Improved effective equation for the Rashba spin-orbit coupling in semiconducting nanowires

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ABSTRACT: Semiconductor Rashba nanowires are quasi-one dimensional materials that have large spin-orbit (SO) coupling arising from a broken crystal potential symmetry due to an external electric field. There exist parametrized multiband models that can describe accurately this effect. However, simplified single band models are highly desirable to study geometries of recent experimental interest, since they may allow to incorporate the effect of the electrostatic environment of the nanowires at a reduced computational cost. We demonstrate here that an effective equation for the linear Rashba SO coupling of the semiconductor conduction band can reproduce the behaviour of more sophisticated eight-band k·p model, what is achieved by adjusting a single effective parameter that depends on the nanowire crystal structure and its chemical composition. We further compare our approach with the Rashba coupling extracted from several experiments.

1. Effective Rashba SO coupling

We solve self-consistently the Schrödinger-Poisson equation to compute the eigenspectrum of *realistic* nanowires. The conduction-band (CB) can be effectively described as

$$\hat{H}_{\mathrm{CB}} = \frac{\hbar^2 \hat{\vec{k}}^2}{2m_{\mathrm{eff}}} + E_F - e\phi(\vec{r}) + \hat{\vec{\alpha}}_{\mathrm{eff}}(\vec{r}) \cdot (\hat{\vec{k}} \times \vec{\sigma}),$$

where φ(r) is the electrostatic potential, and m_{eff} and α_{eff} is the effective mass and SO coupling. For this last parameter, we propose the following expression for type III-V semiconductors

$$\hat{\vec{\alpha}}^{(j)}_{\mathrm{eff}}(\vec{r}) = \frac{P^2_{\mathrm{eff}}}{3} \vec{\nabla} \left\{ \frac{1}{\Delta_g + e\phi(\vec{r}) + E^{(j)}} - \frac{1}{\Delta_g + \Delta_{\mathrm{SOff}} + e\phi(\vec{r}) + E^{(j)}} \right\}$$

where P_{eff} is an effective parameter which depends on the crystal structure and chemical composition of the wire, Δ_g and Δ_{SO} are the (tabulated) semiconducting and split-off band gaps, and $E^{(j)}$ *is* energy of the transverse sub-band.

In previous works, a similar (but oversimplified) expression has been used to describe the SO coupling

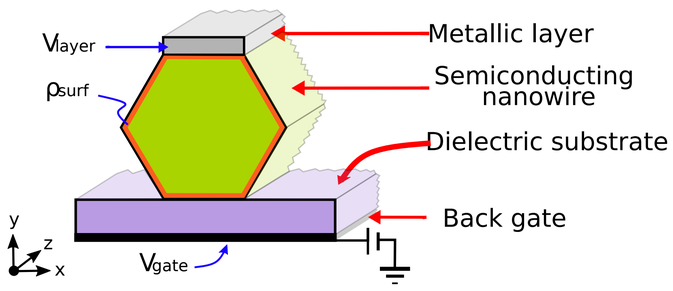
$$\hat{\vec{\alpha}}_{\mathrm{os}}(\vec{r}) \simeq -\frac{P^2}{3} \left[\frac{1}{\Delta_g^2} - \frac{1}{(\Delta_g + \Delta_{\mathrm{SOff}})^2} \right] \vec{\nabla}(e\phi(\vec{r}))$$

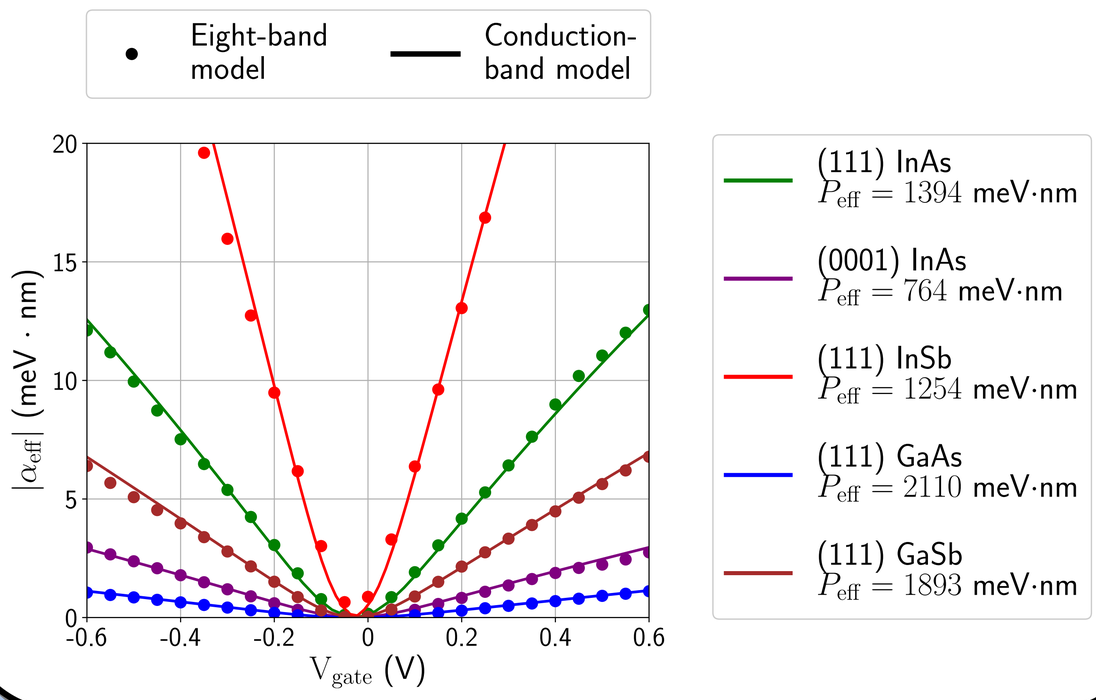
which ignores the energy-dependency with the transverse sub-band, and the precise crystal structure, since *P* only depends on the chemical composition.

2. P_{eff} for different materials

It is possible to extract P_{eff} from fitting α_{eff} to eight-band k·p calculations, which are known to correctly predict the SO effects in semiconductor materials.

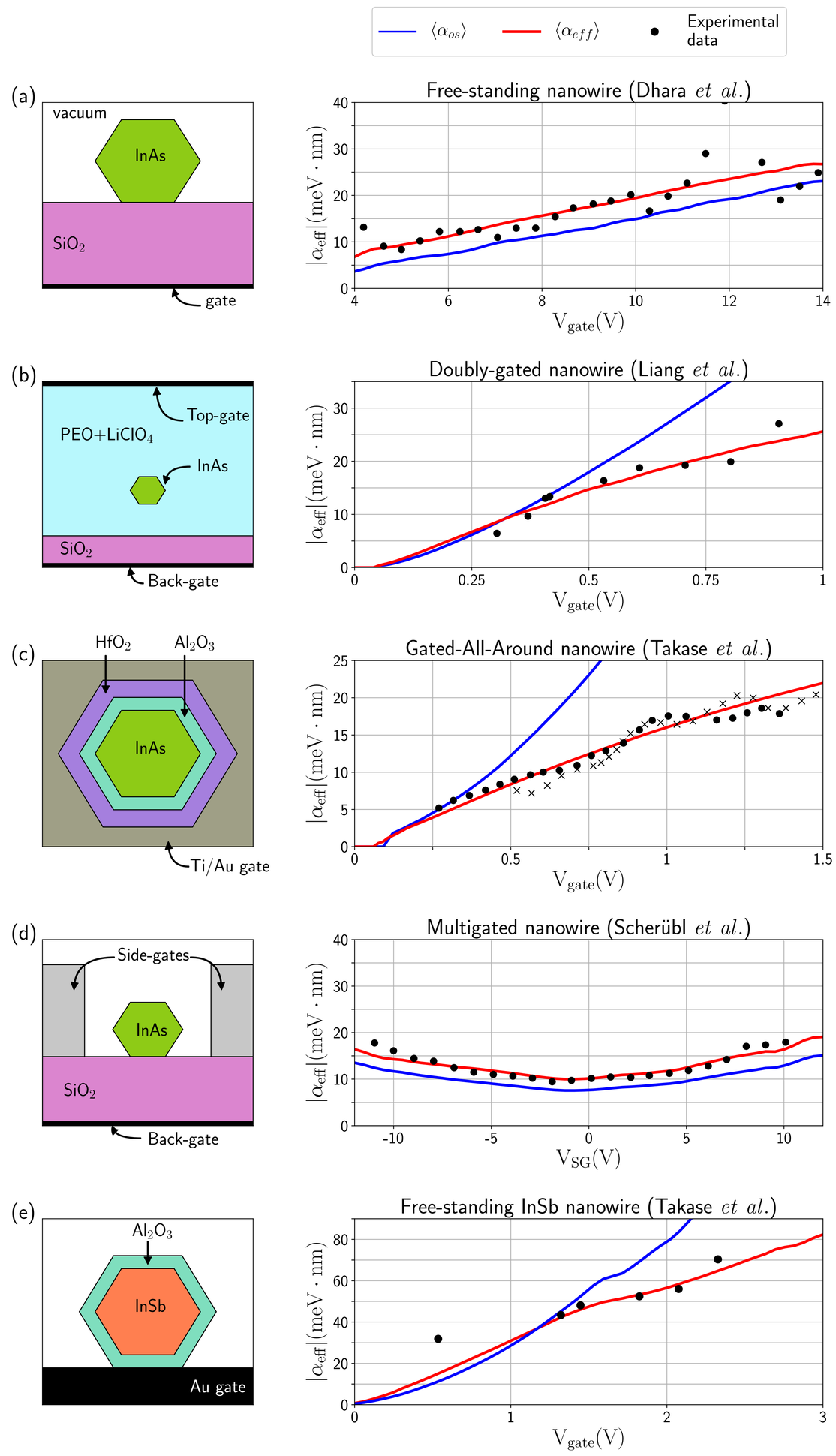
We do so for different crystals and materials. To this end, we simulate an arbitrary electrostatic environment (P_{eff} should not depend on it).





3. Comparison to experiments

To test the validity of our approach, we compare it with several experimental works[1-5] of magneto-conductance



4. Conclusions

- It is possible to describe in a more detailed way than a rough constant the SO coupling in type III-V semiconductor nanowires. This can be done through an effective equation which takes into account the interaction with other bands through one effective parameter. This parameter is found from 8-band k·p calculations.
- We find an excellent agreement between our simulations and the data obtained from magneto-conductance measurements in several references.
- We believe our work could be relevant for spintronics devices or Majorana nanowires, where the SO coupling plays a major role.

Experimental work references.-

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[4] Scherübl *et al.* PRB **94**, 035444 (2016).
[5] Takase *et al.* (InSb) App. Phys. **12**, 117002 (2019).