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Energy-band structure of GaAs and Si: A *sps** k·p method

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A twenty-band $\mathbf{k}\cdot\mathbf{p}$ Hamiltonian taking into account the spin-orbit coupling is used to describe the valence band and the first two conduction bands all over the Brillouin zone. The basis functions are sp^3s^*-like functions used in linear combination of atomic orbitals. To get the right dispersion up to the Brillouin zone edge, the influence of other bands (d bands) is mimicked via Luttinger-like parameters in the valence band and in the conduction band. The method is applied to GaAs and Si. A satisfying agreement is obtained near the band extrema as well in the direct gap semiconductor (GaAs) as in the indirect gap semiconductor (Si). In particular, while the $\mathbf{k}\cdot\mathbf{p}$ Hamiltonian parameters are adjusted to get the longitudinal mass 0.92 of the silicon conduction band, the transverse mass, which results from the calculation without further adjustment, is equal to 0.19 which is the experimental value.

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I. INTRODUCTION

The methods to calculate the band structures of semiconductors (SCs) can be schematically divided in two sets. The first set contains theories with few adjustable parameters such as the pseudopotential method[1] and the linear muffin-tin-orbital method.[2] In the best case only one adjustable parameter, the forbidden band gap, is required. By contrast the second set contains adjustable parameter theories, namely the linear combination of atomic orbitals[3] and the $\mathbf{k}\cdot\mathbf{p}$ method.[4] In linear combination of atomic orbitals it is not possible to account for the indirect forbidden gap if only first neighbor interactions are taken into account.[5] It is then necessary to use second neighbor interactions. From the viewpoint of numerical calculation the method of linear combination of atomic orbitals was greatly improved by Vogl *et al.*[5] who showed that the introduction of "localized pseudo-orbitals" of s symmetry (underlying s in the SC crystal or Γ_1 in group theory notation[6]) is very efficient to account for the first conduction band dispersion. The calculations are much simpler than those taking into account second neighbor interactions because it is a tight-binding (TB) method. The pseudo-orbitals are called s^* so that the Vogl method is known as the sp^3s^* model.[5] Each orbital enters either as a bonding state or an anti-bonding state which means that the model is a ten band model. Taking into account the spin leads to a twenty band model. Jancu *et al.*[3] improved the method taking into account d levels which allows us to cure most of sp^3s^* shortcomings. The method used by Jancu is a sp^3s^*d TB method. In the following, TB will stand as a shorthand notation of the Jancu's method. In the $\mathbf{k}\cdot\mathbf{p}$ method, the use of 15 basis states (at $\mathbf{k}=\mathbf{0}$), without taking into account the spin, allows one to account for the band structure of silicon and germanium as shown in Ref. 4. The $\mathbf{k}\cdot\mathbf{p}$ method was also used for a better understanding of linear-muffin-tin method via a 16×16 $\mathbf{k}\cdot\mathbf{p}$ Hamiltonian.[7] Other calculations including spin and using a 30×30 $\mathbf{k}\cdot\mathbf{p}$ Hamiltonian were also used.[4]

In this article, we propose a $\mathbf{k}\cdot\mathbf{p}$ method which uses a 20×20 basis as in sp^3s^* linear combination of atomic orbitals but which takes into account the influence of other levels, for example d levels, via Luttinger-like parameters. We call the method the sp^3s^*''d'' $\mathbf{k}\cdot\mathbf{p}$ method. The purpose of this article is to show the efficiency of the sp^3s^*''d'' $\mathbf{k}\cdot\mathbf{p}$ method to describe the band structure which is of interest in transport studies. The method is applied to two examples, a direct gap SC (GaAs) and an indirect gap SC (Si) as in Ref. 8. Indeed we are mainly interested to describe the bottom of the first two conduction bands (CBs) and the top of the valence band (VB) which play the main part in different transport phenomena.[8] The layout of the article is as follows: The principle of the calculation is first decribed. The choice of parameters and their influence on the results are then presented. The efficiency and the limits of the present method are finally discussed.

II. THE sp^3s^*''d'' k·p HAMILTONIAN

We start from the 14×14 Hamiltonian given in Ref. 9 which takes into account the Γ_{7V}, Γ_{8V}, Γ_{6C}, Γ_{7C}, and Γ_{8C} levels. First we add the bonding s level Γ_{6V} which describes the lowest level in the VB and whose energy is about ten eV below the Γ_{8V} level: the Hamiltonian dimension is now 16. We keep the notation of T_d group (GaAs) so that Γ_{6V}, Γ_{7V}, Γ_{8V}, Γ_{6C}, Γ_{7C}, Γ_{8C} are to be understood as Γ_6^+, Γ_7^+, Γ_8^+, Γ_7^-, Γ_6^-, Γ_8^- in O_h group (Si). The 16×16 Hamiltonian leads to monotonic band energies. It is necessary to take into account states whose energy is larger than the largest energy of the 16×16 Hamiltonian to find any minimum in X or L directions. The Hamiltonian is then enlarged to include two further levels, four with spin; the s_B^*-like level, which is a bonding level of symmetry Γ_{6V} and the s_A^*-like level, which is an antibonding level of symmetry Γ_{6C}. The dimension of the Hamiltonian including s_B^* and s_A^* is 20: it is the $\mathbf{k}\cdot\mathbf{p}$ Hamiltonian, called H_{20}, in a sp^3s^* model framework. These s^* levels, which have been introduced by Vogl *et al.*[5] to mimic the influence of the second neighbors, allow one to obtain nonmonotonic bands and, finally, to reproduce the correct position of the first CB at the X point. However the

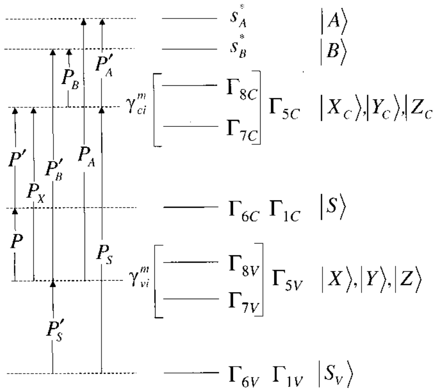

FIG. 1. Wave functions in the sp^3s^*‘‘d’’ $\mathbf{k}\cdot\mathbf{p}$ model at $\mathbf{k}=\mathbf{0}$. We use the notation of T_d group (GaAs) so that Γ_{6V}, Γ_{7V}, Γ_{8V}, Γ_{6C}, Γ_{7C}, Γ_{8C} are to be understood as Γ_6^+, Γ_7^+, Γ_8^+, Γ_7^-, Γ_6^-, Γ_8^- in O_h group (Si). The interband matrix elements are schematically indicated. The Luttinger-like parameters γ_{vi}^m in the $\{\Gamma_{8V},\Gamma_{7V}\}$ levels and γ_{ci}^m in the $\{\Gamma_{8C},\Gamma_{7C}\}$ levels are also indicated. The energies used in the text are $E_G=E(\Gamma_{6C})-E(\Gamma_{8V})$; $\Delta=E(\Gamma_{8V})-E(\Gamma_{7V})$; $E_{GC}=E(\Gamma_{7C})-E(\Gamma_{6C})$; $\Delta_C=E(\Gamma_{8C})-E(\Gamma_{7C})$; $E_A=E(s_A^*)-E(\Gamma_{8V})$; $E_B=E(s_B^*)-E(\Gamma_{8V})$. All these energies are positive except E_{GC} in silicon.

s^* levels are not sufficient to describe the L point and even less the second CB.

The $\mathbf{k}\cdot\mathbf{p}$ H_{20} Hamiltonian gives back the same result for the X point and the same shortcomings for the other points as Vogl's method does. Instead of increasing the Hamiltonian dimension by taking into account the d levels, as it was made in the TB method,[3] we have chosen to introduce the main contributions from far levels (practically the d levels) inside H_{20} via Luttinger-like parameters which play a part in the Γ_{7V} and Γ_{8V} levels and in the Γ_{7C} and Γ_{8C} levels: We call this new Hamiltonian H_{20}^d. In the sp^3s^*‘‘d’’ $\mathbf{k}\cdot\mathbf{p}$ model, ‘‘d’’ reminds us that the d-level influence is taken into account via second order perturbation.

This model is schematically represented at $k=0$ in Fig. 1. In this figure, both the wave functions corresponding to the bands and the matrix elements are indicated. $|S\rangle$ and $|X\rangle$, $|Y\rangle$, $|Z\rangle$ are, respectively, Γ_{1C} (Γ_{6C}) and Γ_{5V} (Γ_{8V},Γ_{7V}) orbital functions as usual. $|S_V\rangle$ and $|X_C\rangle$, $|Y_C\rangle$, $|Z_C\rangle$ are Γ_{1V} (Γ_{6V}) and Γ_{5C} (Γ_{8C},Γ_{7C}) orbital functions, respectively: these eight functions correspond to the sp^3 TB functions. $|A\rangle$ and $|B\rangle$ are, respectively, s_A^*-like and s_B^*-like orbital functions of symmetry Γ_{1C}^* (Γ_{6C}^*) and Γ_{1V}^* (Γ_{6V}^*). The matrix elements of interest are $P=\langle S|p_x|iX\rangle$, $P_S=\langle S_V|p_x|iX_C\rangle$, $P_A=\langle A|p_x|iX\rangle$, $P_B=\langle B|p_x|iX_C\rangle$, $P_X=\langle X_C|p_z|iY\rangle$, $P'=\langle S|p_x|iX_C\rangle$, $P'_S=\langle S_V|p_x|iX\rangle$, $P'_A=\langle A|p_x|iX_C\rangle$, $P'_B=\langle B|p_x|iX\rangle$. The matrix elements P', P'_S, P'_A, P'_B are equal to zero in diamond structure (Si) and are nonzero in zinc blende structure (GaAs). P, P_S, P_A, P_B, P_X are nonzero in both cases. Futhermore we define the related energies as usual, namely the energies $E_{Pj}^{(\prime)}$s are defined by $E_{Pj}^{(\prime)}=2m_0/\hbar^2[P_j^{(\prime)}]^2$. All the matrix elements are real adjustable parameters. As dicussed in Ref. 7 most of them, like for example P and P_X, can be taken positive. Consistent results were obtained by taking only positive parameters. The contributions of the far levels are included by Luttinger-like parameters γ_{vi}^m in the $\{\Gamma_{8V},\Gamma_{7V}\}$ matrix and γ_{ci}^m in the $\{\Gamma_{8C},\Gamma_{7C}\}$ matrix. These parameters are written as γ_j^m where $j=vi$ or ci in the following. The γ_j^ms which describe the interaction of the VB or the CB with far-levels in the H_{20}^d Hamiltonian are adjustable parameters as well. The relations between the Luttinger-like parameters γ_j^m, the matrix elements P and P_X, the forbidden band gap $E_G=E(\Gamma_{6C})-E(\Gamma_{8V})$, the valence spin-orbit splitting $\Delta=E(\Gamma_{8V})-E(\Gamma_{7V})$, $E_{GC}=E(\Gamma_{7C})-E(\Gamma_{6C})$, $\Delta_C=E(\Gamma_{8C})-E(\Gamma_{7C})$, and the Luttinger parameters γ_j are given in Ref. 9. These relations are exact if the spin-orbit splitting is negligible with respect to the direct forbidden band gap as it is the case in silicon. In GaAs, the relations given in Ref. 9 are slightly modified.[10] If the far-level contributions were not taken into account, we would merely have $\gamma_j^m=-1$ if $j=v1$ or $c1$, $\gamma_j^m=0$ if $j=v2,c2,v3,c3$. We define $E_A=E(s_A^*)-E(\Gamma_{8V})$ and $E_B=E(s_B^*)-E(\Gamma_{8V})$ as well.

The m_C^* effective mass of the CB results from the interaction with the Γ_{7V} and Γ_{8V} VB's (Kane formula) via the matrix element P, and from the interaction with the Γ_{7C} and Γ_{8C} CB's (similar to the Kane formula) via P',[11] and from the interaction with far-levels. In the present paper we do not take into account the far-level influence so that m_C^* is merely given by[11]

$$\frac{m_0}{m_c^*}=1+\frac{E_P}{3}\left(\frac{2}{E_G}+\frac{1}{E_G+\Delta}\right)-\frac{E'_P}{3}\left(\frac{2}{E_{GC}+\Delta_c}+\frac{1}{E_{GC}}\right). \tag{1}$$

We did not take any adjustable parameter for the lowest Γ_{6V} CB. The free electron mass m_0 is thus only modified by the influence of P_S and P'_S but not by the contribution of far levels and the Γ_{6V} mass is given by an equation similar to Eq. (1). Concerning the s^* states, described here by $|A\rangle$ and $|B\rangle$, a free electron term ($\hbar^2k^2/2m_0$) was first used, then a nonspherical correction term in the form of $f(\mathbf{k})=3(k_x^4+k_y^4+k_z^4)-k^4$ was introduced as proposed in Ref. 1. Following this approach, the results were not satisfying. The following energies were thus introduced in the diagonal elements of pseudo-orbital s^* in H_{20}^d:

$$\begin{aligned}E_U(\mathbf{k})=E_U&+\alpha_U\frac{\hbar^2k^2}{2m_0}+27(\alpha'_U-\alpha_U)\beta_U\frac{\hbar^2}{2m_0}\frac{k_x^2k_y^2k_z^2}{k^4}\\&+3(\alpha'_U-\alpha_U)(1-\beta_U)\frac{\hbar^2}{2m_0}\frac{k_x^2k_y^2+k_y^2k_z^2+k_z^2k_x^2}{k^2}\\&+\alpha''_U\left(\frac{\hbar^2k^2}{2m_0}\right)^2,\end{aligned} \tag{2}$$

where $U=A$ or B and the αs and the βs are adjustable parameters.

$E_U(\mathbf{k})$ is symmetric with respect to k_x, k_y, k_z as it is the case for $f(\mathbf{k})$. There is neither more nor less justification with the expression of $E_U(\mathbf{k})$ than with the levels s_U^* themselves if not its effectiveness.

TABLE I. Parameters used in the sp^3s^*‘‘d’’ $\mathbf{k}\cdot\mathbf{p}$ model. The Γ_{Ξ} energies are taken from Ref. 12 and are built-in in any $\mathbf{k}\cdot\mathbf{p}$ theory. Γ_{Ξ}, $\Xi=8C$, $7C$, $6C$, $8V$, $7V$, $6V$ are notations in T_d group (GaAs) and are to be understood as Γ_{Ξ}, $\Xi=8^-$, 6^-, 7^-, 8^+, 7^+, 6^+ in O_h group (Si): see text. The 25 other parameters are calculated to obtain the band structure given in Figs. 2 and 3. Energies such as E_A or E'_{Pj} are defined in Fig. 1 or are related to the matrix elements $P_j^{(\prime)}$ of Fig. 1 by $E_{Pj}^{(\prime)}=(2m_0/\hbar^2)[P_j^{(\prime)}]^2$. The parameters like α, β [defined in Eq. (2)], γ (Luttinger-like parameters) are without dimension except α''_A and α''_B which are in eV^{-1}.

eV	GaAs	Si	eV	GaAs	Si		GaAs	Si		GaAs	Si
Γ_{8C}/Γ_8^-	4.659	3.400	E_A	7.2	8.0	γ_{v1}^m	−0.65	−0.07	α_A	−2.35	−4.80
Γ_{7C}/Γ_6^-	4.488	3.400	E_B	7.0	6.5	γ_{v2}^m	0.20	0.03	α'_A	−1.00	5.5
Γ_{6C}/Γ_7^-	1.519	4.185	E_P	22.5	25.0	γ_{v3}^m	−0.26	−0.10	α''_A	0.18	0.10
Γ_{8V}/Γ_8^+	0	0	E'_P	0.025	0	γ_{c1}^m	−0.15	−1.00	β_A	0.78	0.395
Γ_{7V}/Γ_7^+	−0.341	−0.044	E_{PX}	15.0	10.0	γ_{c2}^m	0.104	0.00	α_B	1.40	0.75
Γ_{6V}/Γ_6^+	−12.5	−12.5	E_{PS}	2.3	0	γ_{c3}^m	−0.267	−0.130	α'_B	1.40	0.25
			E'_{PS}	0.2	0				α''_B	0.35	0.00
			E_{PA}	12.0	25.0				β_B	0.00	−2.88
			E'_{PA}	0	0						
			E_{PB}	9.8	13.0						
			E'_{PB}	0	0						

III. RESULTS AND DISCUSSION

Now, we give the values of the parameters use in our $\mathbf{k}\cdot\mathbf{p}$ calculations and describe the results for GaAs and Si. The parameters are listed in Table I. The energies of bands at $\mathbf{k}=\mathbf{0}$ are known.[12] 25 adjustable parameters are present in our model compared to the 13 parameters used by Vogl in his sp^3s^* linear combination of atomic orbitals model.[5]

The parameter values were first estimated by fitting our results at an energy near the forbidden band gap at the center of Brillouin zone then at the extrema X and finally at the extrema L. The accuracy of the CB dispersion near the Brillouin zone surface is strongly dependent on the parameter values like α and β vs energy and on the values of γ_{c2}^m and γ_{c3}^m vs effective masses. These features explain that some parameters are described with three figures (Table I).

The band structure of GaAs and Si calculated according with our $\mathbf{k}\cdot\mathbf{p}$ model, are shown in Figs. 2 and 3, respectively. Numerical results are given in Table II. The band structure is well reproduced on a width of about 6 eV, more precisely the top of the VBs over a one eV scale and the lowest two CBs over a 3 eV scale in four directions namely ΓX, ΓL, ΓK, XU. Indeed it is easy to get right results in the ΓX direction and almost as easy in the ΓL directions. The difficulties come when we try to reproduce results in the ΓK and the XU directions while keeping a good accuracy in the first two directions. The values of the parameters are determined by the calculation in the four directions together and not by four calculations successively. We did not succeed to reproduce the details of the band structure beyond this 6 eV width. This kind of problem was also quoted in Ref. 4 where the authors modified the value of the Γ_{6V} energy to account for the second VB X_{5V} degeneracy. At the L point, the first CB L_{6C} is the right one (see the accuracy in Table II) but the second CB L_{6C} is too high (in Si) as well as the $L_{4,5V}$ point of the first VB. In Ref. 3 the authors did point out that this systematic deviation of L_{6C} cannot be overcome because a nonspherical term cannot be produced correctly in a nearest-neighbor TB model. The second CB is correctly accounted for between X and K but not between K and Γ. This last band

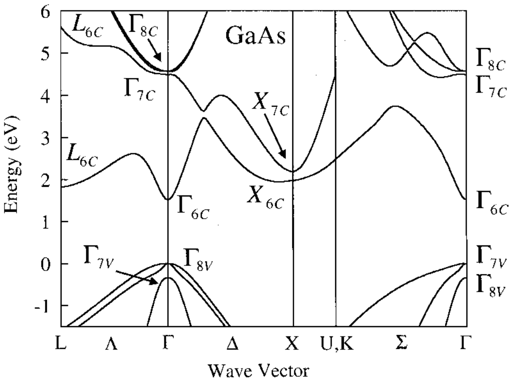

FIG. 2. The GaAs band structure, as calculated according to the present sp^3s^*‘‘d’’ $\mathbf{k}\cdot\mathbf{p}$ model for four directions.

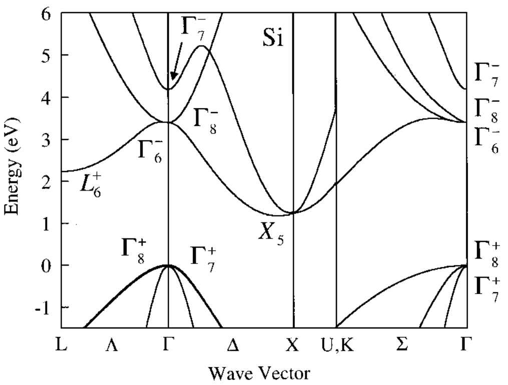

FIG. 3. The Si band structure, as calculated according to the present sp^3s^*‘‘d’’ $\mathbf{k}\cdot\mathbf{p}$ model for four directions.

TABLE II. Comparison of energies and masses obtained in the present work (**k**·**p**) with the $sp^3d^5s^*$ tight-binding calculations (TB) and experimental values (expt). The TB results are taken from Ref. 3 and the experimental data from Ref. 12. Table I parameters are fitted to get energies and m_l longitudinal masses. m_t transverse masses are calculated without further fitting. Masses are in electron free mass unit and *X*, *L*, and $\Delta_{\rm min}$ energies in eV.

	GaAs				Si		
	k·**p**	TB	expt		**k**·**p**	TB	expt
$m_C(\Gamma_6)$	0.067	0.067	0.067	$m_l(\Delta_{\rm min})$	0.920		0.916
$m_t(L_6^c)$	0.13	0.117	0.075	$m_t(L_6^c)$	0.176	0.16	
$m_t(X_6^c)$	0.22	0.237	0.27	$m_t(\Delta_{\rm min})$	0.19	0.22	0.1905
X_{7C}	2.210	2.328	2.35	X_{5C}	1.26	1.35	
X_{6C}	1.945	1.989	1.98	$\Delta_{\rm min}$	1.17	1.17	1.17
X_{7V}	−2.870	−2.929	−2.80	X_{5V}	−3.55	−3.15	−2.90
X_{6V}	−2.968	−3.109	−2.88				
L_{6C}	5.625	5.047	5.7	L_{6C}^+	7.72	4.39	4.15
L_{6C}	1.841	1.837	1.85	L_{6C}^+	2.24	2.14	2.40
$L_{4,5V}$	−1.585	−1.084	−1.20	$L_{4,5V}^-$	−2.02	−1.08	−1.2
L_{6V}	−1.780	−1.33	−1.42	L_{6V}^-	−2.05	−1.12	−1.2

results from the free electron dispersion $(2\pi/a)[2-x,2-x,0]$ $(0<x<3/4)$ which stems from the $(2\pi/a)[220]$ Γ point whose energy is of the order of 20 eV above the bottom of the first CB. This Γ point is out of the scope of the sp^3s^*''*d*'' **k**·**p** model. On the contrary the first two CB's along *XU* are accounted for.

The critical values extracted from our band structures are given in the following. Our results are fitted on the energies and on the masses given in Refs. 8, 12, 13 along the four wave vector directions as stated above. For example, the curves are fitted to give the longitudinal mass m_l in the [100] direction to be equal to 0.92 in the first CB in silicon at **k** corresponding to the CB minimum ($\Delta_{\rm min}$). The top of the VB is at the Γ point while the bottom of the CB is either at the Γ point (GaAs) or in the Δ direction (Si). Table II shows the results of the calculation with the parameters of the Table I and the comparison with TB theoretical results of Ref. 3 and experimental results given in Ref. 12. More specifically the values of the m_t transverse mass of the first CB at *L* and *X* is given for GaAs and at *L* and at the $\mathbf{k}(\Delta_{\rm min})$ point of the first CB minimum in Si. It is worth noting that the transverse mass $m_t(\Delta_{\rm min})$ in Si is the right one when the parameters of Table I are fitted to account for the m_l longitudinal mass. We emphasize that this result is better than the TB results. This feature makes the present method reliable to describe the energies around the forbidden band gap.

As for the VB, the masses and the Luttinger parameters are shown in Table III. These two sets are not deduced one from another as it is usually the case.[14] The masses are calculated from the dispersion curves while the Luttinger parameters are calculated via the set of the 25 adjustable parameters using formula like Eq. (9) of Ref. 9 or the ones of Ref. 10. When the Luttinger parameters are known the calculation of masses is straightforward:[14] in the worst case the masses deduced from the Luttinger parameters differ from the masses calculated from the dispersion curve by less than 10%. This shows that our calculations are consistent even though the results are not excellent for the silicon VB.

We now want to discuss the value of the E_P' parameter which is highly controversial in GaAs ($E_P'=0$ in Si). In Ref. 11, E_P' is equal to 11 eV or 6 eV whether the perturbations

TABLE III. Heavy and light masses for two directions and Luttinger parameters in the Γ_8 valence band. The **k**·**p** masses result from the band structures given in Figs. 2 and 3. The corresponding γ_j Luttinger parameters result from the equations who link the γ_js to the γ_{vj}^m and γ_{cj}^m Luttinger-like parameters and the E_P and E_{PX} parameters via the equations given in Ref. 9. The agreement between masses calculated from the band structures and from Luttinger parameters is of the order of 10% in the worst case (m_{lh}^{111}). See comments in the text.

	m_{hh}^{100}	m_{hh}^{111}	m_{lh}^{100}	m_{lh}^{111}	γ_1	γ_2	γ_3
GaAs (**k**·**p**)	0.46	0.95	0.089	0.085	7.07	2.40	3.05
GaAs[a]	0.43	0.95	0.085	0.077	7.05	2.35	3.00
Si (**k**·**p**)	0.35	0.92	0.15	0.117	4.92	1.06	1.91
Si[b]	0.29	0.88	0.20	0.135	4.26	0.38	1.56

[a] Reference 15.

[b] Reference 12.

due to far-level bands are taken into account or not. In Ref. 9, E_P' is equal to 2.36 eV. The influence of E_p' is all the larger as the magnitude k of the wave vector is large. E_P' determines the energies both at the edge of the Brillouin zone and the E_{1-2} splitting between the first and the second CB in zinc blende structure ($E_{1-2}=0$ in diamond structure). In GaAs the E_{1-2} splitting equals 0.2 eV[8] and the relevant wave vector is $k_1=0.34$ Å^{-1} in [100] direction. E_{1-2} is equal to $2\sqrt{E_P'(\hbar^2 k_1^2/2m_0)}$ as far as the only matrix element P' has to be considered. If we successively take $E_P'=11$, 6, 2.36 we get $E_{1-2}=2\sqrt{E_P'(\hbar^2 k_1^2/2m_0)}=4.4,3.2,2.0$ eV. Whatever the above E_P' value, E_{1-2} is far too large. $E_{1-2}=0.2$ eV leads to $E_P'=0.025$ eV. The complete numerical calculation taking into account all the bands leads to the same value $E_P'=0.025$ eV and eventually gives the value $E_{1-2}=0.18$ eV which is quite reasonable. Once E_P' is known, we use Eq. (1) to get E_P. Finally we find $E_P=22.5$ eV which is the value given in Table I.

IV. CONCLUSION

In conclusion, the sp^3s^*‘‘d’’ **k**·**p** model allows one to get a quantitatively correct description of the top of the valence bands and of the lowest two conduction bands, both in terms of energies and masses. The contribution of the pseudo-orbitals s^* along with the contribution of the far levels via modified Luttinger parameters was found to be determinant for the conduction bands at L and X points. The s^* levels give rise to nonmonotonic bands and the far-level contribution allows one to obtain the correct masses and energies. We have shown that some parameter values reported up to now prevent to reproduce the dispersion on the Brillouin zone which leads us to propose new values. The conduction band dispersion is comparable to that obtained with a $sp^3d^5s^*$ tight binding method. We emphasize that near the band extrema the sp^3s^*‘‘d’’ **k**·**p** model leads to more precise values, in particular for the masses at the bottom of the silicon conduction band. The sp^3s^*‘‘d’’ **k**·**p** model is thus efficient to calculate the band structures all over the Brillouin zone for energies of interest in transport phenomena.

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