Improving the tight-binding description of spin-orbit interaction in a Si/Ge heterostructure for qubits applications

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***Abstract*—Hole spin qubits realized in Ge heterostructures are a promising quantum computing platform. An accurate description of spin-orbit effects is mandatory in numerical methods for device modelling, such as Tight-Binding, to properly describe the spin physics. This work presents a methodology to improve the spin-orbit interaction in Tight-Binding, and to match reference *ab initio* results. We apply this methodology to a prototypical Si/Ge heterostructure, and we achieve such improvement by tuning the Si/Ge band alignment and the onsite potential of the interface atoms, which indicates that the confinement potential is the primary factor for the accurate description of spin-orbit interaction.**

***Index Terms*—Si/Ge heterostructure, spin-orbit coupling, Tight Binding, DFT, Spin Qubits**

I. Introduction

The current research on semiconductor hole spin qubits shows a strong interest in Ge/SiGe heterostructures due to their low level of disorder and the inherent spin-orbit coupling (SOC) of holes, which allows robust electric control and manipulation of the spin qubits [1]–[4]. Furthermore, the light in-plane effective masses of germanium allow the creation of large quantum dots, which reduces the constraints on the device fabrication [5].

The modelling of such spin qubits is typically tackled with semi-empirical methods, such as $k \cdot p$ or Tight-Binding (TB). The proper description of SOC using these methods still remains to be validated. On the other hand, $ab\ initio$ methods, such as density functional theory (DFT), are able to provide a truthful description of SOC effects but are computationally too costly to simulate a full device.

We propose a practical approach to refine the TB parameters based on $ab\ initio$ results and reproduce the same SOC effects. The adjusted set of TB parameters, when extracted from the relevant heterostructures, should provide an improved description of hole spin qubit physics in full device simulations.

In this work, we illustrate the proposed methodology by adjusting the TB spin splitting of the topmost valence bands in a prototypical Si/Ge heterostructure. We tailor the correct SOC in TB by tuning first the valence band offset to achieve an identical confinement potential, and then by introducing different onsite potentials for atoms at the Si/Ge interface to reach the reference spin splitting.

II. Methods

To obtain the reference spin-orbit coupling parameters, non-collinear DFT simulations are performed using the Vienna $ab\ initio$ simulation package (VASP) and the Perdew-Burke-Ernzerhof (PBE) functional, an energy cutoff of 350 eV and a $8 \times 8 \times 1$ k-mesh [6]–[8]. Dipole corrections are applied for the simulations including an external electric field. TB calculations are carried out using the TB_Sim code and a $sp^3d^5s^*$ basis set [9]. This work focuses on a Si/Ge/Si heterostructure, where 21 layers (2.9 nm) of Ge slab are sandwiched by two Si slabs of 20 layers (2.8 nm). We stick to an odd number of Ge layers to have a finite spin splitting in the absence of electric field (note that a Ge slab with an even number of layers has an inversion center, which suppresses all SOC effects). The lattice parameter is set to 5.58 Å [10] for both Si and Ge, which leads to a hydrostatic strain in the heterostructure. The dangling bonds of the outermost silicon surfaces are passivated with hydrogen, and we verified that 20 layers is enough to ensure that the thickness of the Si slabs has no impact on the results. Finally, a 1.5 nm thick vacuum is inserted in the unit cell.

Even though PBE is known to generally underestimate the band gap, which may lead to an inaccurate band offset, we restrict this study to a hydrostatically-strained thin heterostructure (21 Ge layers). The strain and the confinement, by increasing the band gap, allow the study of the SOC with PBE. We therefore take the PBE results as reference, even if meaningful studies for thicker films would require a careful evaluation of the DFT accuracy.

III. Results

Figure 1(a) presents the band structure of the simulated heterostructure, with the reference energy set at the maximum of the valence band. The two topmost valence bands are degenerate at Γ and split at finite k, as shown in Fig. 1(b). The spin splitting ΔE_{spin} arises due to spin-orbit interaction, and it is the main physical quantity we compare in this study. Nonetheless, describing the spin splitting correctly requires an accurate assessment of the confinement potential in the heterostructure, so the first step towards a good estimation of ΔE_{spin} in TB is to reproduce the DFT confinement.

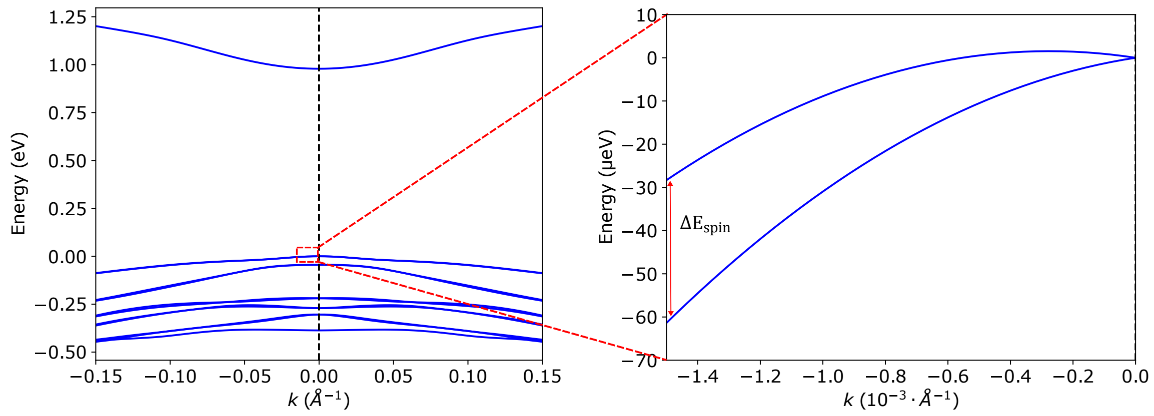

Fig. 1: (a) Band structure of Si/Ge/Si heterostructure with 20/21/20 layers along $[110]$-Γ-$[\bar{1}10]$ direction computed with TB. The reference energy is set at the maximum of the valence band. (b) Zoom on the topmost valence band near the Γ point. The valence band is twofold degenerate at Γ, and split at finite k. The energy difference, ΔE_{spin}, is the spin splitting due to SOC.

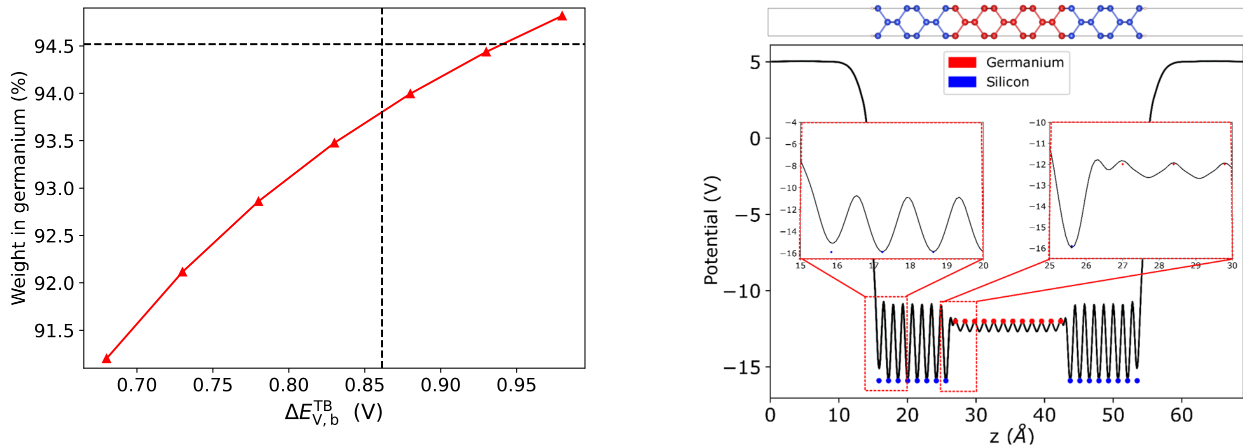

Fig. 2: The weight of the topmost valence band wavefunction in the germanium versus the Si/Ge bulk valence band offset. The horizontal black-dashed line is the weight from the *ab initio* calculation, the vertical one is the $\Delta E^{\mathrm{TB}}_{\mathrm{V,b}}$ that provides $\Delta E^{\mathrm{TB}}_{\mathrm{V,s}} = \Delta E^{\mathrm{DFT}}_{\mathrm{V,s}}$, and blue square is the result of a calculation with the original TB parameters [9].

Fig. 3: Averaged electrostatic potential in the x-y plane along the z direction (perpendicular to the slab) for a 8/12/8 Si/Ge/Si heterostructure. The two insets are the zooms on the potential at a Si/Ge interface (on the right) and on the Si interface (on the left). Blue dots are the positions of the Si, and red dots are for Ge. The atomic structure of the corresponding heterostructure is presented on top, which is chosen purposely small for illustrative purposes.

A. Confinement of the hole wavefunction

The original TB parameters [9] provide a topmost valence band wavefunction which is only 91.2% confined in the Ge slab, in contrast with the 94.5% from *ab initio*. Such a discrepancy might be a consequence of the different effective masses predicted by TB and DFT, which indeed result in a different quantum confinement effect on the heterostructure. The TB parameter to tune in order to modify the confinement is the bulk valence band offset ($\Delta E^{\mathrm{TB}}_{\mathrm{V,b}}$). It is an input parameter which is defined as the difference between the valence band position in bulk Si and Ge. Changes on this parameter result on a rigid shift on all onsite matrix elements of the germanium atoms.

Figure 2 shows that by adjusting the bulk valence band offset we can correct the discrepancy between TB and DFT. In this case, we require $\Delta E^{\mathrm{TB}}_{\mathrm{V,b}} = 0.94$ V in TB to reproduce the *ab initio* hole confinement, which is far from the original $\Delta E^{\mathrm{TB}}_{\mathrm{V,b}} = 0.68$ V [9]. Consequently, we fix the Si/Ge bulk band offset at 0.94 V hereafter.

To validate this value, the valence band offsets from DFT and TB are compared. The estimation of the DFT value is made from a simulation of the slab, and we extract the position of the valence band of Ge in the Si/Ge heterostructure using the following equation:

$$E_v = E_v^0 - V^0 + V, \tag{1}$$

where E_v^0 is the position of the Ge valence band in the isolated Ge slab, and V^0 and V are the electrostatic potential in the isolated Ge slab and in Si/Ge heterostructure, respectively. Eq.1 also applies to Si in the Si/Ge heterostructure. The physical meaning of such an operation is to shift the valence band of isolated Si and Ge slabs by the electrostatic potential difference in the isolated slab and heterostructure. The DFT Si/Ge band offset $\Delta E_{\mathrm{V,s}}^{\mathrm{DFT}}$ is then simply the difference between the Si and Ge valence band position in the heterostructure. Using this methodology, we obtain a DFT estimation for $\Delta E_{\mathrm{V,s}}^{\mathrm{DFT}}$ of 0.54 V.

The extracted DFT value is not yet comparable to TB results, as the former is obtained for the slab, and the latter refers to the bulk and misses the effect of confinement and strains. Each TB bulk band offset can be converted into a slab offset ($\Delta E_{\mathrm{V,s}}^{\mathrm{TB}}$) by evaluating the difference in energy between the valence bands of the isolated, strained Si (20 layers) and Ge (21 layers) slabs, both computed with the desired $\Delta E_{\mathrm{V,b}}^{\mathrm{DFT}}$ as input parameter. The resultant $\Delta E_{\mathrm{V,s}}^{\mathrm{TB}}$ can be directly compared to the DFT value, and are 0.36 V and 0.62 V for the initial and adjusted TB parameters, respectively. Additionally, we can find the input $\Delta E_{\mathrm{V,b}}^{\mathrm{TB}}$ that provides $\Delta E_{\mathrm{V,s}}^{\mathrm{TB}} = \Delta E_{\mathrm{V,s}}^{\mathrm{DFT}}$. We found this value to be 0.86 V, which is reasonably close to the $\Delta E_{\mathrm{V,b}}^{\mathrm{TB}} = 0.94$ V that reproduces the DFT confinement. This indeed confirms that tuning $\Delta E_{\mathrm{V,b}}^{\mathrm{TB}}$ is not only meaningful to reproduce the DFT confinement, yet it also improves the description of the DFT slab band offset.

B. *Spin splitting at zero electric field*

Once the confinement is properly described in TB, we can adjust the spin splitting itself. The dependence of the spin splitting with the k-vector shown in Figure 1b can be fitted to a linear and a cubic term as

$$\Delta E_{\text{spin}}(E) = 2 \cdot \alpha_1(E)k + \alpha_3(E)k^3, \tag{2}$$

where $\alpha_1(E)$ and $\alpha_3(E)$ are the electric field (E) dependent linear and cubic coefficients, respectively. We first focus on the case of zero electric field. The original TB parameters provide a description of the spin splitting that differs considerably from the reference DFT results, see Table I and Fig. 5.

To adjust the TB spin splitting we introduce an extra onsite potential δ to the Si and Ge atoms at the Si/Ge interface. This correction is applied as a shift of $-\delta$ and $+\delta$ to the TB onsite matrix elements of the interface Ge and Si atoms, respectively. Fig. 3 shows the averaged electrostatic potential in the x-y plane along the z direction from a DFT calculation on a smaller heterostructure. The potential on Si/Ge atoms at the interface show significant differences from those of the inner layers, which are all essentially equal. Such a phenomenon is due to the Si-Ge bonds at the interface, which induce a charge redistribution between Si and Ge atoms and differ from a bulk situation. This is certainly missing in the original TB parameters, where the onsite terms are the same for all atoms of each kind.

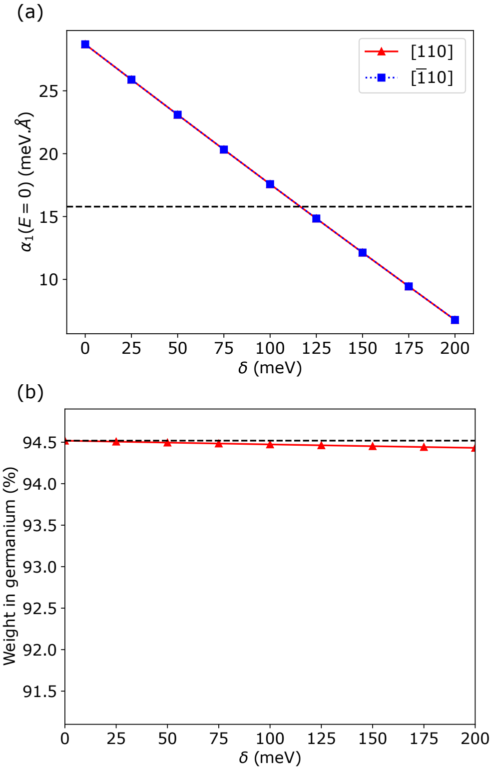

Fig. 4: Impact of the onsite potential of the interface atoms δ on (a) the coefficient of the linear term in the spin splitting fit of Eq. 2, (b) the weight of the topmost valence band wavefunction in germanium. The x-axis gives the magnitude of the onsite potential. The black dashed line is the *ab initio* reference.

For the adjustment of the spin splitting we focus on the linear term in Eq. 2. Fig. 4(a) shows that modifying the onsite potential of the interface atoms has a strong impact on $\alpha_1(E = 0)$, and we can reach a perfect agreement between TB and DFT when $\delta = 116$ meV. Remarkably, the modifications of δ have a negligible impact on the confinement of hole wavefunction, as shown in Fig. 4(b). This allows to keep the correct confinement reached by tuning the band offset while adjusting the spin splitting.

With a TB interface onsite correction of 116 meV, we reach a perfect description of the DFT spin splitting in a large range of k, see Fig. 5. Even if the corrections were applied to adjust the linear part, also the cubic term is well captured. We also recover the expected equality between the spin splitting along the [110] and [$\bar{1}$10] directions, which must indeed be identical due to symmetry. The comparison of the fitting parameters of Eq. 2, given in Table I, highlights the excellent agreement between the corrected TB and the DFT results.

C. *Spin splitting at finite electric field*

In the context of spin qubits, a meaningful description of SOC effects at finite electric fields is crucial, as they are formed by electrically confined quantum dots. To address the

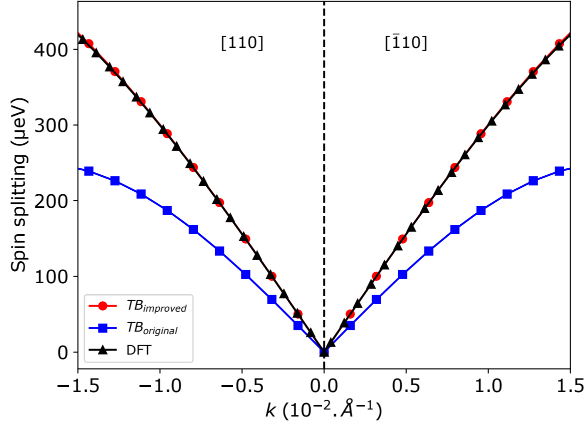

Fig. 5: Spin splitting (ΔE_{spin}) along $[110]$-Γ-$[\bar{1}10]$ direction for DFT, the original and the corrected TB calculations.

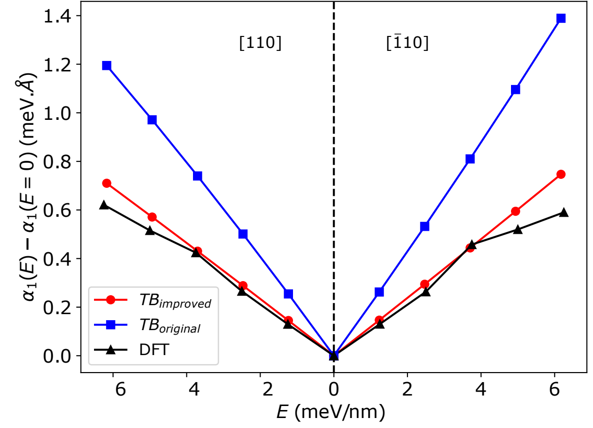

Fig. 6: The linear term coefficient on the fit of Eq. 2 as a function of the Ge internal electric field along [110] and $[\bar{1}10]$ directions.

validity of the new TB parameters in such conditions (they have been adjusted at zero electric field), we performed DFT and TB calculations with an electric field perpendicular to the slab. For the DFT calculations, we apply an external electric field ranging from 0 to 100 meV/nm, which results in an internal field up to 7.9 and 6.25 meV/nm in Si and Ge, respectively (the external/internal field ratio yields to a static dielectric constant of 12.6 and 16 for Si and Ge, which are consistent with experiments [11]). The same internal fields are applied in TB to have a proper comparison.

Fig. 6 shows the variation of α_1 along the [110] and $[\bar{1}10]$ directions with the magnitude of the electric field. The zero field spin splitting is subtracted for each method to ease the comparison. Note that the presence of an electric field yields to a different spin splitting along the two directions. The original TB parameters fail to describe the correct impact of E-field dependence. Notably, the same corrections that ensure an optimal description of the zero-field SOC effects provide an accurate description of their electric field dependence.

The DFT dependence of the spin splitting on E can only be reproduced in TB with an accurate description of the wavefunction confinement. As for the case $E = 0$, the correct spin splitting cannot be obtained only by adjusting δ, which highlights again the relevance of the two introduced parameters. Therefore, the general method to adjust the description of SOC effects in TB to a reference DFT result requires first the tuning of the valence band offset to ensure the correct confinement, and the subsequent introduction of an onsite potential to the interface atoms to adjust the spin splitting.

TABLE I: Linear and cubic coefficients extracted from Eq. 2 for the different calculations. The linear coefficient has the units of meV·Å, and the cubic one is eV·Å^3.

	$\alpha_1(E=0)$	$\alpha_3(E=0)$
DFT	15.79	16.06
TB_{improved}	15.80	15.51
TB_{original}	10.99	25.80

The realization of these steps for $E = 0$ captures the electric field effects, at least for the test heterostructure simulated here.

IV. Conclusion

In this work, we demonstrated a general approach to improve the Tight-Binding description of SOC in Si/Ge heterostructures by refining the quantum confinement with the TB band offset, and then adjusting the spin splitting of the topmost valence bands with an onsite potential on the interface atoms. Even though the methodology was here illustrated with a simple functional (PBE) and a prototypical heterostructure for demonstration purposes, such an approach could in principle reproduce the targeted *ab initio* results regardless of the functional and heterostructure complexity. Better TB models, when fitted for the relevant heterostructures, should improve the modelling of Ge spin qubits physics.

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