted.

We note that analysis of infrared absorption data for GaAs, to which many scattering mechanisms contribute, yields  $|\bar{a}_c| = 15.7$  eV.<sup>35</sup> We believe this value to be too high. High values ( $|\bar{a}_c| = 17.5$  eV) were also found from transport measurements in Ref. 36.

Low-field transport data are also available for InP. Their analysis yields the values  $|\bar{a}_c| = 14.5$  (Ref. 37) and 18 eV (Ref. 38) which would be compatible with our unscreened data ( $|\bar{a}_c| = 12.4$  eV) but cannot be reconciled with the screened value (5.9 eV). For InAs, the value  $|\bar{a}_c| = 11.5$  has been reported in Ref. 37, also higher than the calculated (screened) one (7.3 eV). It is not very likely that quadrupole scattering, of the type discussed by Lawaetz,<sup>39</sup> will provide the additional scattering mechanism to harmonize the theoretical and experimental values of  $|\bar{a}_c|$ .

The uncertainties just described get even worse for electron valleys off  $\mathbf{k} = 0$ , such as found in Ge, Si, GaP, and the Al compounds, as one has to include in the analysis the shear components of both TA and LA phonons. The value  $|\bar{a}_c| = 5.7$  eV found in Ref. 40 for Ge is in reasonable agreement with our calculations (4.5 eV). That given for Si in the same work  $|\bar{a}_c| = 3$  eV seems a little high (ours is 0.6 eV) although it agrees with the predictions of Ref. 24 ( $a_c = 2$  eV). Other experimental data are given in Ref. 2. We point out that a method to determine  $\bar{a}_c$ , including its sign, has been suggested in Ref. 41. It involves the measurement of LA-phonon self-energies versus  $\bar{q}$  in heavily doped silicon with neutron scattering. The experimental data seemed to favor  $\bar{a}_c \simeq -5$  eV. We have reevaluated these data for  $\bar{a}_c = 0$ . While the calculated curve seems to *deviate* from the experimental data twice as much as that obtained for  $\bar{a}_c = -5$ , we feel that the uncertainty of the data and the theoretical processing (which ignores electron mean-free path) is large enough to make  $\bar{a}_c \simeq 0$  acceptable.

The value  $|\bar{a}_c| = 9 \pm 1$  eV has been obtained by Kocsis for an analysis of transport data in GaP.<sup>42</sup> It is also much higher than that predicted here (0.8 eV).

#### V. DEPENDENCE OF LATTICE CONSTANT ON DOPING

Doping with electrically active atoms (donors or acceptors) is known to change the lattice constant of semiconductors.<sup>2,43,44</sup> We treat here the case of heavy doping, by "shallow" hydrogenic impurities, in which the excess electrons or holes have no ionization energy. As first suggested by Yokota,<sup>43</sup> the effect can be broken up into two components, one due to the cores of the dopant ions and the other to the hydrostatic deformation potential of the band

edge occupied by the free carriers. We shall describe the effect by the parameter  $\beta$ :

$$(\Delta a_0)/a_0 = \beta N_i, \quad (3)$$

where  $N_i$  is the dopant concentration and  $\beta$  will be given in units of  $10^{-24} \text{ cm}^3$ . Thus  $\beta = \beta_{\text{size}} + \beta_{e,h}$ , where  $\beta_{\text{size}}$  corresponds to the hard-core effect of the ions and  $\beta_e$  ( $\beta_h$ ) is the deformation potential effect for electrons (holes) given by:

$$\beta_{e,h} = \pm(\bar{a}_{c,v})/3B, \quad (4)$$

where  $B$  is the bulk modulus and the  $- (+)$  sign corresponds to electrons (holes). It was shown in Ref. 2 that the unscreened deformation potentials  $a_c$  ( $a_v$ ) give the correct sign of  $\beta_e$  ( $\beta_h$ ) but too large a magnitude (a factor of 2). As we shall see below (Table IV), agreement is improved if the screened  $\bar{a}_{e,h}$  are used. If no pinning of the Fermi energy at the surface would take place, the argument for using an unscreened deformation potential may be made since the corresponding strain would be uniform. In samples exposed to air, however, the Fermi energy is pinned at the surface, somewhere in the gap, and the strain produced by the free carriers will not be uniform, relaxing when the surface is approached to within a few tens of an angstrom (screening length). The material in this region will thus polarize and screen the deformation potential in the manner discussed in Sec. II. Thus we conjecture that the screened  $\bar{a}_c$  ( $\bar{a}_v$ ) should be used in Eq. (4).

We present in Table IV the total values of  $\beta$  determined experimentally ( $\beta_{\text{expt}}$ ) and those of  $\beta_e^{\text{expt}}$  ( $\beta_h^{\text{expt}}$ ) obtained from the experimental ones after subtracting the hard-core effect calculated from the ionic radii as discussed in Ref. 2 (see also Ref. 44) for Si, Ge, GaAs, and GaP with different dopants. With the exception of electrons in  $X$  valleys (Si and GaP), the agreement between  $\beta_e^{\text{expt}}$  and the values calculated from the  $\bar{a}_{c,v}$  with Eq. (4) is rather satisfactory, especially in view of the scatter in the experimental data. For the case of the  $X$  valleys, the opposite sign is obtained for  $\beta_{e,h}^{\text{expt}}$  and  $\beta_{e,h}^{\text{calc}}$ . We should keep in mind, however, that in this case  $\bar{a}_c$  is very small. A slight decrease in the screening  $\epsilon$  would suffice to reverse its sign and thus restore sign agreement between theory and experiment. In any case, the agreement in Table IV is considerably better than that shown in Table V of Ref. 2 for unscreened deformation potentials.

## VI. VALENCE-BAND OFFSETS AT HETEROJUNCTIONS

### A. Lattice-matched heterojunctions

As can be seen from the lattice constants  $a_0$  in Table I, many lattice-matched heterojunctions can be constructed with the materials under consideration here. It will become obvious in Sec. VIB that mismatches in  $a_0$  of less than 1% are negligible within the type of accuracy aimed at here ( $\approx 0.1 \text{ eV}$ ). We shall consider heterojunctions with  $a_0$  mismatches of less than 1% to be lattice matched; for the materials under consideration, the list of such heterojunctions is given in Table V. For each pair of materials, we give first that with the deeper valence-band top ( $\Gamma_{15}$ )

TABLE IV. Experimental values of  $\beta$ , the constant which expresses the doping-induced changes in  $a_0$ , for several semiconductors. The sources are given in Ref. 2 unless otherwise specified.  $\beta_{e,h}^{\text{expt}}$  represents the electronic contribution to  $\beta_{e,h}$  obtained as specified in the text while  $\beta_{e,h}^{\text{calc}}$  was obtained with Eq. (4).

Material Dopant and type	Germanium						GaAs			GaP		
	Si:e	P:e	As:e	Sb:e	Si:h	Ga:h	Si:e	Se:e	Te:e	Si:e	Ge:h	Te:e
$\beta^{\text{expt}}$	-1.3 <sup>a</sup>	+7.4 <sup>d</sup>	+1.3	+11	+3	+1.7 <sup>b</sup>	+3	+9.4	+11.6	+1	+1	+3.0 <sup>c</sup>
$\beta_{e,h}^{\text{expt}}$	+3.7	+9.0	+5.8	+12.4	+9.9	-1.9	+9.9	+16	+11	-2.2	-2.2	+0
$\beta_{e,h}^{\text{calc}}$	-0.7	+9.0	+9.0	+9.0	+18	-2.6	+18	+18	+18	-2.7	-2.7	-2.9

<sup>a</sup>Reference 66.

<sup>b</sup>Reference 67.

<sup>c</sup>Reference 68.

<sup>d</sup>Reference 69.

TABLE V. Valence-band ( $\Delta E_{\nu}^{A,B}$ ) offsets (in eV) for nearly lattice matched heterojunctions between several group-IV elements and III-V and II-VI compounds calculated by different methods compared with recent experimental data. The compound with the deeper valence band is listed first. A value of 0.7 eV has also been calculated *ab initio* by Ihm and Cohen for ZnSe-GaAs (Ref. 70).

	LMTO <sup>a</sup>	LMTO <sup>b</sup>	SCIC <sup>c</sup>	CNP <sup>d</sup>	Experiment
AlP/Si	0.92	0.91	1.03	0.91	
AlP/GaP	0.38	0.34	0.36	0.46	
AlAs/Ge	0.87	0.84	1.05	0.87	0.95 <sup>e</sup>
AlAs/GaAs	0.43	0.43	0.37	0.55	0.55, <sup>f</sup> 0.42 <sup>g</sup>
AlSb/GaSb	0.34	0.30	0.38	0.38	0.4 <sup>h</sup>
GaP/Si	0.53	0.57	0.61	0.45	0.80 <sup>i</sup>
GaAs/Ge	0.51	0.45	0.63	0.32	0.56 <sup>j</sup>
InSb/ $\alpha$ -Sn	0.34	0.39			
InAs/GaSb	0.55	0.54	0.38	0.43	0.51, <sup>k</sup> 0.57 <sup>l</sup>
ZnSe/Ge	1.46	1.57	2.17	1.52	1.52, <sup>m</sup> 1.29 <sup>m</sup>
ZnSe/GaAs	0.99	1.13	1.59	1.20	1.10 <sup>m</sup>
CdTe/ $\alpha$ -Sn	0.99	1.12			1.0 <sup>q</sup>
CdTe/InSb	0.66	0.73		0.84	0.87 <sup>n</sup>
CdTe/HgTe	0.64	0.61	0.23	0.51	0.35, <sup>o</sup> 0.12 <sup>p</sup>

<sup>a</sup>Present calculations, Eq. (5) with  $\bar{\epsilon}$  equal to  $\epsilon$  of Table III.

<sup>b</sup>Present calculations, Eq. (5) with  $\bar{\epsilon}=3.5$ .

<sup>c</sup>Self-consistent interface calculations (SCIC), from Refs. 45 and 46.

<sup>d</sup>Calculations based on charge-neutrality point, from Ref. 10.

<sup>e</sup>Reference 71.

<sup>f</sup>Reference 72.

<sup>g</sup>Reference 73.

<sup>h</sup>Reference 74.

<sup>i</sup>Reference 75.

<sup>j</sup>Reference 76.

<sup>k</sup>Reference 77.

<sup>l</sup>References 63 and 78.

<sup>m</sup>Reference 79.

<sup>n</sup>Reference 80.

<sup>o</sup>Reference 81.

<sup>p</sup>Reference 82.

<sup>q</sup>Reference 83.

after heterojunction formation.

The band offsets for the  $\Gamma_{15}$  states calculated by us, by Tersoff<sup>10</sup> and by Van de Walle and Martin<sup>45,46</sup> are given in Table V compared with the most recent (or reliable, as judged by the present authors) experimental data. Other theoretical and experimental data can be found in Refs. 10, 45, and 46.

The procedure we have used for our calculations is based on the calculation of the  $\Gamma_{15}$  valence bands using the LMTO method with respect to the reference level of the ASA which, except for surface dipoles, should represent the potential at infinity.<sup>2,7</sup> When bringing two materials together to form a heterojunction, a potential difference will appear which will be screened by the electronic polarizability in a way similar to that discussed in Secs. II and III for acoustic phonons. The phonons of relevance, however, are of wavelength much larger than the lattice constants while for the heterojunction the potential variation occurs in a region of a depth typically equal to about  $a_0/2$ .<sup>4,46</sup> It is therefore questionable whether it is legitimate to screen with the full dielectric constant. We thus use now an effective dielectric constant  $\bar{\epsilon}$  and consider this question in more detail below. The expression for the band offset between two materials  $A$  and

$B$  can thus be written:

$$\Delta E_{\nu}^{A,B} = E_{\nu}^B - E_{\nu}^A - (E_D^B - E_D^A)(\bar{\epsilon} - 1)/\bar{\epsilon} \quad (5)$$

where  $E_{\nu}$ 's represent the energies of the  $\Gamma_{15}$  top of the valence band (including s.o. splitting), which are listed in Table I. The sign of Eq. (5) has been chosen such that if  $A$  has a deeper valence band,  $\Delta E_{\nu}^{A,B}$  is positive. The effective dielectric constant  $\bar{\epsilon}$  can be taken to be an average of the  $q=0, \omega=0$  data for both materials, listed in Table III. As already mentioned, however, this probably overestimates the screening. A possible approach to correct this deficiency would be to estimate or assume a one-dimensional variation of  $E_B$  with  $z$  at the interface, decompose it into one-dimensional Fourier components and screen each according to the calculated  $\epsilon(q)$  averaged, of course, for both materials.<sup>47</sup> For an interface with a transition region of width  $\approx a_0/2$ , as expected for [100] heterojunction planes, and a linear variation of the potential within this region, we find a maximum in the Fourier component of the potential for  $q_M \approx 5.6 \times d^{-1}$ . Figure 7 of Ref. 47 shows that for Ge, GaAs, and ZnSe,  $\epsilon(q_M) \approx 2.3$ . One may, therefore, be tempted to use this value for  $\bar{\epsilon}$  in Eq. (5), regardless of material. This is a point of view similar to that adopted in Ref. 7, where it



was suggested, as a result of microscopic calculations for the interface, that  $\bar{\epsilon}=3.5$  regardless of material. The work of Tersoff, however, requiring exact lineup of  $E_V^A$  and  $E_V^B$ , implies  $\bar{\epsilon}=\infty$  in the spirit of Eq. (5). ( $E_T \approx E_D$  according to Table II.) (See Note added in proof.)

Fortunately, the band offsets  $\Delta E_V^{A,B}$  calculated with our formulation do not depend critically on the value of  $\bar{\epsilon}$  because the values of  $E_D$  are very similar for materials which yield well-ordered heterojunctions (see Table II). In order to illustrate the differences in band offset estimates produced by the uncertainty of  $\bar{\epsilon}$ , we present in Table V calculations for lattice-matched pairs of materials performed by replacing into Eq. (1) the energies of Tables I and II, with two values of  $\bar{\epsilon}$ , the average of those listed in Table III for both components ( $q=0$  assumption), and  $\bar{\epsilon}=3.5$  as suggested in Ref. 7. The difference between both predictions is small and no trends are apparent that may help us to describe which ansatz is preferable for  $\bar{\epsilon}$ . Table V clearly exposes the fallacy of the so-called common anion rule<sup>48,49</sup> (small band offset for common anions), a fact which has been also recently recognized by Tersoff.<sup>50</sup> The band offsets for pairs of materials with

common anions are not particularly smaller than for other cases in which the anions are not common (e.g., InAs-GaSb).

## B. Lattice-mismatched heterojunctions

Several heterojunctions with constituents differing in their lattice constants up to  $\sim 7\%$  can be prepared. We discuss here the pairs Ge-Si ( $\delta=\Delta a_0/a_0=0.04$ ), GaAs-Si ( $\delta=0.04$ ), and GaAs-InAs ( $\delta=0.07$ ). If the thickness of one of the materials is small ( $< 50$  Å for the cases mentioned) and that of the other large (substrate), the lattice constant of the thin component along the interface will match that of the substrate: the thin material will thus be strained. As it becomes thicker, the lattice mismatch (strain) is relieved through misfit dislocations. In the latter case, the theory of the previous subsection is applicable. In the former, one must correct for the hydrostatic and shear components of the strain. We thus decompose the strain tensor of the strained component as follows:

$$\delta \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -2C_{12}/C_{11} \end{pmatrix} = \delta_H \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} + \delta_S \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 2 \end{pmatrix},$$

$$\delta_H = \frac{2}{3}\delta(1 - C_{12}/C_{11}), \quad \delta_S = -\frac{1}{3}\delta(1 + 2C_{12}/C_{11}), \quad (6)$$

where  $C_{12}$  and  $C_{11}$  are elastic stiffness constants. Equation (6) is valid for a (001) interface; generalization to other interfaces is trivial.

The correction of the values of  $\Delta E_V^{A,B}$  obtained with Eq. (5) from the energies of the unstrained components (Tables I and II) for the hydrostatic component of the strain is straightforward. If  $A$  is the strained component of the heterojunction, one must add to  $\Delta E_V^{A,B}$ :

$$\Delta E_H^{A,B} = (-a_V^A + a_D^A(\bar{\epsilon}-1)/\bar{\epsilon})\delta_H.$$

The values of the volume coefficients of the  $\Gamma_{15}$  valence band  $a_V^{A,B}$  and those for the DME  $a_D^{A,B}$  are listed in Tables I and III. We note that the  $a_V$ 's and  $a_D$ 's have the same sign and about the same magnitude for all materials. Hence, effects of  $\delta_H$  on  $\Gamma_{15}$  and the DME are nearly the same and compensate each other. Actually, the  $a_V$ 's are somewhat larger in magnitude than the  $a_D$ 's and this effect is accentuated through multiplication by  $(\bar{\epsilon}-1)/\bar{\epsilon}$ . Hence a residual effect remains which tends to lower the  $\Gamma_{15}$  valence edge for the  $A$  material in the case  $\delta_H > 0$  (i.e.,  $a_0^A > a_0^B$ ). We consider next the cases of special interest.

### 1. Silicon-germanium

Let us take material  $A$  to be silicon (strained) and  $B$  germanium (unstrained). We find

$$\Delta E_H^{A,B} = 1.6\delta_H = +0.02 \text{ eV}.$$

Thus in this case  $\delta_H$  slightly increases the band offset be-

tween Si and Ge which for the unstrained materials is calculated to be 0.19 eV. If the strain is in the germanium side (compression), we find similarly:

$$\Delta E_H^{A,B} = -1.6\delta_H = -0.02 \text{ eV}, \quad (7)$$

thus the magnitude of the effect is the same in both cases.

The treatment of the pure shear component of the strain is more complicated, especially if the strained component is silicon. In this case, the  $\Gamma_8$  valence band splits into two and the strain couples it to its spin-orbit-split component  $\Gamma_7$ .<sup>51</sup> Since the coupling energy is larger than the spin-orbit splitting of Si (0.04 eV), the resulting shifts are strongly nonlinear in strain. These complications can be eliminated by treating the band offset for the average of the six  $\Gamma_{15}$  valence bands, the four  $\Gamma_8$ 's and two  $\Gamma_7$ 's, as discussed in Refs. 46 and 52: the effect of the pure shear component of the strain  $\delta_S$  on the valence bands then disappears. The offset for the average valence bands of Ge and Si thus becomes  $\Delta E_{V,av}^{A,B} = 0.12$  eV, much smaller than the values calculated by Van de Walle and Martin (0.54 eV) (Refs. 46 and 52) with an "ab initio" pseudopotential method which is expected to give a better representation of the interface than the calculations performed here.

The experimental situation is, as for most heterojunctions, somewhat confused. Maybe the most reliable relevant data are those recently obtained for Si-Si<sub>1-x</sub>Ge<sub>x</sub> multiple quantum wells, for  $x$  up to  $\simeq 0.5$ .<sup>53,54</sup> An analysis of transport and other data enables the authors to

deduce the relative positions of the lowest conduction bands in the two components, now split by the uniaxial stress. It is concluded in Refs. 46 and 52 that these data require band offsets which extrapolate for  $x \rightarrow 1$  to  $\Delta E_{V,av}^{A,B} > 0.5$  eV. Most other experimental data, however, yield somewhat smaller values of this offset, although neither the nature of the interface nor the strain is usually specified.<sup>55-57</sup> The photoemission work of Margaritondo *et al.*<sup>56</sup> yields  $\Delta E_{V,av}^{A,B} = 0.2$  eV which, assuming that no uniaxial strain is present, would correspond to  $\Delta E_{V,av}^{A,B} = 0.1$  eV, a result which would agree with ours. However,  $\Delta E_{V,av}^{A,B} = 0.4 \pm 0.1$  eV was obtained in Ref. 57, using the same technique.

We note that Tersoff's calculations<sup>10</sup> yield a value of  $\Delta E_{V,av}^{A,B} = 0.25$  eV for Si-Ge. Since these calculations do not include any uniaxial stress, they correspond to  $\Delta E_{V,av}^{A,B} = 0.15$  eV, a number which agrees with our estimates. In view of the reliability of the calculations of Van de Walle and Martin,<sup>52</sup> we should examine the possibility that the difference between data based on midgap points (Tersoff's, ours) and theirs may be due to the uniaxial component of the stress.

For a (001) interface between materials with different lattice constants, the first Baldereschi points [Eq. (1)] are not all equivalent after the strain of Eq. (6) appears: they split into three groups of eight each. The question then arises of which of the split points must be matched with that of the unstrained material. We have not calculated the splitting of these points because of the complications which arise in the LMTO method when shear strain is present. We give, however, a simple model which enables us to make a crude estimate of the splitting and its effects on the matching across the interface.

Let us consider the Penn model of the electronic polarizability and the changes induced by strain, of both types described in Eq. (6), on the Penn gap and on  $E_D$ . The changes induced by  $\delta_H$  and  $\delta_S$  are, in principle, independent of each other. If we assume, however, that the change along a direction  $\mathbf{k}$  of  $\mathbf{k}$  space is given solely by the compression along this direction, the hydrostatic and the shear change become related through the expression (for  $E_D$ ):

$$\Delta E_D(\mathbf{k}) = (\Delta a_D)(\mathbf{k} \cdot \underline{\epsilon} \cdot \mathbf{k}) \quad (8)$$

where  $\underline{\epsilon}$  represents the strain tensor. Thus, for a shear strain  $E_D$  will depend on the direction of  $\mathbf{k}$  and we must consider how to average the various  $E_D(\mathbf{k})$  so as to obtain the one to be matched across a (001) interface. We note that a similar model was successfully used in Ref. 14 to explain the sign and magnitude of the long-wavelength stress-induced birefringence.

We call  $\theta$  the angle between  $\mathbf{k}$  and the (001) direction.  $\Delta E_D(k)$  can thus be written, for the pure shear component of the strain of Eq. (6):

$$\Delta E_D(k) = (\Delta a_D)\delta_S(2\cos^2\theta - \sin^2\theta) \quad (9)$$

In order to decide which value of  $\Delta E_D(\mathbf{k})$  to use for the matching across the interface, we consider the fact that in the Penn model, the states along  $\mathbf{k}$  only contribute to the polarizability along  $\mathbf{k}$ . Hence, if we want to consider the effect of the dielectric response on the  $\Delta E_D(\mathbf{k})$  of Eq. (9),

we must multiply this equation by  $\cos^2\theta$  and average it for all directions of  $k$ . We find

$$\begin{aligned} \langle \Delta E_D \rangle_{(001)} &= (\Delta a_D)\delta_S(2\langle \cos^4\theta - \sin^2\theta\cos^2\theta \rangle) / \langle \cos^2\theta \rangle \\ &= \frac{4}{5}(\Delta a_D)\delta_S \end{aligned} \quad (10)$$

The average of  $\cos^2\theta$  in the denominator of Eq. (10) has been introduced to take into account that such average appears for a pure hydrostatic strain. For a Si-Ge interface with Si under strain and Ge unstrained, we find with Eq. (6) that  $\delta_S = -0.024$ . With  $\Delta a_D = 6.3$  eV (Table III), we finally obtain  $\langle \Delta E_D \rangle_{001} = -0.12$  eV. The sign of  $\langle \Delta E_D \rangle_{001}$  just found is such that it increases the band offset between Si and Ge and thus brings our calculated value closer to those of Van de Walle and Martin. Nevertheless, our calculated value will now be 0.22, still too small when compared with that of those authors (0.54 eV). Van de Walle and Martin also calculated a Si-Ge heterojunction between *cubic* Si and Ge with *the same* lattice constant. They found a band offset of 0.40 eV. The difference to the case in which Si was allowed to expand along the  $z$  axis, 0.14 eV,<sup>52</sup> does agree with the estimate of the effect of the uniaxial stress performed above. Hence the discrepancy between our result of 0.27 eV and that of Ref. 52 (0.54 eV) is still unanswered.

A reason for this discrepancy may be found in the fact that the spectrum of  $\epsilon_2(\omega)$  of Si differs considerably from that of Ge.<sup>20</sup> This is the spectrum of virtual transitions which contribute to the polarizability for  $\omega = 0$ . Both Ge and Si have a peak in  $\epsilon_2(\omega)$  at  $\sim 4.3$  eV (listed as  $E_2$  in Table II). They also have a peak, usually labeled  $E_1$ , at 2.1 in the case of Ge and at 3.4 for Si. Hence the shape of  $\epsilon(\omega)$  is considerably changed in Ge with respect to that of Si. The increase in  $E_1$  in the latter is responsible for the fact that the dielectric gap  $E_g$  of Si is  $\simeq 4.8$  eV, as compared to 4.3 for Ge. The  $E_1$  peak, due to transitions along  $\langle 111 \rangle$ , is not well sampled by the first Baldereschi point (see Table II; actually  $E_D = 4.73$  eV for Si, smaller than the value of 4.85 eV calculated for Ge!). Inclusion of two Baldereschi points,  $(2\pi/a_0)(\frac{3}{4}, \frac{1}{4}, \frac{1}{4})$  and  $(2\pi/a_0)(\frac{1}{4}, \frac{1}{4}, \frac{1}{4})$ , would remedy this problem as they include the transitions along the  $\langle 111 \rangle$  directions responsible for  $E_1$ . Since the valence bands of both materials are very similar, the discrepancy just discussed must reflect itself in a higher  $E_D$  for Si than for Ge, in excess of the difference between the  $E_D$  calculated at the  $\mathbf{k}_B$  (Table II). We estimate this additional increase in the  $E_D$  of Si to be  $\simeq 0.3$  eV, which would bring our estimate of the offset to 0.52 eV, now in agreement with the data of Ref. 52.

## 2. GaAs-Si

We now discuss the GaAs-Si heterojunction ( $\delta = 0.04$ ). Using the method described above, we find for a lattice-mismatched cubic heterojunction an average band offset ( $\Delta E_{av}^{A,B}$ ) of 0.48 eV. For lattice-matched heterojunctions, the hydrostatic strain lowers this value to 0.35 eV if only the GaAs is strained and to 0.34 eV if only Si is strained. The shear correction of Eq. (10) brings this value down to 0.21 eV in the former case and to 0.22 eV in the latter. This is in reasonable agreement with Van de Walle's cal-

culations, which yield 0.12 eV for strained GaAs and 0.14 eV for strained Si.<sup>46</sup>

We note that an offset of 0.05 eV has been measured for this system by Margaritondo<sup>58</sup> for layers of GaAs deposited on Si. The state of the strain in this layer, however, was not known.

### 3. GaAs-InAs

We discuss next the GaAs-InAs heterojunction for which  $\delta=0.07$ . Our calculation without taking into account the strain yields actually an average  $\Gamma_{15}$  valence band for InAs lower than that for GaAs ( $\Delta E_{av}^{A,B} = -0.15$  eV). The hydrostatic correction brings this value up to  $-0.12$  eV. The uniaxial correction of Eq. (10) raises this value by 0.30 eV, up to  $\Delta E_{av}^{A,B} = +0.18$  eV, with the GaAs side now deeper than InAs. This is in rather good agreement with the value of 0.11 eV calculated by Martin and Van de Walle.<sup>46,59</sup> The same value (+0.18 eV) is found with our method for a strained GaAs layer. It agrees even better with the results of Refs. 46 and 58 (+0.21 eV).

We note that for this system, an offset  $\Delta E_V = 0.17 \pm 0.07$  eV was measured by Kowalczyk *et al.*<sup>60</sup> The heterojunction was formed by a thin layer of InAs deposited on a GaAs substrate. Because of the large spin-orbit splittings of the  $\Gamma_{15}$  valence states ( $\Delta_0 = 0.34$  for GaAs, 0.38 for InAs), the nonlinear contributions to the strain splittings of the top of the valence band are negligible. So is the difference in the spin-orbit splittings. The linear splitting of the  $\Gamma_8$  valence band of InAs by the uniaxial strain, however, should lift the top of the valence band of InAs by about 0.34 eV with respect to that of unstrained GaAs (we have used for this estimate the strain deformation potential  $b = -1.8$  eV given in Ref. 61), thus increasing the band offset estimated here to  $\Delta E^{A,B} = 0.52$  eV, now much higher than the experimental one [ $0.17 \pm 0.07$  eV (Ref. 60)]. A plausible explanation for the discrepancy is partial relaxation of the large shear component of the strain in the deposited InAs layer.

## VII. CONCLUSIONS

We have shown that the valence- and conduction-band edges calculated at the first Baldereschi special points ( $\mathbf{k}_B$ ) for group-IV elemental and III-V and II-VI compound semiconductors can be successfully used to estimate the effect of screening on the hydrostatic deformation potentials used to calculate the electron-phonon interaction. This procedure introduces the concept of a dielectric midgap point, somewhat similar to Tersoff's charge-neutrality point, but arrived at in a rather different, simpler manner. The results so obtained for the electron-phonon coupling constant yield reasonable agreement with available experimental data when the most reliable ones of the many available and conflicting data are chosen. They probably can be used as a guide to choose among such conflicting data. The screened deformation potentials so obtained also improve agreement of experimental and calculated values of the change in lattice constant with doping in heavily doped semiconductors.

The ideas used for the evaluation of screening effects on electron-phonon interaction constants can also be used to calculate the effect of screening on the band offset at heterojunctions obtained from the absolute energies calculated with the LMTO method. This procedure is straightforward in the case of nearly lattice-constant-matched pairs of materials (less than 1% mismatch). For strongly mismatched pairs, the effects of the hydrostatic and the uniaxial components of the resulting strain must be included. The former is straightforward to evaluate. The latter is estimated on the basis of a generalized Penn model which considers the inequivalence of the various points of the star of  $\mathbf{k}_B$  after a shear strain is applied. Reasonable agreement with *ab initio* pseudopotential calculations for the same interfaces is obtained. The screening of the shear strain should also contribute small additional terms to the electron-phonon interaction constants which are similar to the octopole terms discussed by Lawaetz.<sup>39</sup> They have not been considered here any further.

In a recent paper, Priester *et al.* have performed a self-consistent tight binding calculation of the Ge-GaAs interface.<sup>62</sup> They use as reference  $sp^3$  hybrids instead of the DME utilized here. They find for that system a band offset of 0.65 eV, only slightly higher than ours (0.51 eV). It has also come to our attention that Claessen *et al.*<sup>63</sup> have measured the dependence of the valence-band offsets on pressure for InAs-GaSb superlattices. They find this offset to increase at the rate 4.2 meV/kbar. Using the method discussed here, we also find an increase of this offset with pressure, but at a smaller rate, namely, 1.5 meV/kbar.

*Note added in proof.* W. A. Harrison and also J. C. Durán, F. Flores, C. Tejedor, and A. Muñoz (unpublished) have recently calculated that the effective dielectric constant  $\bar{\epsilon}$  of Eq. (5) should be rather close to that for  $q=0$ . If we accept this conclusion, the LMTO<sup>a</sup> data of Table V should be preferred to the corresponding LMTO<sup>b</sup> data. A value of  $\bar{\epsilon}_c = 11 \pm 1$  eV has been recently obtained by K. Hirakawa and H. Sakaki [Appl. Phys. Lett. 49, 14 (1986)] by investigating electron relaxation processes in AlGaAs-GaAs heterojunctions.

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## APPENDIX

The dielectric response of a semiconductor to a low-frequency potential  $V(r) = V_0 e^{iqr}$  (time dependence omitted), such as that created by longitudinal acoustic phonons, can be approximately obtained with the Penn

model.<sup>4</sup> This model replaces the Jones zone by a sphere of radius  $k_p$  and introduces an isotropic gap, the Penn gap  $E_p$ , between the occupied and unoccupied states at the boundary of the spherical Jones zone. The model is basically equivalent to that of a one-dimensional semiconductor with a gap at the edge of the Brillouin (Jones) zone. In order to obtain the dielectric response, we must evaluate the matrix element of  $V(r)$  for virtual transitions between the valence and the conduction band in the neighborhood of  $E_p$  (we implicitly neglect umklapp processes in the dielectric response). For  $q \rightarrow 0$ , this matrix element tends to zero, hence we evaluate it for  $q$  small but finite. The

gap then takes place between valence states at  $k_p - q/2$  and conduction states at  $k_p + q/2$ . Using  $\mathbf{k} \cdot \mathbf{p}$ -perturbation theory, the corresponding eigenstates can be written as

$$\begin{aligned} |c, k_p + q/2\rangle &= (|c, k_p\rangle + (Pq/2E_p)|v, k_p\rangle)e^{iqr/2}, \\ |v, k_p - q/2\rangle &= (|v, k_p\rangle + (Pq/2E_p)|c, k_p\rangle)e^{-iqr/2}, \end{aligned} \quad (\text{A1})$$

where  $c$  and  $v$  denote the conduction and valence bands, respectively, and  $P$  is the interband matrix element of  $\mathbf{p}$ . The interband matrix element of  $V(r)$  is readily obtained from Eqs. (A1):

$$\langle c, k_p + q/2 | V(r) | v, k_p - q/2 \rangle = \frac{1}{2} Pq/E_p [\langle c, k_p | V_q | c, k_p \rangle + \langle v, k_p | V_q | v, k_p \rangle]. \quad (\text{A2})$$

$V_q$  must be understood as the self-consistent sum of the applied unscreened potential and the dielectric response. If the former is an external electrostatic potential, both matrix elements in the rhs of Eq. (A1) become equal and the dielectric response reduces the external potential  $V_{\text{ex},q}$  to a total potential  $V_q = V_{\text{ex},q}/\epsilon(q)$ , where  $\epsilon(q)$  is the static,  $q$ -dependent dielectric function. For  $q$  smaller than about 0.2 times  $2\pi/a_0$  ( $a_0$  = crystallographic lattice constant),  $\epsilon(q)$  is nearly equal to the value at  $q=0$ . At  $q = 2\pi/a_0$ , it reduces to a smaller value, close to that obtained by Tejedor and Flores<sup>7</sup> for the screening of band offsets in heterojunctions.

In the case of the unscreened potential induced by the hydrostatic component of the strain of a longitudinal acoustic phonon,  $\langle c, k_p | V_q | c, k_p \rangle$  and  $\langle v, k_p | V_q | v, k_p \rangle$  are not equal since the corresponding deformation poten-

tials usually differ (the Penn gap depends on hydrostatic strain). Nevertheless, Eq. (A2) indicates that the calculation of the screened response is basically the same as that for an electrostatic potential provided one replaces this potential by the average of the potentials seen by the valence and the conduction bands. This *average* must be screened by dividing by  $\epsilon(q)$ . Hence the deformation potentials obtained in Ref. 2 must be corrected for the effect of screening on the deformation potential of the *dielectric midpoint energy* (average of the conduction and valence bands which form the Penn gap) before using them to evaluate the electron-phonon interaction. A similar correction should be applied to the difference in absolute band energies in order to obtain band offsets in heterojunctions.

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