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Tight-binding model and interactions scaling laws for silicon and germanium

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We provide a set of parameters for second-neighbor tight binding model Hamiltonians, including spin-orbit interaction, in silicon and germanium. Our attempt is the construction of a simple Hamiltonian, useful as a stepping stone for the description of more complex systems. We introduce a criterion for establishing transferable scaling laws of the parameters. The results obtained, checked versus determination of deformation potentials under hydrostatic and uniaxial [001] stress, indicate a clear deviation from the d^{-2} Harrison scaling law.

I. INTRODUCTION

The determination of energy band structures in semiconductors under pressure, has recently been the object of renewed interest, due to the development of epitaxial techniques for the growth of lattice mismatched nanostructures.[1] Among them an important role is played by Si/Ge strained-layer superlattices,[2] also in the form of $\mathrm{Ge}_x\mathrm{Si}_{1-x}$ alloys,[3] as promising candidates for device applications. A natural request has thus emerged, for the construction of transferable Hamiltonians,[4] which can provide reliable bulk band structures (energy gaps and masses), with the further bonus of being so manageable as to be easily employed also for the description of band structure and structural properties of very large scale system. Hydrostatic and uniaxial deformations as well as alloying are additional physical effects to be properly accounted for by these Hamiltonians.

The semiempirical tight-binding (TB) method is well suited to describe situations where periodicity is partially or totally disrupted and provides a simple description of bands and density of states in the solid. A wide literature exists on its merits and limits (for a review see Ref. 5), moreover its connection with self-consistent density-functional theory has recently been explored,[6] providing a more fundamental ground to the matrix elements entering in the tight-binding procedure.

The need for simplified reliable tight-binding Hamiltonians is evident, for instance, from their use in molecular-dynamics simulations,[7,8] total energy calculations,[9] determination of elastic constants, phonon frequencies, defect formation energies,[4] etc.

In this paper, we provide a very economical tight-binding sp^3 Hamiltonian for silicon and germanium, considering first and few selected second nearest neighbors, with the inclusion of spin orbit interaction. We describe in Sec. II, our procedure for the determination of the Slater and Köster (SK) parameters for bulk crystals:[10] our results have the accuracy of other tight-binding calculations obtained with a larger number of parameters.[11–13] We also provide in Sec. III a criterion for the determination of scaling laws for these parameters as a function of distances. We test in Sec. IV these laws calculating deformation potentials for direct and indirect transitions under hydrostatic pressure and in the case of uniaxial deformation. Section V contains the conclusions.

II. THE METHOD FOR BULK DIAMONDLIKE BAND STRUCTURE

We use a Slater Köster[10] tight-binding model with an orthogonal basis built from s and p orbitals for each atom in the unit cell. Interactions up to second neighbors and spin orbit are considered; inclusion of second neighbors is essential for accurate description of the region around the fundamental gap and of the lowest conduction bands.

The (8×8) second neighbor Hamiltonian matrix elements for diamondlike structures are given in terms of *four* transfer energy integrals involving nearest neighbors, i.e., $E_{ss}(\frac{1}{2}\frac{1}{2}\frac{1}{2})$, $E_{sx}(\frac{1}{2}\frac{1}{2}\frac{1}{2})$, $E_{xx}(\frac{1}{2}\frac{1}{2}\frac{1}{2})$, and $E_{xy}(\frac{1}{2}\frac{1}{2}\frac{1}{2})$, *seven* transfer energy integrals involving second neighbors, i.e., $E_{ss}(110)$, $E_{sx}(110)$, $E_{xx}(110)$, $E_{xx}(011)$, $E_{xy}(110)$, $E_{xy}(011)$, and $E_{sx}(011)$, and *two* on site energies, E_s and E_p, for the outer s and p orbitals, respectively, in the crystal. Since the original work of Slater and Köster, a long list of attemps and recipes have been presented in the literature to determine the value of these parameters looking for best fit with experimental data or other semiempirical calculations.

Of course, in the use of TB as interpolation scheme, the higher the number of parameters considered (as, for instance, including larger distances), the better is the fit; however, if one plans to introduce the TB Hamiltonian as a stepping stone to another calculation (as, for instance, in the transfer matrix procedure and renormalization of multilayer structures),[14] it is often useful to consider only an economical small number of optimized parameters.

In this philosophy is the five orbitals per atom, sp^3s^*, model introduced by Vogl *et al.*[15] including only first neighbors: following Slater and Köster, by diagonalizing the TB matrix at high symmetry points, they exploit the analytic expression of the crystal eigenvalues at Γ and X points to fit the values of nearest neighbors parameters. The importance of the inclusion of second neighbors in this model has then been stressed by Newmann and Dow.[16]

In our method, we follow the spirit of Refs. 15 and 16, including selected second-neighbor parameters and spin-orbit interaction. The procedure can be summarized in the following steps. First, we consider the close analytic expression for the eigenvalues at Γ and X, without spin-orbit interaction; we realized that these expressions do not contain the parameters $E_{sx}(110)$, $E_{sx}(011)$, $E_{xy}(110)$, and $E_{xy}(011)$, thus, we are faced with four eigenvalues at X, i.e., $X_{1v}, X_{4v}, X_{1c}, X_{3c}$, four eigenvalues at Γ, i.e., $\Gamma_{1v}, \Gamma'_{25v}, \Gamma_{15c}, \Gamma'_{2c}$, and nine SK parameters. If we introduce the constraint $E_{ss}(110) = 0$, which is reasonable because the energy integral involving s functions at second-neighbor distances is smaller than the other parameters, we have an exactly soluble problem, which gives analytic expression for the values of the SK parameters in terms of the known eigenvalues at X and Γ points.

These expressions which are at the basis of our procedure are given below:

$$E_s = \frac{\Gamma_1 + \Gamma'_2}{2} , \tag{1a}$$

$$E_p = \frac{X_{1v} + X_{1c} + X_3 + X_4}{4} + \frac{\Gamma'_{25} + \Gamma_{15} - \Gamma_1 - \Gamma'_2}{8} , \tag{1b}$$

$$E_{ss}\left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right) = \frac{\Gamma_1 - \Gamma'_2}{8} , \tag{1c}$$

$$E_{xx}\left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right) = \frac{\Gamma_{15} - \Gamma'_{25}}{8} , \tag{1d}$$

$$E_{xy}\left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right) = \frac{X_3 - X_4}{8} , \tag{1e}$$

$$E^2_{sx}\left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right) = \frac{(\Gamma_1 + \Gamma'_2)(2X_{1v} + 2X_{1c} - \Gamma_1 - \Gamma'_2)}{64} - \frac{X_{1v}X_{1c}}{16} , \tag{1f}$$

$$E_{xx}(110) = \frac{\Gamma'_{25} + \Gamma_{15} + \Gamma_1 + \Gamma'_2}{32} - \frac{X_{1v} + X_{1c}}{16} , \tag{1g}$$

$$E_{xx}(011) = \frac{\Gamma'_{25} + \Gamma_{15} - \Gamma_1 - \Gamma'_2}{32} + \frac{X_{1v} + X_{1c} - X_4 - X_3}{16} . \tag{1h}$$

We need further relations to determine the value of the four parameters not included in the above Eqs. (1). If we introduce the *two-center approximation*,[10] the SK parameters assume the following expressions in terms of two-center integrals:

$$E_{ss}\left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right) = (ss\sigma)_1 ,$$

$$E_{sx}\left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right) = \frac{1}{\sqrt{3}}(sp\sigma)_1 ,$$

$$E_{xx}\left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right) = \frac{1}{3}(pp\sigma)_1 + \frac{2}{3}(pp\pi)_1 ,$$

$$E_{xy}\left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right) = \frac{1}{3}(pp\sigma)_1 - \frac{1}{3}(pp\pi)_1 ,$$

for the nearest neighbors, and

$$E_{ss}(110) = (ss\sigma)_2 ,$$

$$E_{sx}(110) = \frac{1}{\sqrt{2}}(sp\sigma)_2 ,$$

$$E_{xx}(110) = \frac{1}{2}(pp\sigma)_2 + \frac{1}{2}(pp\pi)_2 ,$$

$$E_{xx}(011) = (pp\pi)_2 ,$$

for the second neighbors. For the remaining SK parameters, in the two-center approximation, we have

$$E_{xy}(011) = E_{sx}(011) = 0 \tag{2}$$

and

$$E_{xy}(110) \equiv E_{xx}(110) - E_{xx}(011) = \frac{1}{2}\left[(pp\sigma)_2 - (pp\pi)_2\right] . \tag{3}$$

The value of $E_{xy}(110)$ has no effect on the eigenvalues along the Δ line from Γ to X, but is very important at the L point, in fact it is linked to the barycenter of L_3 and L'_3 eigenvalues through the relation,

$$E_{xy}(110) = -\frac{1}{4}\left(E_p - \frac{L_3 + L'_3}{2}\right) . \tag{4}$$

Equation 4 is obtained from diagonalization of the H at L point and considering the submatrix with degenerate eigenvalues. It has already been noticed[13] that the expression for the energy distance $L'_3 - L_3$, as obtained from the same diagonalization, in the form

$$L'_3 - L_3 = 4\left[E_{xy}\left(\frac{1}{2}\frac{1}{2}\frac{1}{2}\right) + E_{xx}\left(\frac{1}{2}\frac{1}{2}\frac{1}{2}\right)\right] ,$$

is not consistent with the energy distance revealed experimentally when we use the SK parameters given in Eqs. (1). This means that this distance cannot be obtained if we do not include higher orders of neighbors, or if we do not consider higher angular momentum contributions to the wave functions, even if we abandon the two-center approximation. The above argument has led[13] us to consider an empirical parameter A to correct the value of $E_{xy}(110)$ in the form

$$E_{xy}(110) = E_{xx}(110) - E_{xx}(011) - A, \tag{5}$$

the parameter A does not affect the eigenvalues at Γ and X points, thus, we also use it to adjust the barycentre between L_3 and L'_3 eigenvalues and, consequently, the band structure along the Λ segment in the energy region near the fundamental gap; we have found $A = 0.445$ for Si and $A = 0.4438$ for Ge. Finally, in the search of smallest number of parameters, the $E_{sx}(110)$ parameter is also neglected at this stage because we have verified that it has a negligible effect on the band structures.

With this first choices, our procedure gives a reasonably good valence and conduction band structure scheme, when we exploit known eigenvalues obtained in the literature by other methods.[17]

As a further improvement, we double the secular problem to properly take into account the spin-orbit interaction in the form proposed by Chadi.[18] Let λ be the matrix element of the spin-orbit interaction between different p orbitals with different spin, on the same site. At Γ, the topmost valence band is split by spin orbit as follows:[18]

$$E(\Gamma_8^+) = E(\Gamma_{25}') + \lambda \,,$$
$$E(\Gamma_7^+) = E(\Gamma_{25}') - 2\lambda \,,$$

thus λ is determined from the band structure as

$$\lambda \equiv \frac{\Delta_0}{3} = \frac{E(\Gamma_8^+) - E(\Gamma_7^+)}{3} \,. \tag{6}$$

In the same way at the topmost valence L point, we have the spin-orbit splitting:[18]

$$\Delta_0' = \frac{2}{3}\Delta_0 .$$

Finally, we have shifted the on site energy E_p so to exactly reproduce the fundamental gap. We list in Table I the parameters obtained for Si and Ge. The corresponding band structures are reported in Figs. 1 and 2. We obtain a realistic dispersion for conduction states; this goal is generally very difficult to be reached using sp^3 TB Hamiltonians with up to second-neighbor interactions. The above parametrization gives a good agreement also between theoretical and experimental values of effective masses for electrons and holes as can be seen from Tables II and III.

III. TIGHT-BINDING PARAMETERS SCALING

TABLE I. Silicon and germanium parameters obtained with our method (units are in eV).

Parameter	Silicon	Germanium
$E_p - E_s$	5.0794	6.9311
$E_{ss}(\frac{1}{2}\frac{1}{2}\frac{1}{2})$	-2.0662	-1.6862
$E_{sx}(\frac{1}{2}\frac{1}{2}\frac{1}{2})$	1.2038	1.2412
$E_{xx}(\frac{1}{2}\frac{1}{2}\frac{1}{2})$	0.4287	0.4001
$E_{xy}(\frac{1}{2}\frac{1}{2}\frac{1}{2})$	1.3775	1.3937
$E_{xx}(110)$	0.2644	0.2341
$E_{xx}(011)$	-0.3612	-0.3372
$E_{xy}(110)$	0.1800	0.1275
λ	0.0147	0.0967

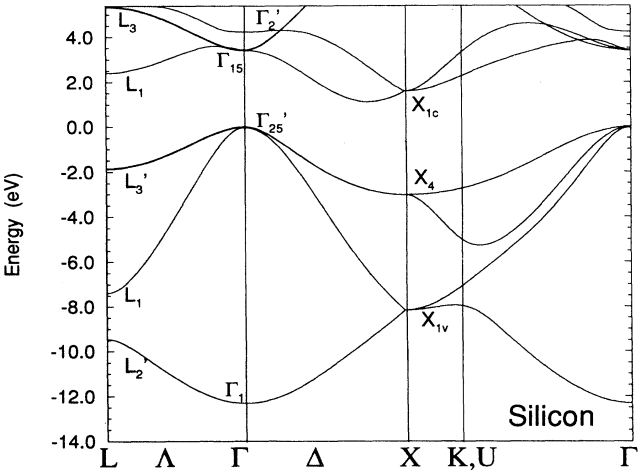

FIG. 1. Band structure of silicon obtained with the parameters of Table I. Spin-orbit effects are included; they cannot be distinguished on the chosen scale, thus single group notations are used.

The semiempirical TB method presented in Sec. II is particulary suited to describe electronic structures when the crystal arrangement is distorted by pressure or alloying effects; it is also precious in the search of transferable TB Hamiltonians for group IV semiconductors and in total energy calculation.[4,8,9] In all these situations, the knowledge of the change of SK parameters with the distance is essential. For this aim an often used prescription is the d^{-2} Harrison scaling law.[19]

The inadequacy of the Harrison law has been pointed out in literature,[20–22] and more or less complicated expressions have been introduced to selectively correct each parameter involved in TB matrix elements.[23–25,9,13] To determine the analytic trends of the energy parameters with pressure, an approach has been to fit TB parameters to closely reproduce a good variation of the band gap at several pressure points;[23] alternatively cluster calculations have been proposed[8] to extract the TB matrix elements and to study their dependence on the atomic

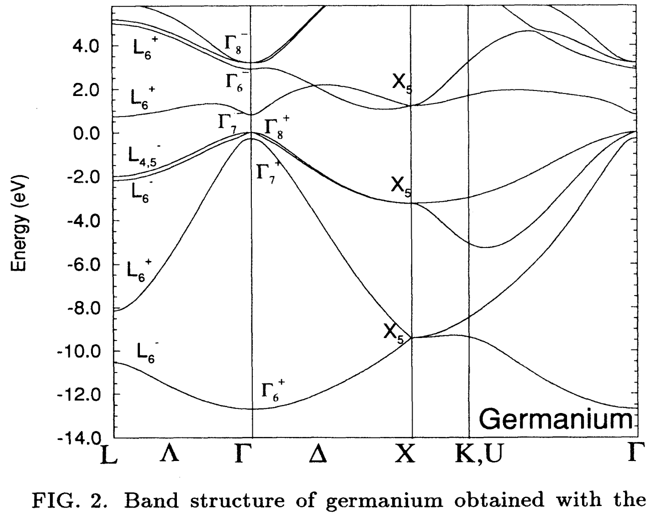

FIG. 2. Band structure of germanium obtained with the parameters of Table I. Spin-orbit effects are included.

TABLE II. Values of the fundamental gap, of masses (in units of electron mass), and of spin-orbit separation Δ_0 for silicon. $m_{\parallel}$ and $m_{\perp}$ refer to the conduction electron mass along direction Δ, and perpendicular to it. $m_{\rm hh}$ and $m_{\rm lh}$ refer to the topmost heavy and light valence bands, along Λ and Δ directions.

	Present	Expt.[a]
$E_{\rm gap}$ (eV)	1.12	1.12
$m_{\parallel}$	0.51	0.9
$m_{\perp}$	0.20	0.19
$m_{\rm hh}(\Lambda)$	0.54	0.54
$m_{\rm lh}(\Lambda)$	0.17	0.15
$m_{\rm hh}(\Delta)$	0.28	
$m_{\rm lh}(\Delta)$	0.25	
Δ_0 (eV)	0.044	0.044

[a] Reference 32.

distance.

The scaling technique that we introduce in this paper, derives from the numerical evaluation of the SK two-center parameters for different interatomic distances. We start from single-ζ Slater-type atomic wave functions in the form deduced by Clementi *et al.*[26] From them the crystal potential is built as a sum of atomiclike potentials each of them made by nuclear, Hartree, and exchange-correlation terms in the form

$$V_a(r) = -\frac{2Z_a}{r} + \frac{8\pi}{r}\int_0^r r'^2\rho(r')\,dr' + 8\pi\int_r^\infty r'\rho(r')\,dr' -6\left(\frac{3}{8\pi}\rho(r')\right)^{1/3} F(\alpha)\ . \qquad (7)$$

The density dependent correlation factor F, which corrects the Slater exchange potential to include electron correlation on pair interactions, introduces an active screening in the low density region far from nuclei; it is given by[27]

$$F(\alpha) = 1 - \frac{4}{3}\,\alpha\,\tan^{-1}\left(\frac{2}{\alpha}\right) + \frac{1}{2}\,\alpha^2\,\ln(1+4\alpha^{-2}) -\frac{1}{6}\,\alpha^2\left[1-\frac{1}{4}\alpha^2\,\ln(1-4\alpha^{-2})\right]\ ,$$

with $\alpha = 0.646\ \rho^{1/6}$.

TABLE III. Values of the fundamental gap, of masses (in units of electron mass), and of spin-orbit separation Δ_0 for germanium. $m_{\parallel}$ and $m_{\perp}$ refer to the conduction electron mass at the L point along direction Λ, and perpendicular to it. $m_{\rm hh}$ and $m_{\rm lh}$ refer to the topmost heavy and light valence bands, along Λ and Δ directions.

	Present	Expt.[a]
$E_{\rm gap}$ (eV)	0.74	0.74
$m_{\parallel}$	1.64	1.64
$m_{\perp}$	0.18	0.08
$m_{\rm hh}(\Lambda)$	0.45	0.37
$m_{\rm lh}(\Lambda)$	0.06	0.04
$m_{\rm hh}(\Delta)$	0.22	0.28
$m_{\rm lh}(\Delta)$	0.07	0.04
Δ_0 (eV)	0.29	0.29

[a] Reference 32.

The two-center integrals are numerically evaluated for different distances between centers, considering deformation of these distances up to 5% of their values without applied stresses: this corresponds to consider pressures up to 100 Kbar. The numerical values can be well interpolated by the relations

$$h_J = h_J^0\left(\frac{d_0}{d}\right)^{n_J}\ , \qquad (8)$$

where the index α identifies the type of two-center integral. We give the resulting values of n_J in Table IV for silicon and germanium. The departure from the d^{-2} law is evident. We stress that our determination of scaling laws is completely *ab initio*, and that our results agree qualitatively with the calculations of Refs. 9 and 4, where a semiempirical approach is used. The strong scaling law for second neighbors interactions represents, in the case of small deformations, a useful alternative to the introduction of an exponential type cutoff.[9,4,24] In what concerns the TB diagonal parameters E_p and E_s, they are made by free atomic eigenvalues corrected by the crystal field. We have evaluated analytically the two-center crystal field integrals at different distances and have obtained *ab initio* scaling laws also for them. As generally done in the literature, in the search of very simple TB Hamiltonians, we have used the parameters E_p and E_s deduced for the unstrained crystal also in the case of hydrostatic deformation; in fact, we have verified that the role of variation of crystal field integrals with hydrostatic pressure has a negligible effect on the band structure. The effect of uniaxial strain on the crystal field contribution to E_p is discussed below. We now verify the quality of the above scalings by using them for the SK parameters introduced in Sec. II, and evaluating deformation potentials for hydrostatic and uniaxial pressure.

IV. CALCULATION OF DEFORMATION POTENTIALS

Strain effects can be easily considered in the tight-binding scheme; strain modifies atomic arrangement and influences the energy parameters and the direction

TABLE IV. Scaling laws for independent integrals for silicon and germanium.

Interaction	n_J	
	Silicon	Germanium
$(ss\sigma)_1$	4.37	5.00
$(sp\sigma)_1$	3.46	3.63
$(pp\sigma)_1$	2.72	2.73
$(pp\pi)_1$	4.51	4.76
$(ss\sigma)_2$	8.97	10.72
$(sp\sigma)_2$	7.12	8.25
$(pp\sigma)_2$	7.18	8.09
$(pp\pi)_2$	8.56	9.59

cosines, which enter in the definition of the TB matrix elements. These latter quantities are deduced from the new geometrical arrangement of the atoms as indicated by Slater and Köster,[10] the dependence of the SK parameters from the distance between centers needs an appropriate scaling procedure. For this aim we use the scaling laws obtained in the previous section and perform several band structure calculations for different pressures; from them we can compare the results obtained versus the known experimental values of the deformation potentials. Different methods have been employed for calculation of the pressure coefficients in silicon and germanium; we mention the semiempirical TB,[11,21,22] first-principle pseudopotential,[28] LMTO,[29] first principle quasiparticle approach,[30] and LCGO methods.[31]

We study both hydrostatic and uniaxial [001] stress conditions on Si and Ge. To consider the effect of uniaxial stress on the energy parameter E_p, and thus the induced modification of crystal field interactions, we can write[11,22]

$$E_p^{(x,y)} = E_p + b_p(\epsilon_{xx} - \epsilon_{zz}) \ ,$$

$$E_p^{(z)} = E_p - 2b_p(\epsilon_{xx} - \epsilon_{zz}),$$

where $\epsilon_{xx} = \frac{a_{\|} - a_0}{a_0}$ and $\epsilon_{zz} = \frac{a_{\perp} - a_0}{a_0}$; a_0 is the unstrained bulk lattice constant, $a_{\|}$ and $a_{\perp}$ are the in-plane and the interplane lattice constants, respectively. The parameter b_p is a deformation potential for the p eigenvalue when uniaxial stress is applied to the crystal. We introduce the empirical values $b_p = 2.9$ eV and $b_p = 3.5$ eV for Si and Ge, respectively, because they satisfactory reproduce the distances of nonequivalent minima in the lowest conduction band valleys. Moreover, due to the effect of the empirical parameter A only at the L point, we have deduced the scaling laws exponents $n_A = 4.0$ for Si, and $n_A = 6.0$ for Ge, from the behavior of the energies at the L point.

We have first evaluated the deformation potential for selected direct and indirect transitions under hydrostatic pressure; these are given from the relation that connects the variation of the corresponding gap energies per relative variation of the cell volume:

$$a(E_g) = \frac{dE_g}{d\ln V} = -\frac{dE_g}{dp} B \ , \tag{9}$$

where B is the Bulk modulus ($B = 0.99$ Mbar for Si and $B = 0.758$ Mbar for Ge).[32]

We have thus considered the deformation potentials $a(E_0)$, corresponding to the transitions $\Gamma'_{25v} \rightarrow \Gamma'_{2c}$, and the deformation potential $a(E_1)$, corresponding to the transition $L'_{3v} \rightarrow L_{1c}$; the above transition are direct. We have also considered the deformation potential for the indirect transitions $\Gamma'_{25v} \rightarrow \Delta_{\min}$ and $\Gamma'_{25v} \rightarrow L_{1c}$; by convention, these are indicated as $\left[\Xi_d + \frac{1}{3}\Xi_u - a\right]^{\Delta,L}$, respectively, in the literature.[33]

TABLE V. Deformation potentials for silicon (units are in eV).

	Present	Expt.[a]
$a(E_0)$	-12.3	
$a(E_1)$	-4.8	-5.2
$(\Xi_d + \frac{1}{3}\Xi_u - a^v)^\Delta$	1.8	1.4, 3.8
$(\Xi_d + \frac{1}{3}\Xi_u - a^v)^L$	-5.8	
Ξ_u^Δ	6.2	7.9[b], 11.3[b]
b	-1.6	-1.95, -2.27

[a] Reference 32.

[b] Reference 34.

The uniaxial stress lifts the degeneracy of the topmost valence band. Useful relations for pressure variation of the three topmost valence bands at Γ, under application of an uniaxial stress much smaller than spin-orbit interaction, have been obtained by Pollak and Cardona;[38] the linear split of the $P_{3/2}$ multiplet, δE_{001}, can be expressed in terms of the deformation potential b and the strain component ϵ_{zz} and ϵ_{xx} as follows:

$$\delta E_{001} = 2b(\epsilon_{zz} - \epsilon_{xx}). \tag{10}$$

The minima of the six equivalent valleys along Δ direction in Si, are differently shifted under application of uniaxial strain: if the strain is along [001], the bands along [001] and [00$\bar{1}$] are shifted by $-\frac{2}{3}\Xi_u(\epsilon_{xx} - \epsilon_{zz})$, while the remaining four equivalent bands are shifted by $\frac{1}{3}\Xi_u(\epsilon_{xx} - \epsilon_{zz})$ with respect to the mean energy, thus the relative shift of inequivalent minima is

$$\delta E = \Xi_u(\epsilon_{xx} - \epsilon_{zz}). \tag{11}$$

Equation (11) defines the shear deformation potential Ξ_u.[33]

The deformation potentials calculated with our procedure are shown in Tables V and VI, in comparison with the experimental results. Due to the uncertainties which often affect the experimental results (for a discussion see Refs. 34 and 39) and the wide amount of theoretical values (see, for instance, Refs. 11, 21, and 22 for TB calculations and the list of data collected in Ref. 29 for other computational schemes), we can conclude that quite satisfactory values for deformation potentials are provided by our results.

V. CONCLUSIONS

There are two main results of this paper: the operative derivation of a simple sp^3 TB Hamiltonian and

TABLE VI. Deformation potentials for germanium (units are in eV).

	Present	Expt.[a]
$a(E_0)$	-11.7	-12.7
$a(E_1)$	-4.3	-4.7,[b] -5.7
$(\Xi_d + \frac{1}{3}\Xi_u - a^v)^\Delta$	1.7	1.14[c]
$(\Xi_d + \frac{1}{3}\Xi_u - a^v)^L$	-4.5	-2.0, -3.8[d]
Ξ_u^Δ	6.2	
b	-1.6	-2.2, -2.86

[a] Reference 32.

[b] Reference 35.

[c] Reference 36.

[d] Reference 37.

scaling laws proposed for the TB parameters. The analytic expressions of Eq. (1) for first- and second-neighbor TB parameters in terms of known eigenvalues at Γ and X points, and the further refinements introduced, are indeed very effective procedures for semiempirical TB Hamiltonians for group IV semiconductors. These Hamiltonians provide satisfactory conduction and valence electronic band structures, as well as effective masses.

We have also presented an *ab initio* criterion for obtaining scaling laws of TB parameters as a function of distances between centers. Deformation potentials under hydrostatic and uniaxial pressures obtained from the knowledge of these scaling laws show satisfactory comparison with existing experimental and theoretical values.

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