Modelling of electronic and transport properties in semiconductor nanowires

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The NODE project

- NODE – Nanowire-based One Dimensional Electronics
- Bottom up approach to nanowire based electronics
- Evaluate and deliver replacement and add-on technologies to silicon CMOS
- Partners within academia and industry in Europe
  - Lund University (Coordinator)
  - TU Delft, Max-Planck Institute (Halle), Scuola Normale Superiore (Pisa)
  - Würzburg University, CEA, IBM Research, IMEC, Philips, Infinieon, Qumat
- CEA Grenoble is contributing with theory and structural analysis of nanowires

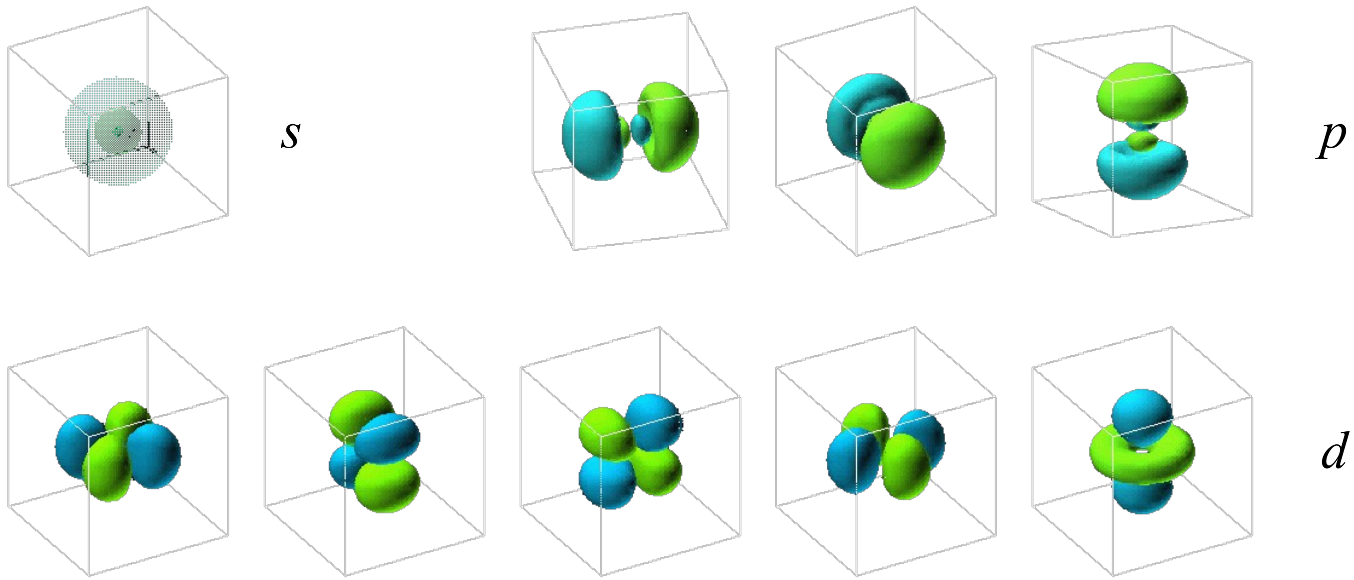
Outline

- **Strains in nanowire heterostructures**.
  - Effects of strain relaxation of nanowire heterostructures.
  - Barrier lowering due to strain.

- Doping of nanowires
  - Dielectric effects
  - Increased binding energies

- **Transport properties of semiconductor nanowires**.
  - The Kubo-Greenwood and Landauer-Büttiker approach.
  - Application : Surface disorder.

The tight-binding method



- Principle : Expand the wavefunctions as linear combination of atomic orbitals.
  - The **range** of the model is limited to first, second or third-nearest neighbors.
  - The matrix elements of the hamiltonian are considered as adjustable parameters usually fitted on bulk band structures then **transferred** to the nanostructures.
  - **The computation time scales (at least linearly) with the number of atoms** (up to a few millions of atoms today).

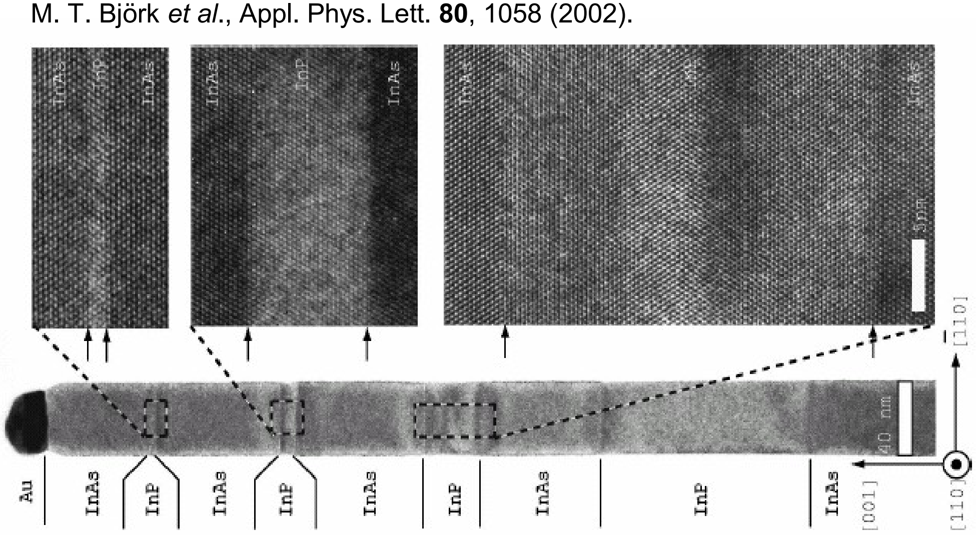
Part I :

Strains in nanowire heterostructures

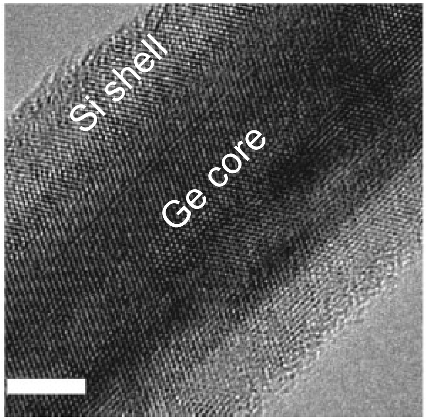
Nanowire heterostructures

- Large interest in nanowire « heterostructures » for optics & transport :

M. T. Björk *et al.*, Appl. Phys. Lett. **80**, 1058 (2002).



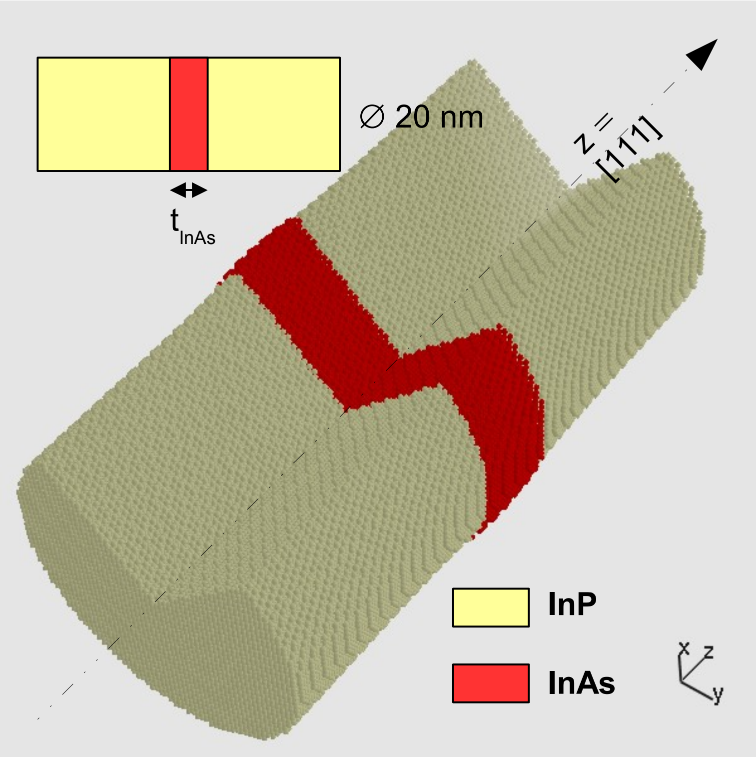
W. Lu *et al.*, PNAS. **102**, 10046 (2005).



- Strain relaxation is believed to be efficient in these structures, likely allowing the growth of thick lattice mismatched layers.

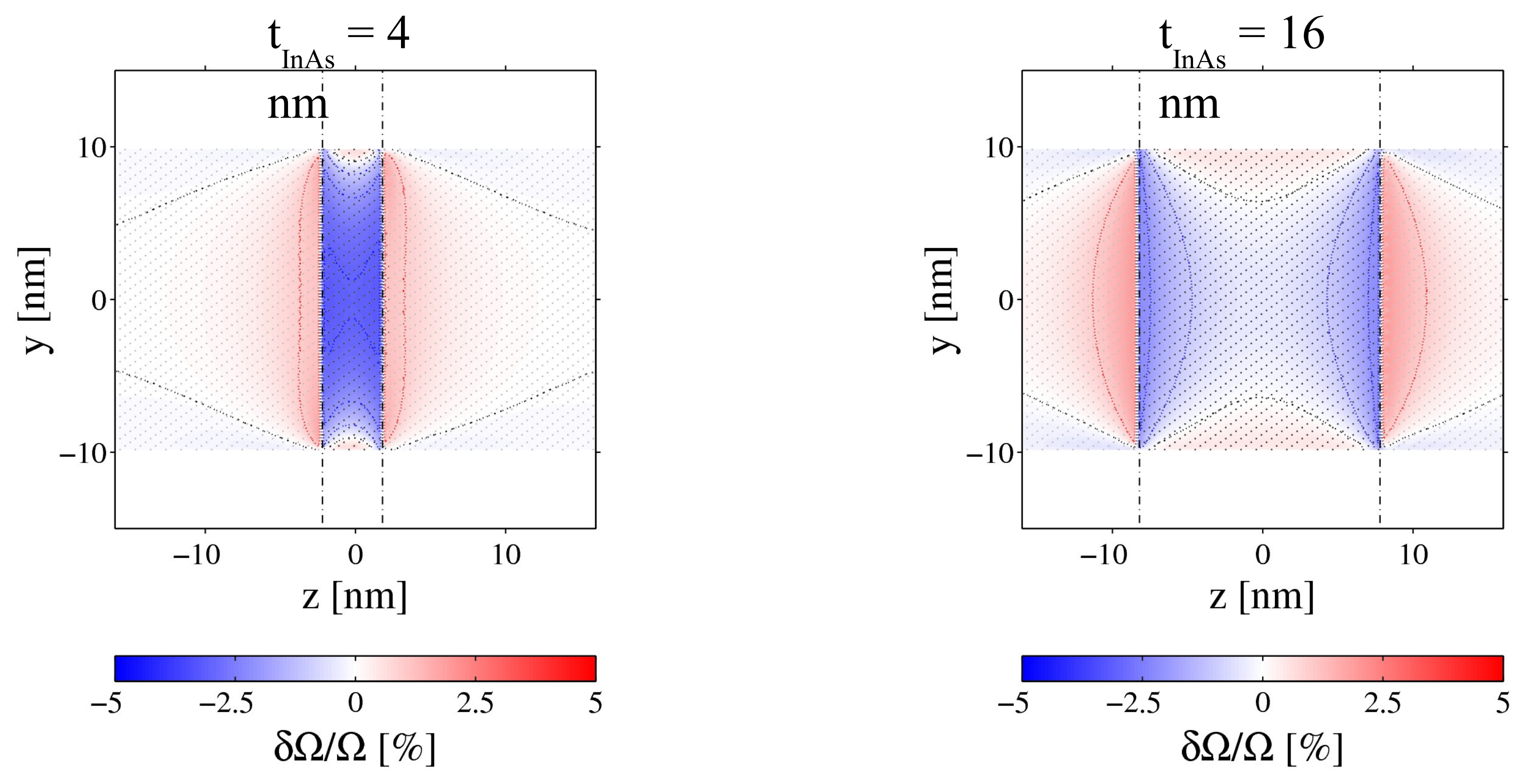
- A few issues :
  - **What is the effect of strain relaxation on the electronic properties of nanowire heterostructures ?**
  - **What is the effect of an overgrown shell ?**

InAs/InP heterostructures



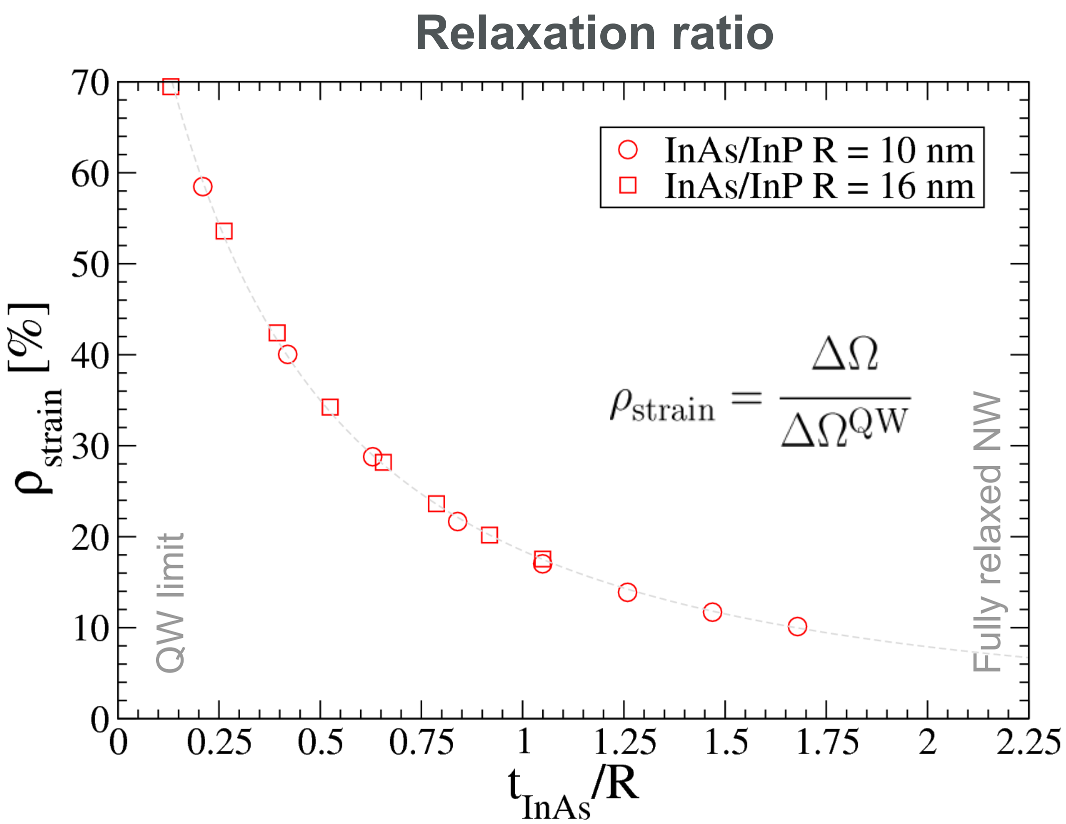
- The bond length is 3.13% shorter in InP than in InAs. The InAs layer is thus **compressed** by the InP core, but can partly **relax** strains at the surface of the nanowire.
- Strain relaxation is computed using Keating's Valence Force Field model

Strain relaxation



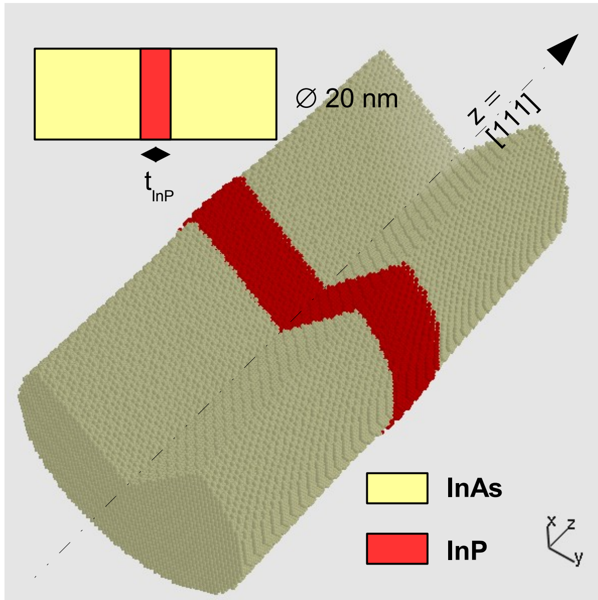
- Strain relaxation is very **efficient** in nanowire heterostructures. The InAs layer expands outwards and distorts the surface of the nanowire. The strain distribution is however very **inhomogeneous** in thin InAs layers : the surface is overrelaxed while the axis is still significantly compressed.

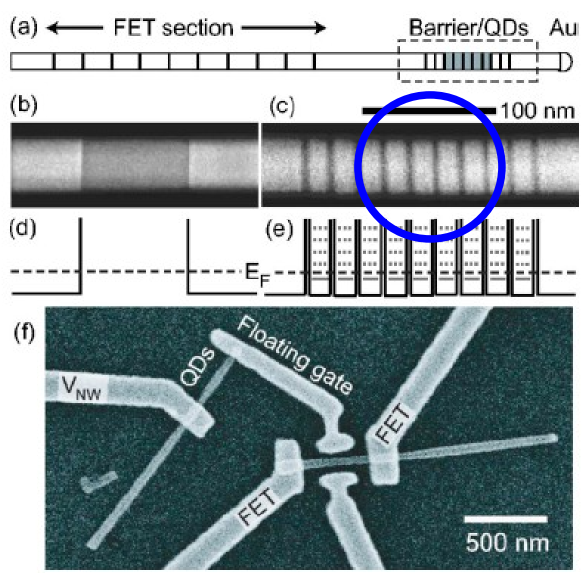
Strain relaxation



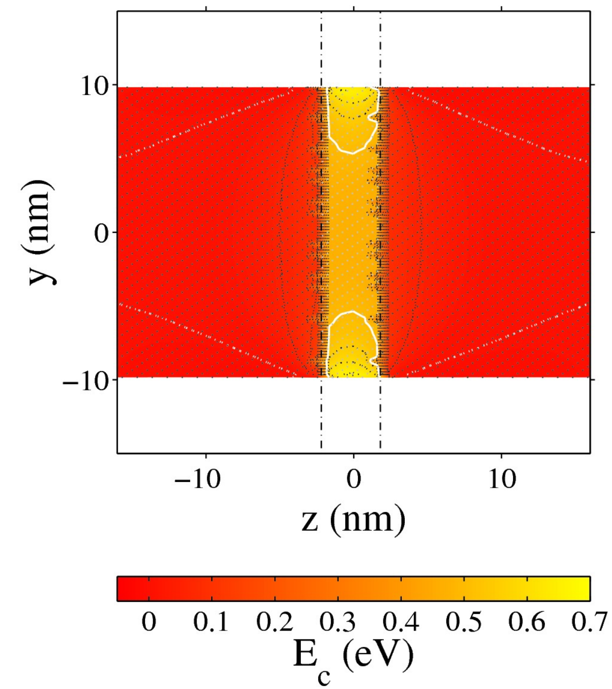
- The InAs layers are almost **completely relaxed** when $t_{\text{InAs}} > 2R$.

InP tunnel barriers in InAs nanowires



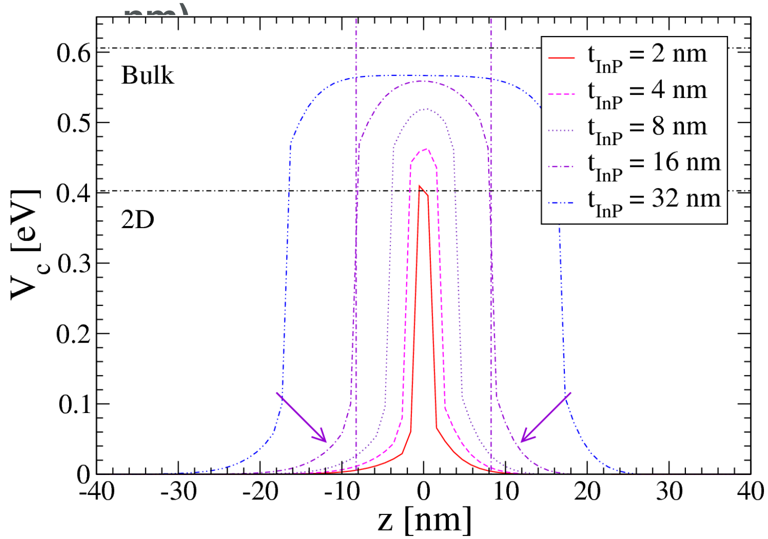


H. A. Nilsson *et al.*, Applied Phys. Lett. **89**, 163101 (2006).

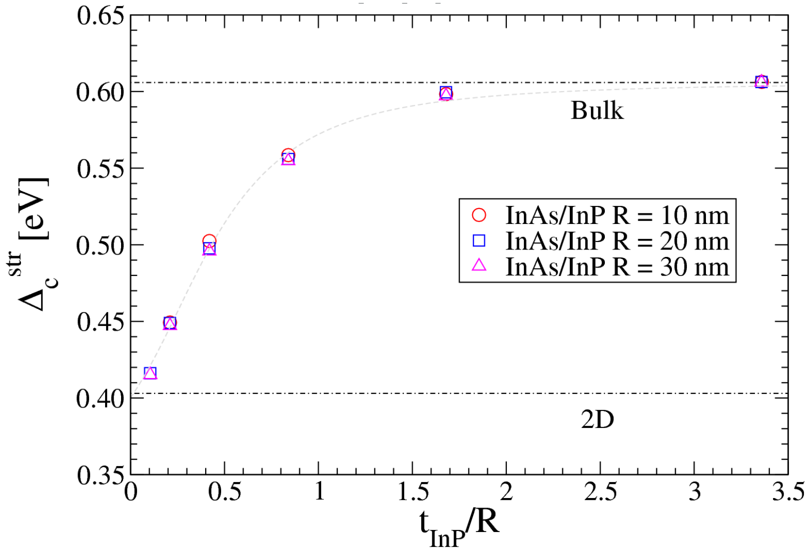


- The InP barrier is dilated by the InAs core, which tends to **lower the conduction band energy**.

Conduction band profile (R = 10 nm)



Barrier



- The barrier height is **close to the bulk value (0.6 eV)** in thick InP layers (t_{InP} > 1.5R), but tends to the **2D limit (0.4 eV)** in thin ones.

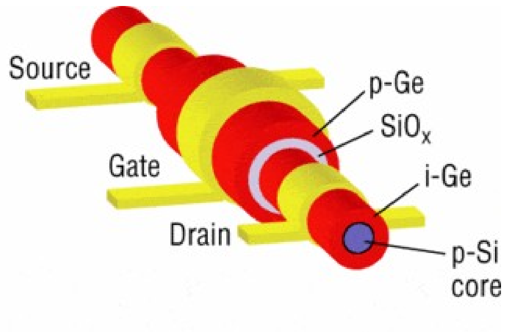
Quantum dots and tunnel barriers in InAs/InP nanowire heterostructures : Electronic and optical properties
Y. M. Niquet and D. Camacho, Phys. Rev. B. **77**, 15316 (2008).

Part II :

Doping in nanowires

Doping in nanowires

- Doping of semiconductor nanowires is an important issue and challenge.



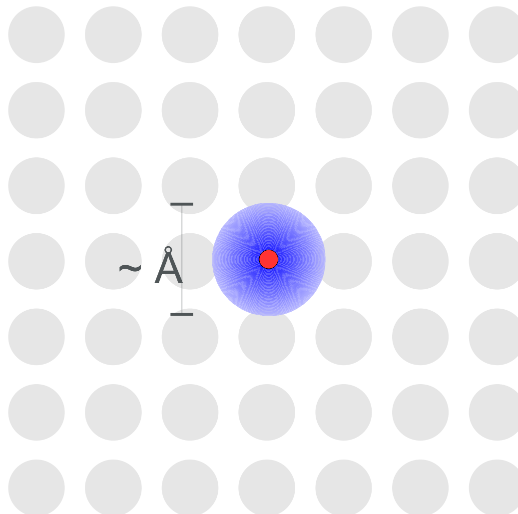
L. J. Lauhon *et al.*, Nature **420**, 57 (2002)

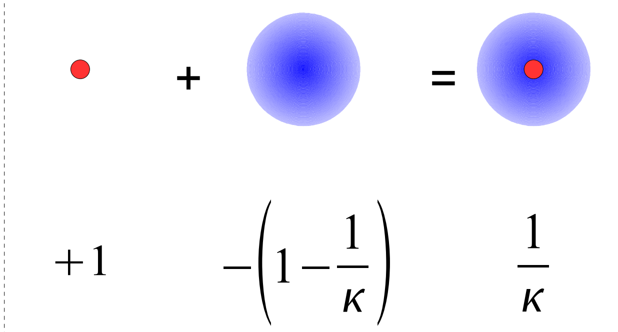
- Non uniform dielectric environments ⇒ Complex electrostatics.

What is the binding energy of donor and acceptor impurities ?
What is the doping efficiency ?
How can we improve doping efficiency?

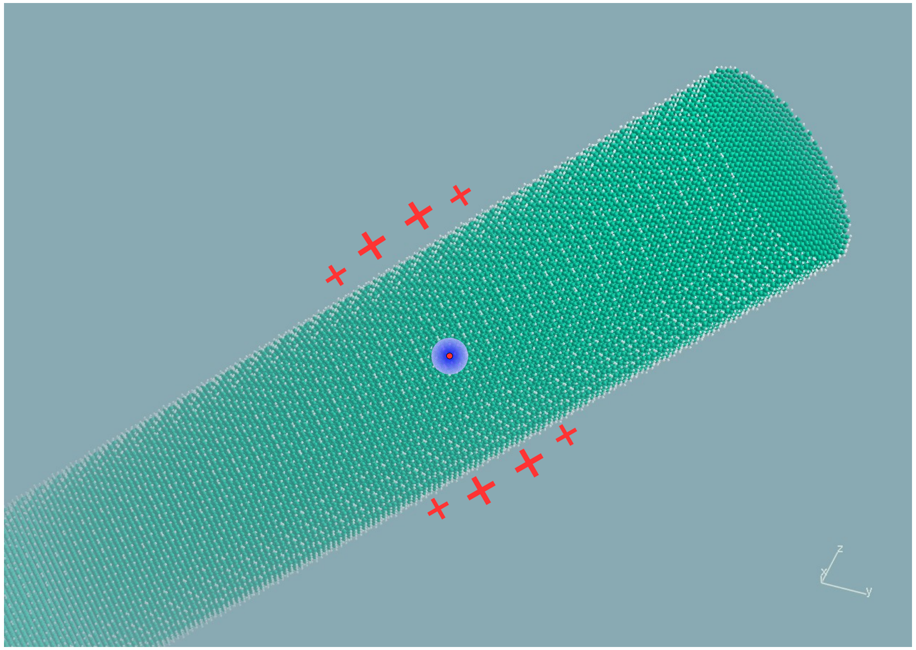
- <u>Conclusions</u> :
  - **The binding energy of donor and acceptor impurities can be greatly enhanced in thin (*R* < 10 nm) silicon nanowires in vacuum.**
  - **High-κ dielectrics and all-around metallic gates for example can help to improve the doping efficiency.**

The microscopic interpretation of classical electrostatics





- An ionized donor attracts nearby valence electrons and **gets screened by a short-range « cloud » of negative charges**.
- **The impurity and its cloud behave as a total charge $1/\kappa$** creating a potential $V(\mathbf{r},\mathbf{r}') = 1/\kappa|\mathbf{r}-\mathbf{r}'|$ at long distances.
- In bulk materials, the charge $-\left(1-\frac{1}{\kappa}\right)$ in this cloud comes « from infinity ».



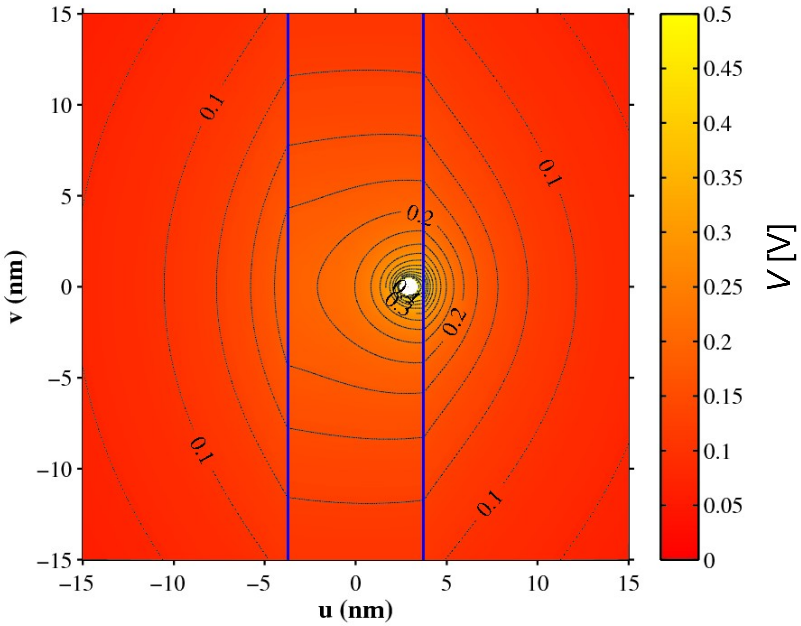
- In a nanowire, however, **the charge in the cloud comes from the surface** (« **image charges** » distribution).

- The solution of Poisson equation :

$$\nabla_{\mathbf{r}'} \left[\kappa(\mathbf{r}') \nabla_{\mathbf{r}'} V(\mathbf{r}, \mathbf{r}')\right] = 4\pi\delta(\mathbf{r} - \mathbf{r}')$$

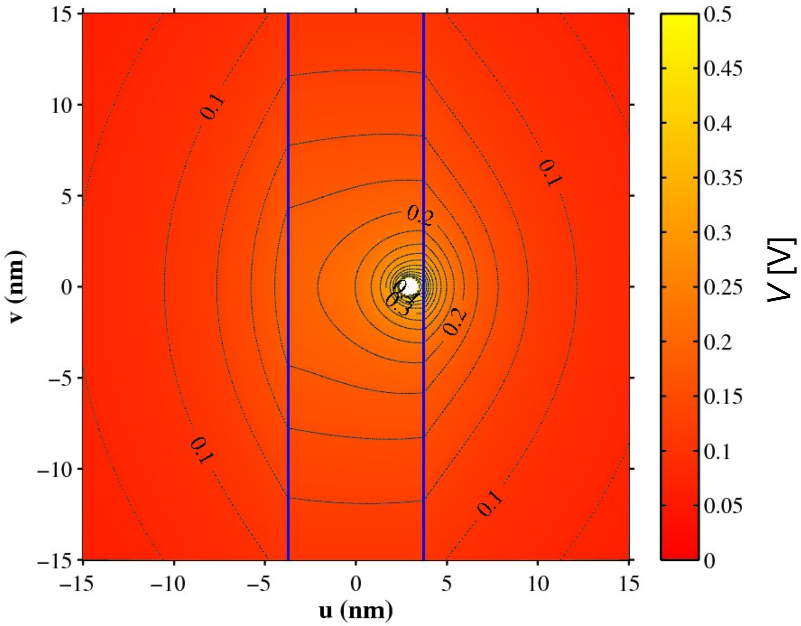
is actually the potential created in vacuum by the (unscreened) impurity, its cloud and its image charges.

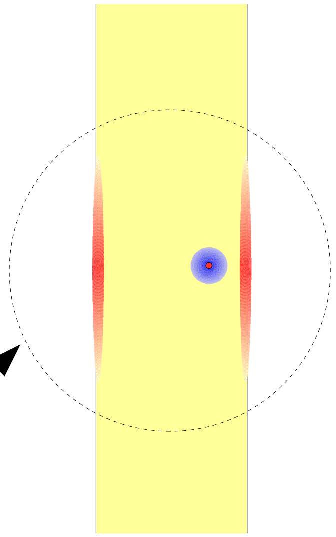
The hydrogenoid impurity problem in nanowires



- The potential is not isotropic due to the image charges.

The microscopic interpretation of classical electrostatics



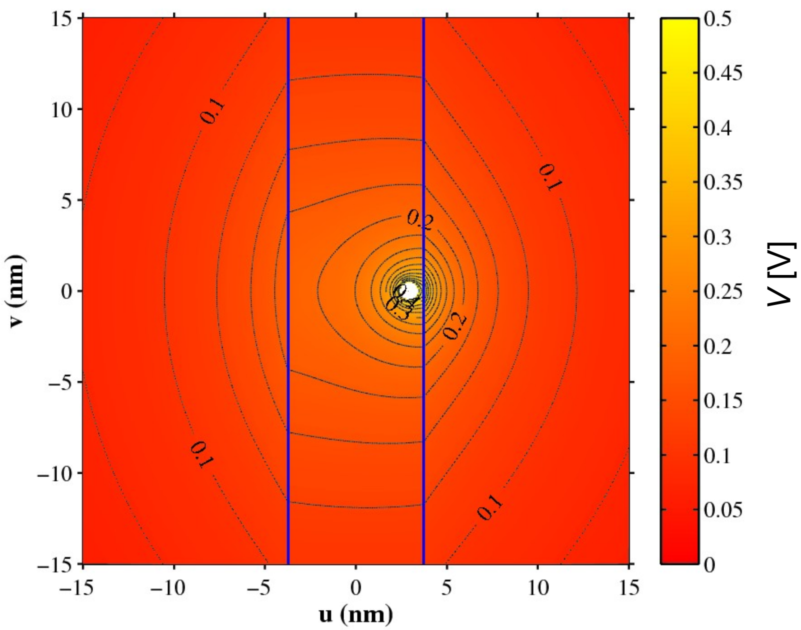


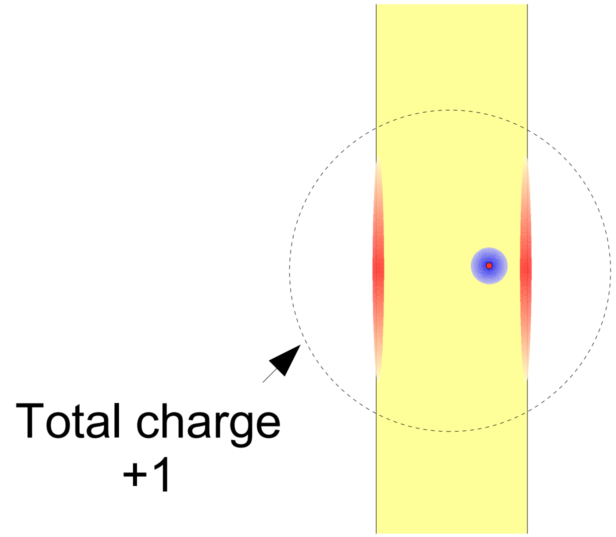
Total charge
+1

- The potential is not isotropic due to the image charges.

- The total charge of the system (impurity + cloud + image charges) is +1 ; hence the potential decreases as $1/|\mathbf{r}-\mathbf{r}'|$ far enough (a few R's) from the impurity. As a consequence, **the potential around the impurity is deeper than in bulk**.

The microscopic interpretation of classical electrostatics





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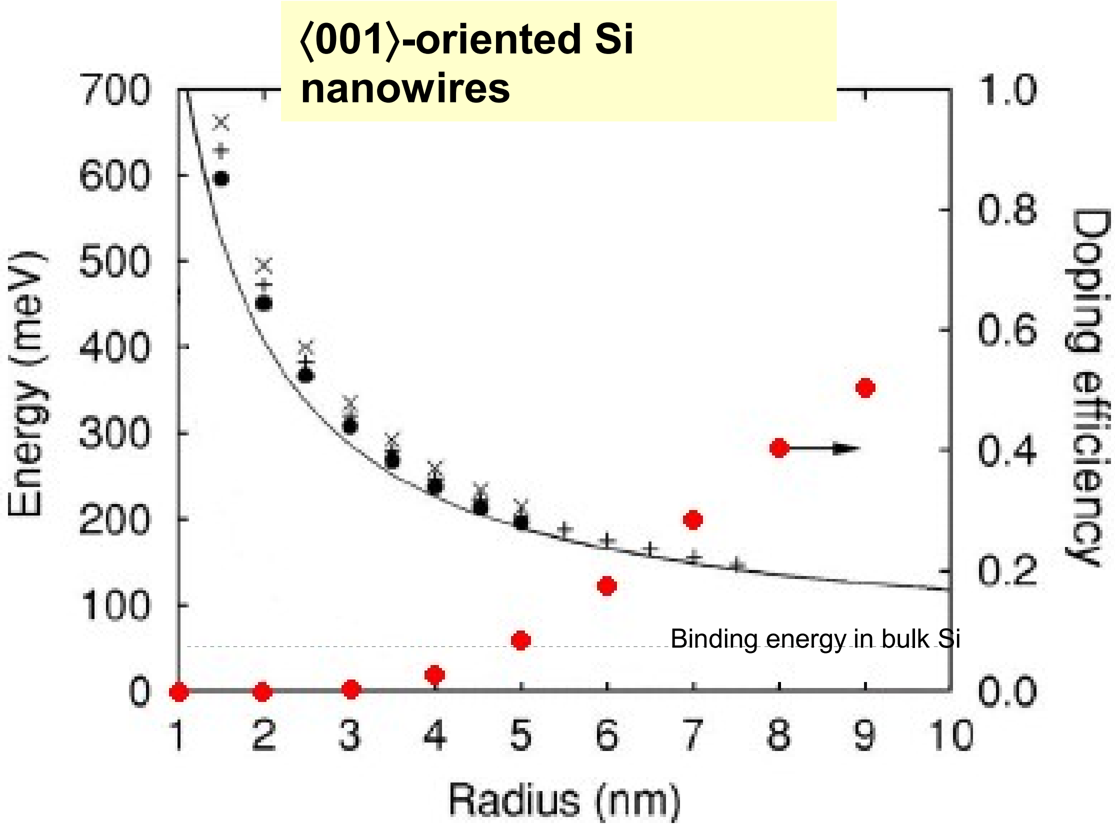
Effects on the binding energies and doping efficiency ?

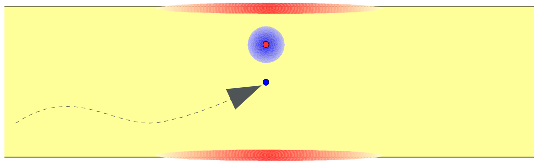


Binding energy of a donor in a Si nanowire as a function of its radius.

The donor is located along the nanowire axis.

+ P (45 meV in bulk)
× As (54 meV in bulk)
• Sb (39 meV in bulk)

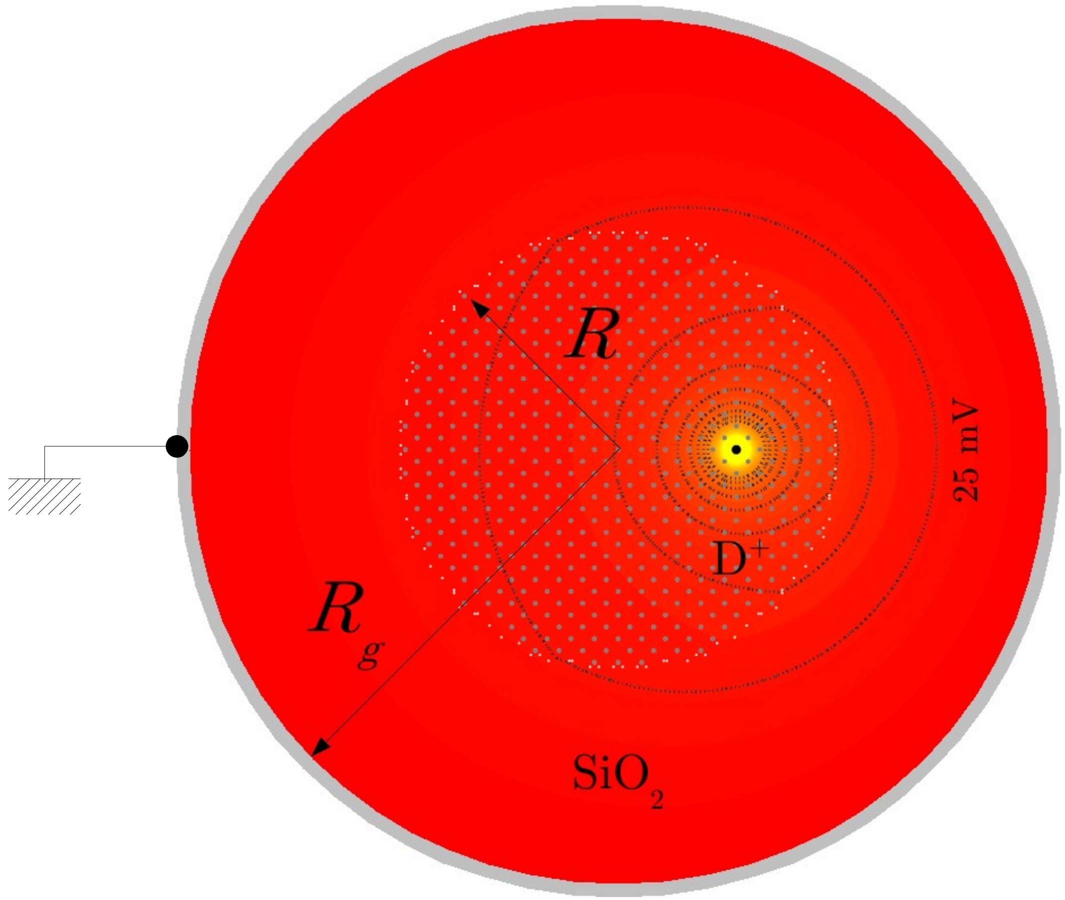
- The image charges **increase the binding energy of the donor up to a few hundreds of meV** in the smallest nanowires !!



The electron is trapped around the donor by the impurity and its image charges.

Ionization energies of donor and acceptor impurities in semiconductor nanowires : importance of dielectric confinement
M. Diarra, Y. M. Niquet, C. Delerue and G. Allan, Phys. Rev. B **75**, 045301 (2007).

Screening in a complex dielectric environment



- Oxides and metallic gates screen the impurity potential...

  ⇒ **Decrease of the binding energy**

  ... BUT ...

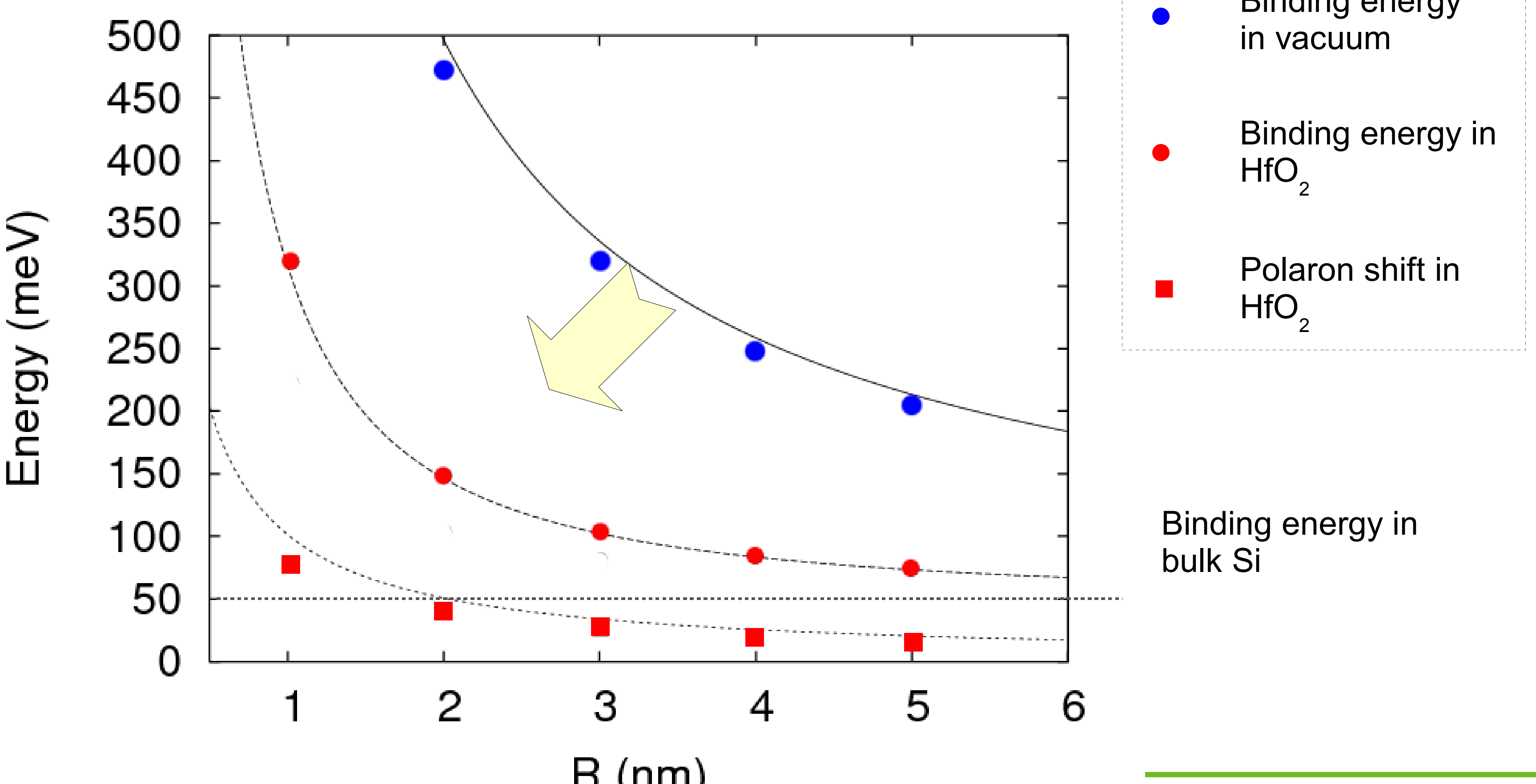
- The dielectric response of the oxides is slow...

  ⇒ **Polaronic enhancement of the binding energy** !

Si nanowires embedded in HfO_2

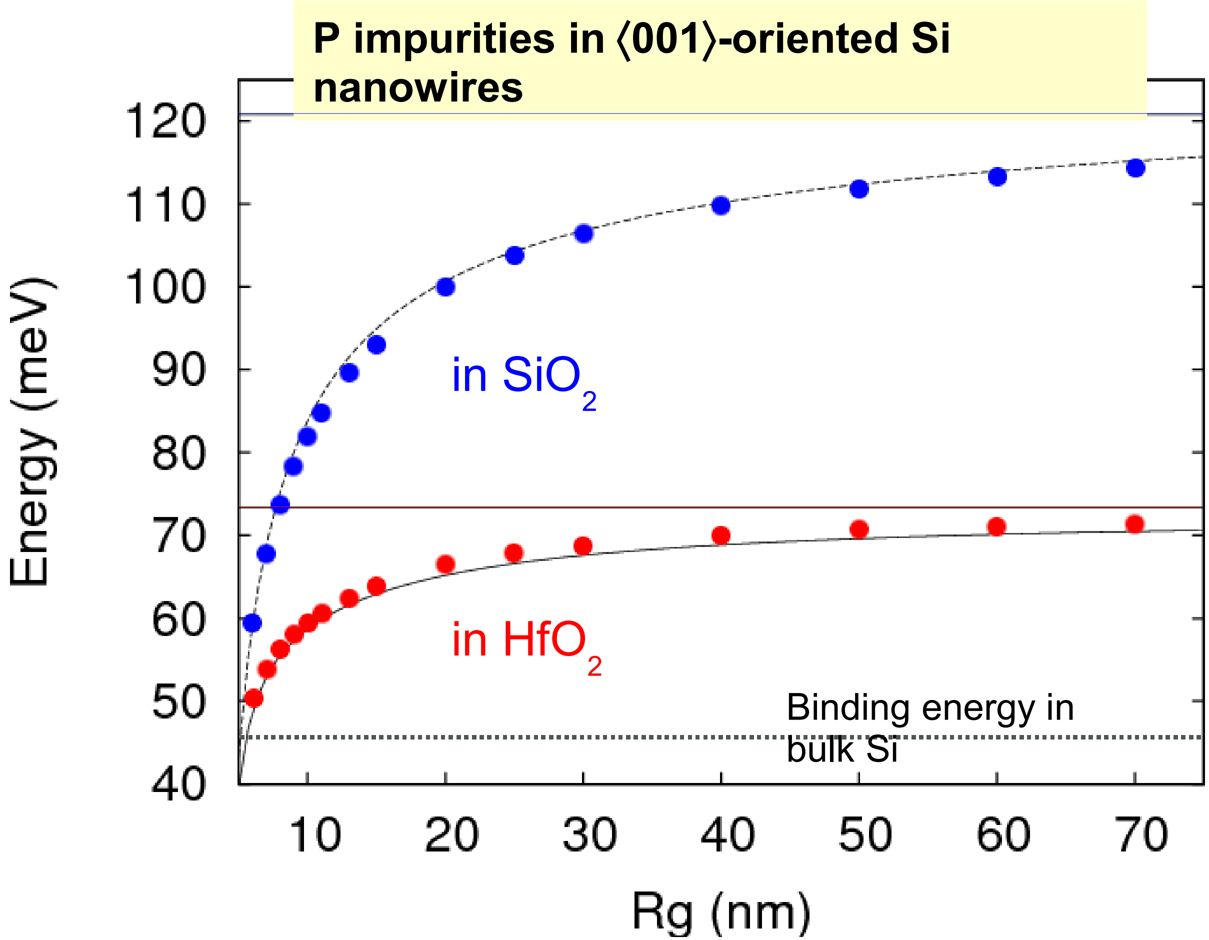
- Strong increase of the doping efficency (T = 300 K) :
  - **$P_{ionization}$ = 6%** @ R = 5 nm in vacuum.
  - $P_{ionization}$ = 47% @ R = 5 nm in SiO_2.
  - **$P_{ionization}$ = 78%** @ R = 5 nm in HfO_2.

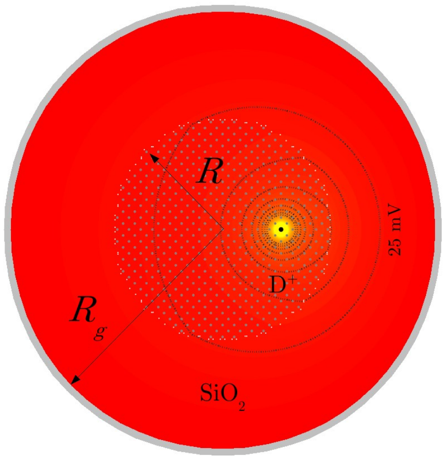
P impurities in ⟨001⟩-oriented Si nanowires



Screening and polaronic effects induced by a metallic gate and a surrounding oxide on donor and acceptor impurities...
M. Diarra, C. Delerue, Y. M. Niquet and G. Allan, Journal of Applied Physics **103** 073703 (2008).

Effect of an « all-around » metallic gate





R = 5 nm

- Strong decrease of the binding energy.

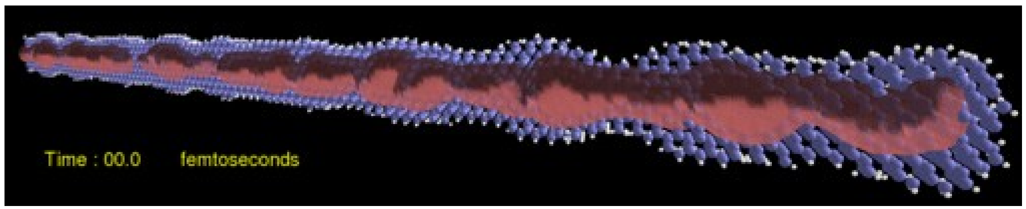
- **Analytical model available for any κ_{in}, κ_{out}, R and R_g ⇒ Can easily be taken into account in device simulation.**

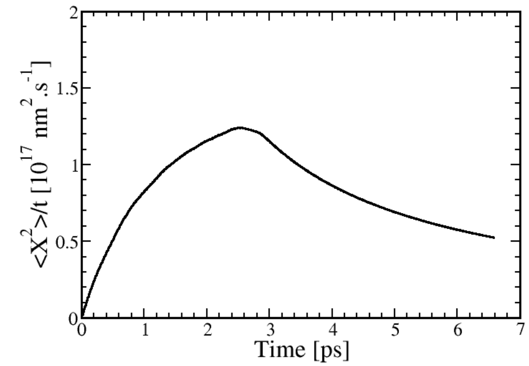
Screening and polaronic effects induced by a metallic gate and a surrounding oxide on donor and acceptor impurities...
M. Diarra, C. Delerue, Y. M. Niquet and G. Allan, Journal of Applied Physics **103** 073703 (2008).

Part III :

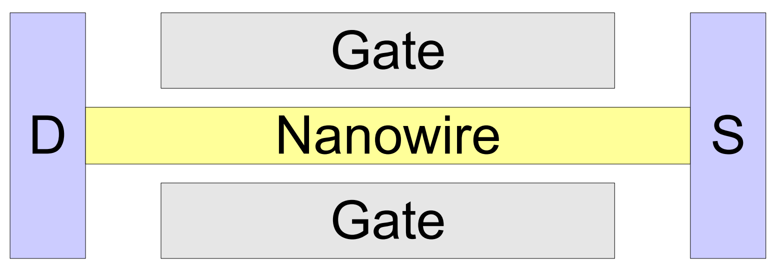
Transport in silicon nanowires

- **Kubo method** : progagate random wavepackets along the nanowires.
  - Yields the « **intrinsic** » transport properties of infinite, disordered nanowires (e.g., mean free paths and mobilities).





- **Green functions method** :
  - Yield the transmission/conductance through a nanowire connected to drain and source **electrodes** (transistor configuration).



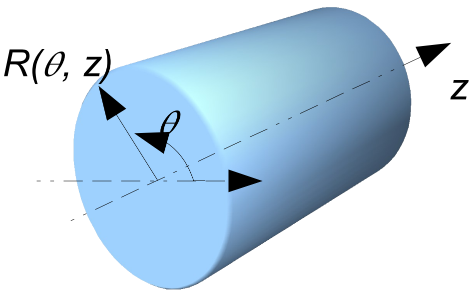
- The two methods are complementary and well suited to localized basis sets.

- **Disorder** : Random fluctuations of the radius of the nanowire, characterized by the auto-correlation function :

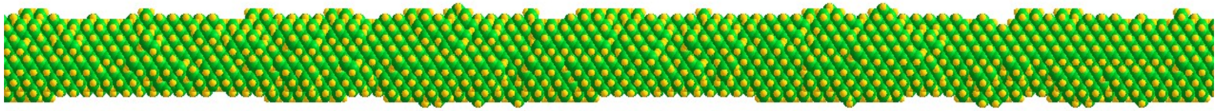
$$\langle \delta R(z,\theta)\delta R(z+\delta z,\theta+\delta\theta)\rangle \equiv \delta R_0^2 e^{-\sqrt{\delta z^2+R_0^2\delta\theta^2}/L_r}$$

<u>Parameters</u> :

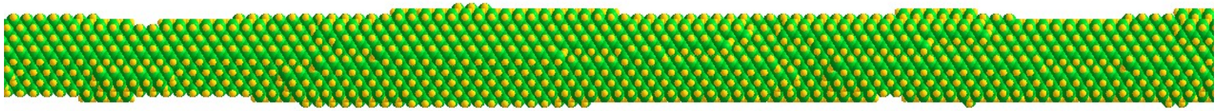
- R_0 : average radius.
- δR_0 : rms fluctuations of the radius.
- L_r : correlation length (~ typical size) of the fluctuations.



Si ⟨110⟩ nanowires R_0 = 1 nm, δR_0 = 1 Å

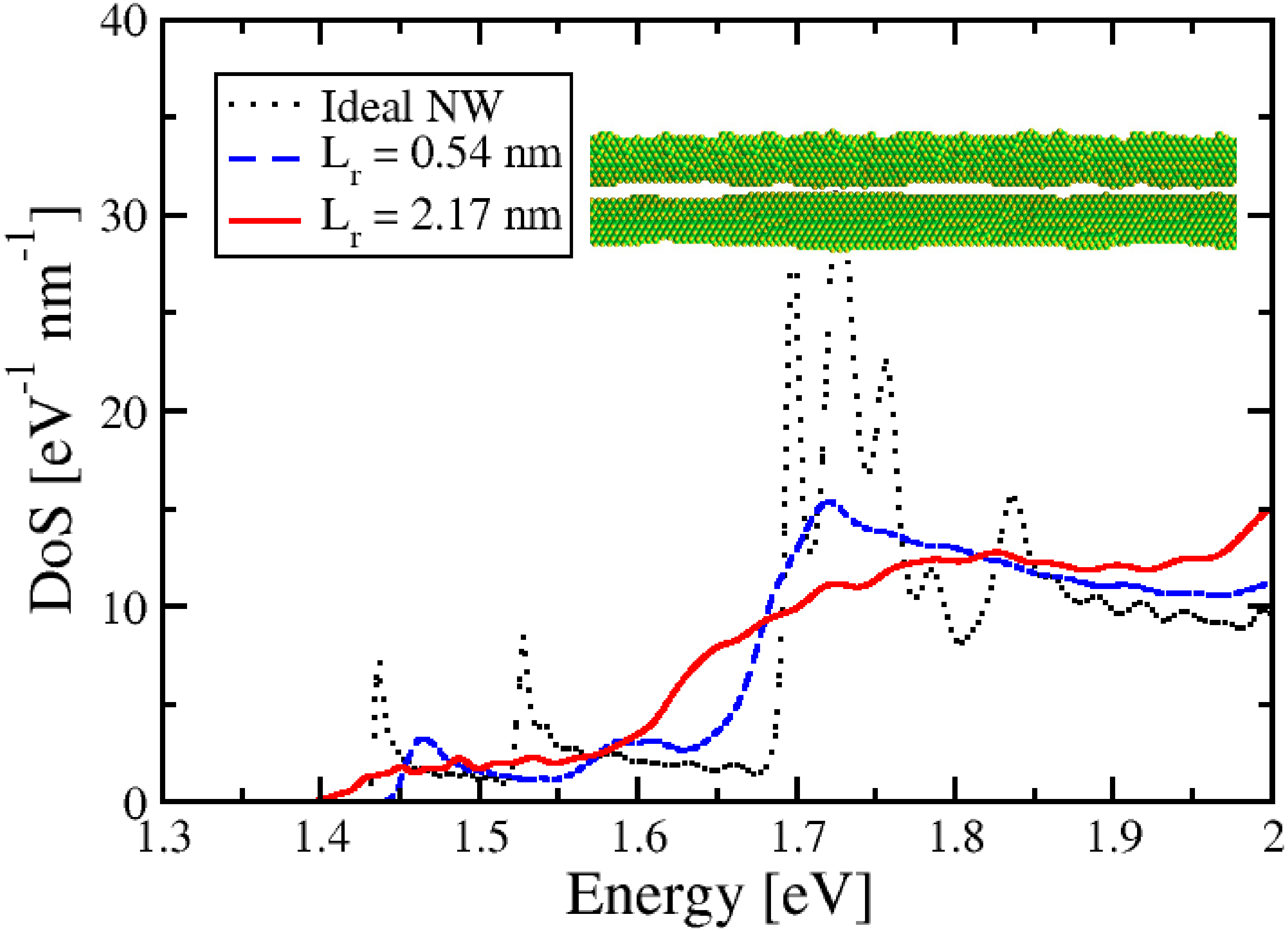


L_r = 5.4 Å



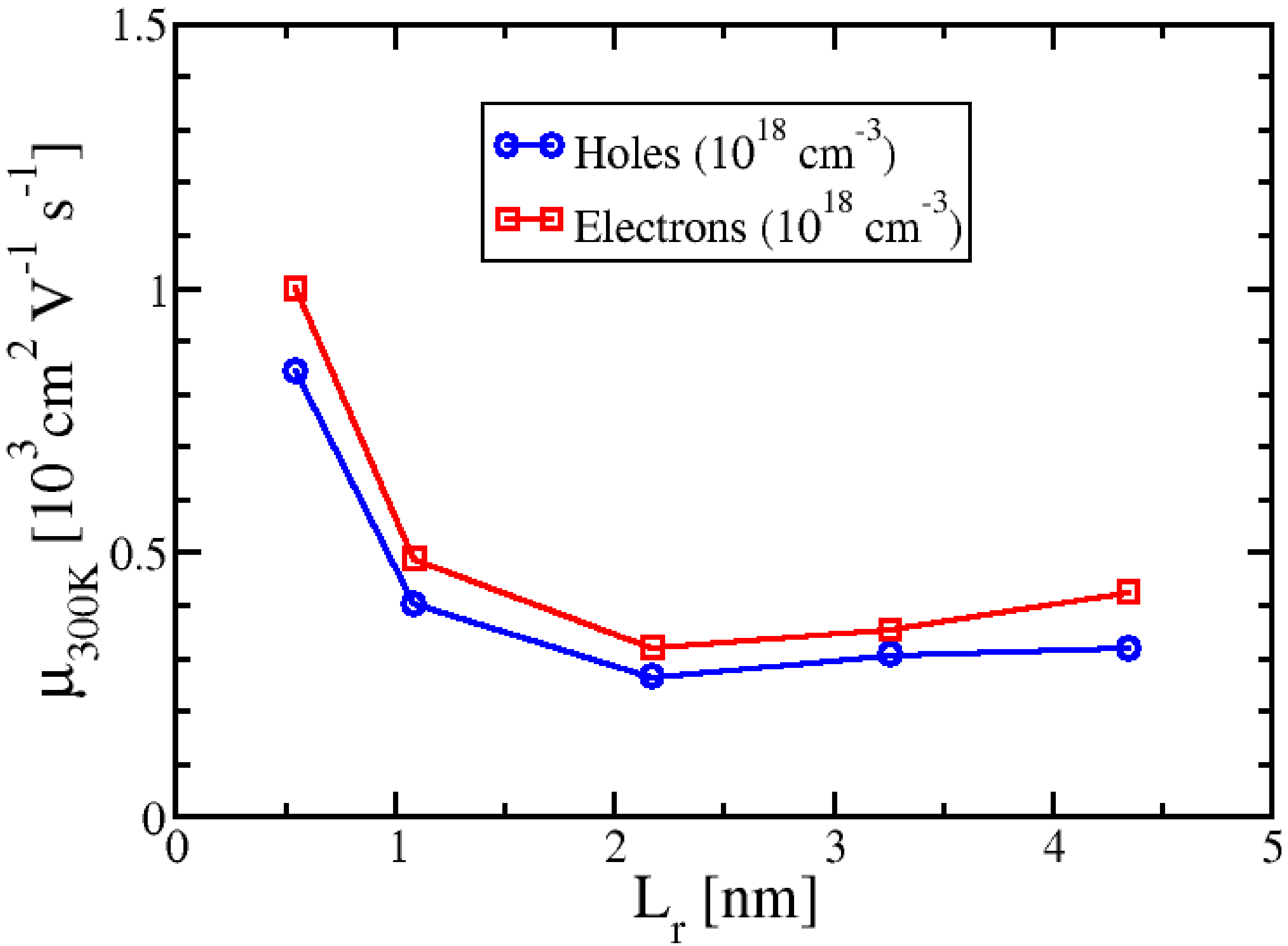
L_r = 21.7 Å

Rough NWs : Density of states



- The Van Hove singularities are smoothed as L_r is increased.

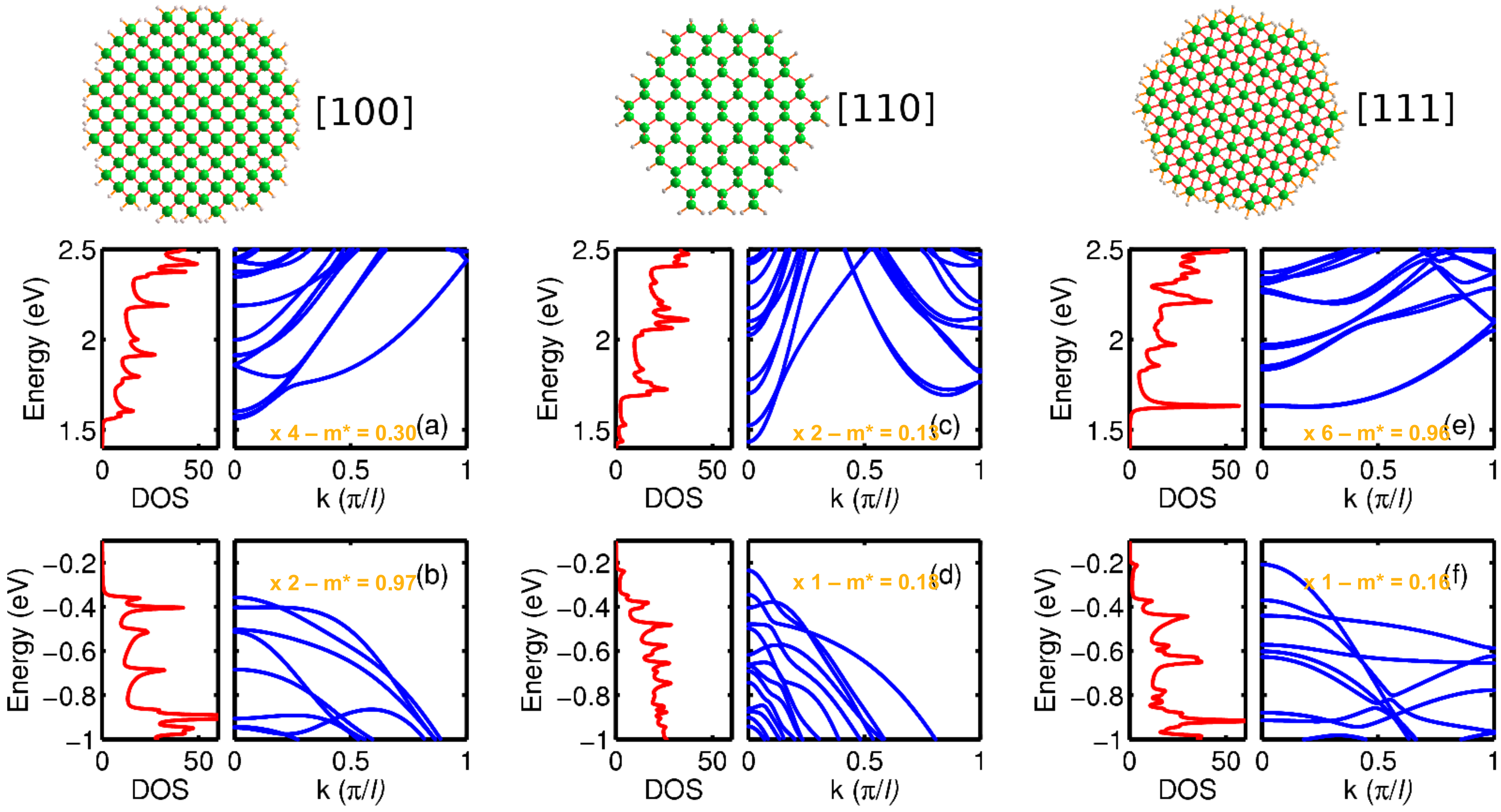
Rough NWs : Mobilities



- The mobility of the electrons and holes shows a minimum around L_r = 2.5 nm.

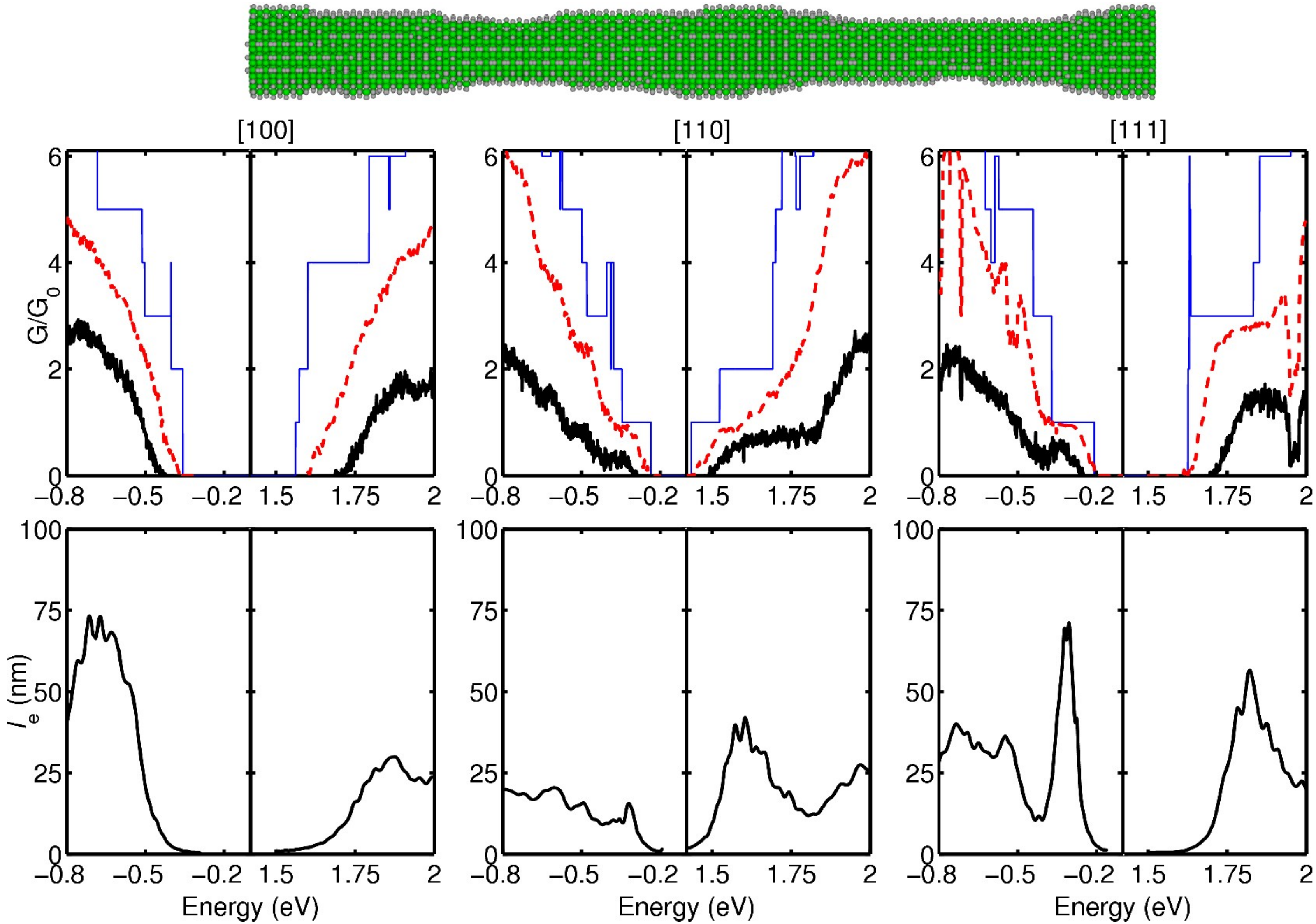
Quantum transport length scales in silicon-based semiconducting nanowires : Surface roughness effects.
A. Lherbier, M. P. Persson, Y. M. Niquet, F. Triozon and S. Roche, Phys. Rev. B. **77**, 085301 (2008).

Band structure of silicon nanowires



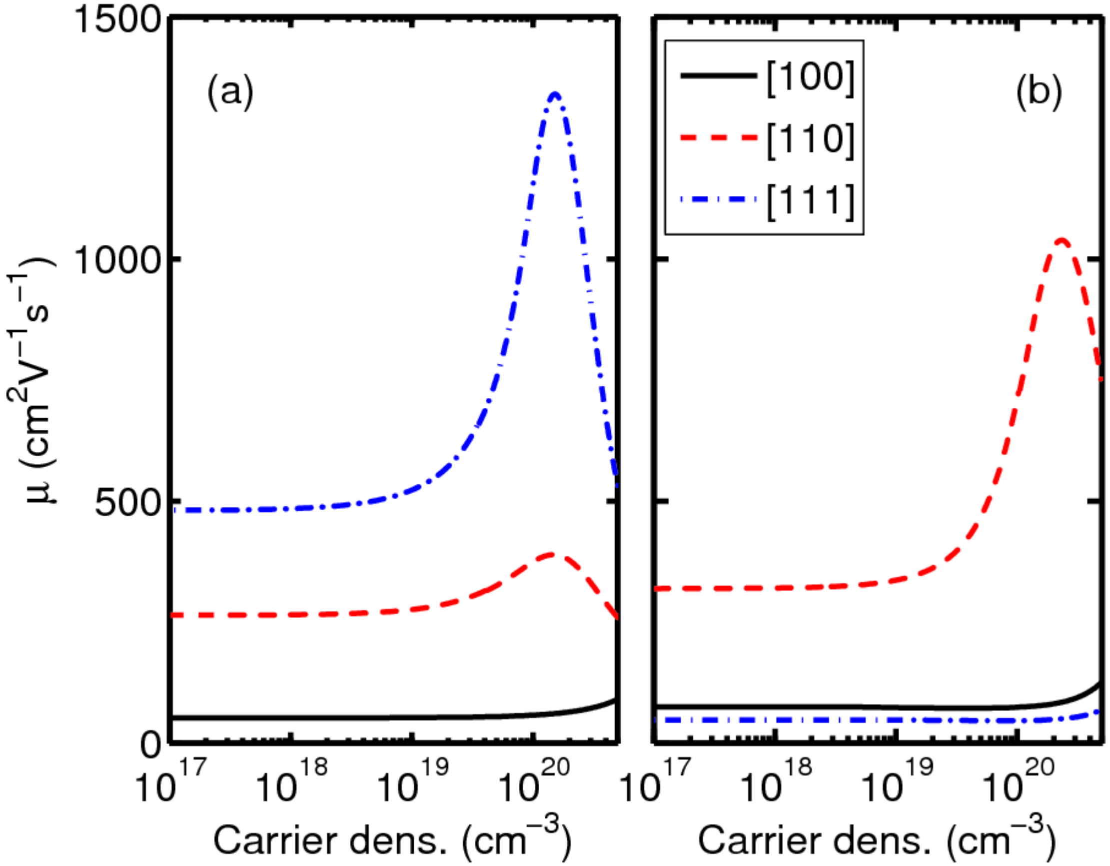
- The band structure of thin Si NWs is strongly dependent on their orientation :
  - Conduction band **valley degeneracy** completely **lifted in [110] Si NWs**.
  - **Lightest hole mass** and largest valence subband splittings **in [111] Si NWs**.

Transport properties of [100], [110] and [111] oriented Si NWs



Orientational dependence of charge transport in disordered silicon nanowires
M. Persson, A. Lherbier, Y. M. Niquet, F. Triozon and S. Roche, submitted.

Mobility as a function of Si NW orientation



- In agreement with the trends evidenced on the band structures,
  - **[111]** is the best orientation for **hole** transport.
  - **[110]** is the best orientation for **electron** transport.

Orientational dependence of charge transport in disordered silicon nanowires
M. Persson, A. Lherbier, Y. M. Niquet, F. Triozon and S. Roche, submitted.

Conclusions

- **Strain relaxation is very efficient in nanowire heterostructures.**
- **In short barriers and quantum-dots the potential barrier is lowered.**

- **The binding energy of donor and acceptor impurities can be greatly enhanced in small semiconductor nanowires, which decreases the doping efficiency.**
- **The binding energy of the impurities however depends on the dielectric environment of the nanowires** (through screening and polaronic effects). High-κ dielectrics and metallic gates can help to increase the doping efficiency.

- **The transport properties of thin silicon nanowires strongly depend on their orientation :**
  - **The best orientation for electron transport is [110].**
  - **The best orientation for hole transport is [111].**

  This can be related to the anisotropy of the band structure of silicon and should not be much sensitive to the nature of the scattering mechanisms.