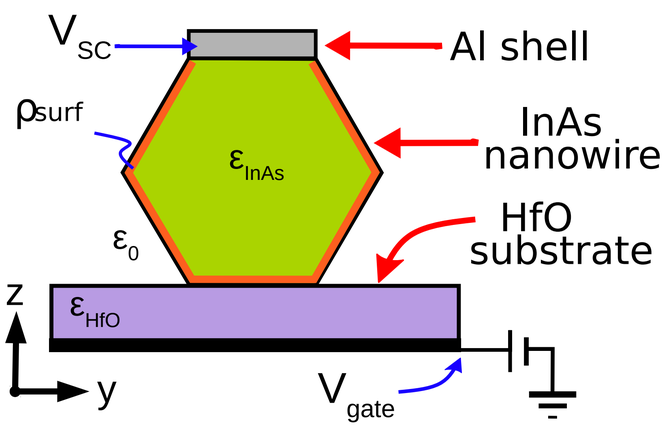
Spin-Orbit coupling in Rashba nanowires: modelling and behaviour

[1]Samuel D. Escribano, [2]Alfredo Levy Yeyati and [1]Elsa Prada

[1]Departamento de Física de la Materia Condensada and [2]Departamento de Física Teórica de la Materia Condensada, IFIMAC and Instituto Nicolás Cabrera, Universidad Autónoma de Madrid, E-28049 Madrid, Spain

ABSTRACT: Semiconductor Rashba nanowires have attracted a great deal of attention due to the large Spin-Orbit (SO) coupling present in their conduction bands. One source of SO interaction can arise in these nanowires when the crystal potential symmetry is broken due to a tunable external and/or internal electric field. Here we look for a phenomenological equation which could be used in a tight-binding (TB) model and which correctly captures this kind of SO interaction for complex crystallographic structures, specifically for type III-V semiconductor compounds. To this end, and following the ideas of Refs. **[1,2]**, we depart from an 8-band k·p model from which the effective Rashba coupling can be adequately extracted. Then, we fit the results to a phenomenological equation that can be used in a TB model regardless of the geometry of the environment. We apply this theoretical description to a Majorana nanowire device (including its electrostatic environment), where the SO coupling is known to play a major role for the formation of topological edge states.

1. System



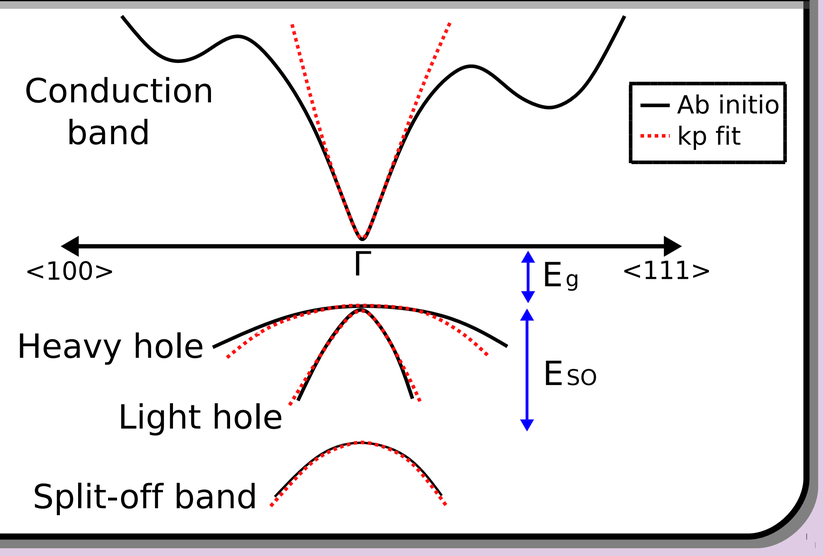
Poisson eq: $\vec{\nabla}\left\{\epsilon(\vec{r})\cdot\vec{\nabla}\phi(\vec{r})\right\}=\rho(\vec{r})$

2. 8-band model

Using k.p theory, the bands of any semiconductor can be described around the Γ-point by fitting *Ab initio* calculations,

$$H_{kp}=\frac{p^2}{2m_0}+\frac{\hbar^2k^2}{2m_0}+\frac{\vec{k}\cdot\vec{p}}{m_0}-e\phi(\vec{r})-\\-\frac{\hbar}{4m_0^2c^2}(\vec{k}+\vec{p})\cdot(\vec{\sigma}\times\vec{\nabla}\phi)$$

The Hamiltonian is projected into the 8-band basis, taking into account the remaining bands through Löwdin perturbation theory.



3. Tight-binding model

The TB model has been proved to be more versatile and less computationally expensive,

$$H_{TB}=\sum_i\frac{\hbar^2k^2}{2m_i^*}-e\phi(\vec{r})+\vec{k}\cdot(\vec{\sigma}\times\vec{\alpha}_i(\vec{r}))$$

band — Effective mass — Effective SOC

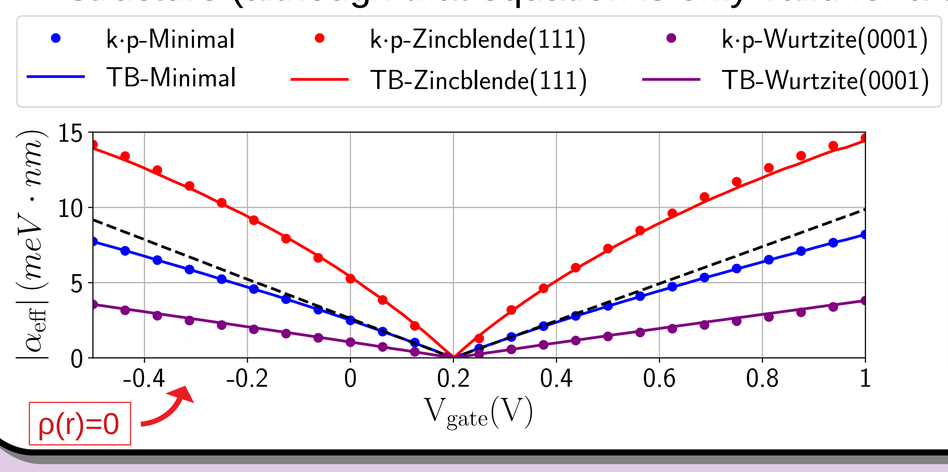
From the simplest 8-band k·p Hamiltonian, it can be extracted an analytical equation for the Rashba coupling:

$$\vec{\alpha}(\vec{r})=\vec{\nabla}\left\{\frac{P_h^2}{(E_g-e\phi(\vec{r})-E)}-\frac{P_{SO}^2}{(E_{SO}+E_g-e\phi(\vec{r})-E)}\right\}$$

$$\xrightarrow[E_g\gg(e\phi+E)]{}\simeq-\left[\frac{P_h^2}{E_g^2}-\frac{P_{SO}^2}{(E_{SO}+E_g)^2}\right]\vec{\nabla}\phi(\vec{r})$$

4. Rashba extraction from k·p theory

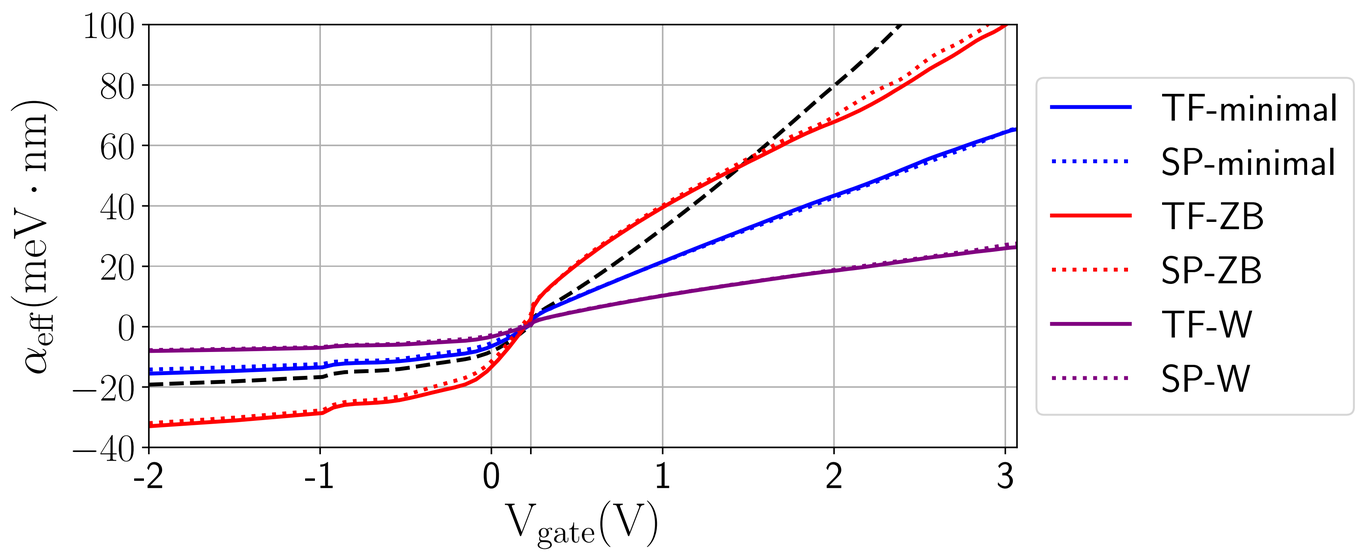
We fit the energy bands of the TB model to the ones of k·p theory in order to adjust the phenomenological parameters P_h and P_{SO} for each crystallographic structure (although that equation is only valid for a simplified model):



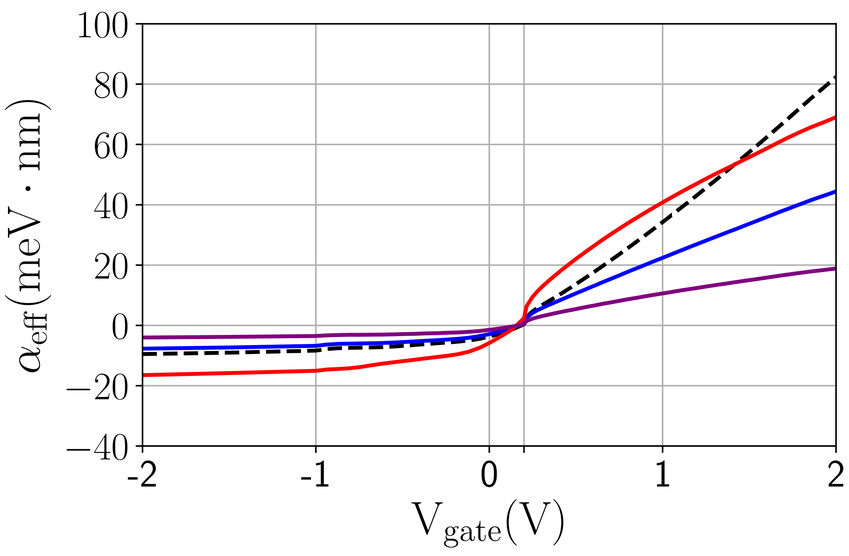
	P_h (meV·nm)	P_{SO} (meV·nm)
Min.	517.4	431.1
ZB	1277.6	1995.4
W	664.8	931.3

5. Results

Using the TB model we can obtain the Rashba coupling for any V_{gate} (and for any subband). We do so by solving self-consistently the Schrödinger-Poisson equation (SP), and in the Thomas-Fermi approximation (TF).



We can include in the TB model the metallic region corresponding to the SC, where we assume that there is a negligible Rashba coupling.



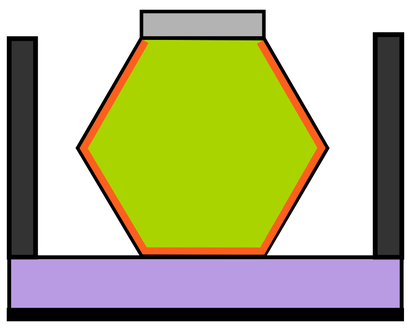
6. Conclusions

It is possible to find a phenomenological equation in a TB model which properly describes the SO coupling in semiconductor (compounds) nanowires, independently of the particular geometry of the environment (*still in progress*). However, it has two limits of applicability: the one imposes by the fitting to the *ab initio* calculations, and the other given by the fitting to the 8 band theory.

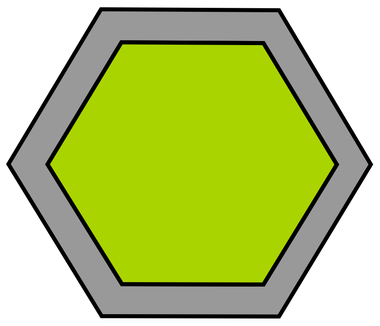
7. Work in progress

We can apply this approach to other geometries:

Multi-gated nanowires



Full-shell nanowires



Parameters.- W_w=80nm, W_{Al}=8nm, W_{HfO}=20nm, V_{Al}=0.2eV, T=10mK, $\rho_{surf}=2\cdot10^{-4}\,e\cdot nm^{-3}$.

References.- **[1]** M. Gmitra and J. Fabian, Phys. Rev. B **94**, 165202 (2016).

[2] P. Wójcik, A. Bertoni and G. Goldoni, Phys. Rev. B **97**, 165401 (2018).