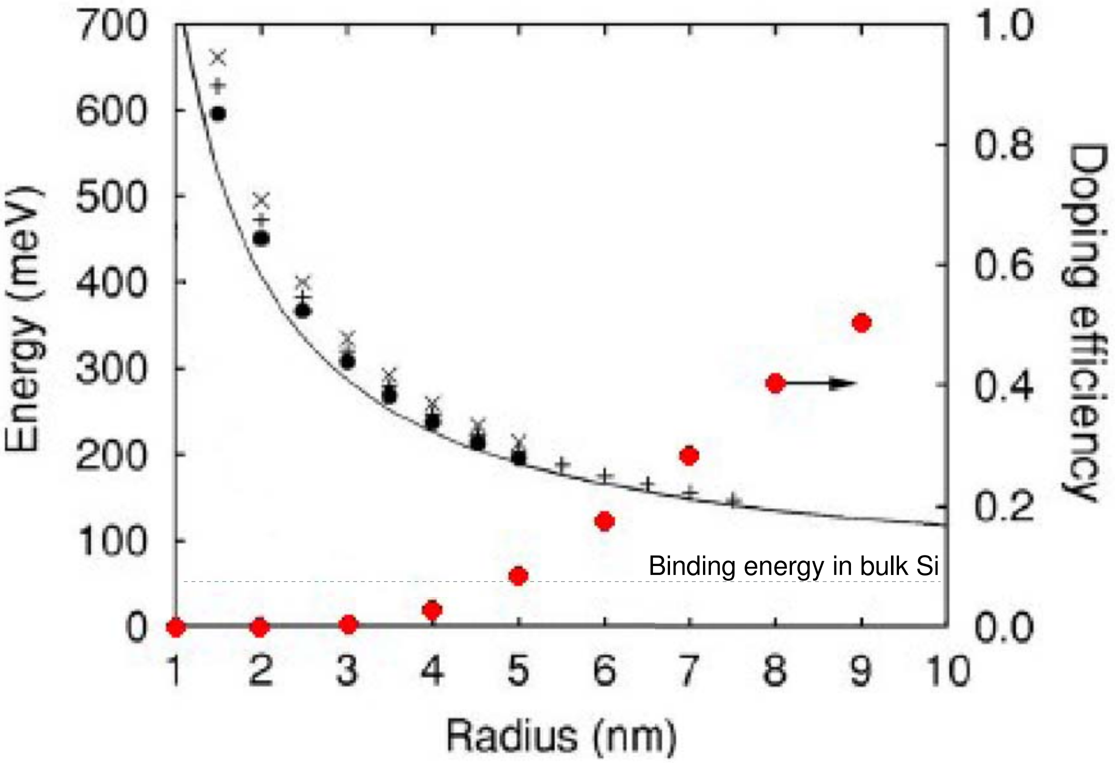
Doping the nanowires

<001>-oriented Si nanowires

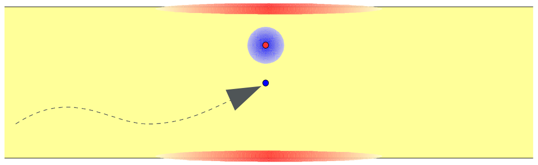


Binding energy of a donor in a Si nanowire as a function of its radius.

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 !!

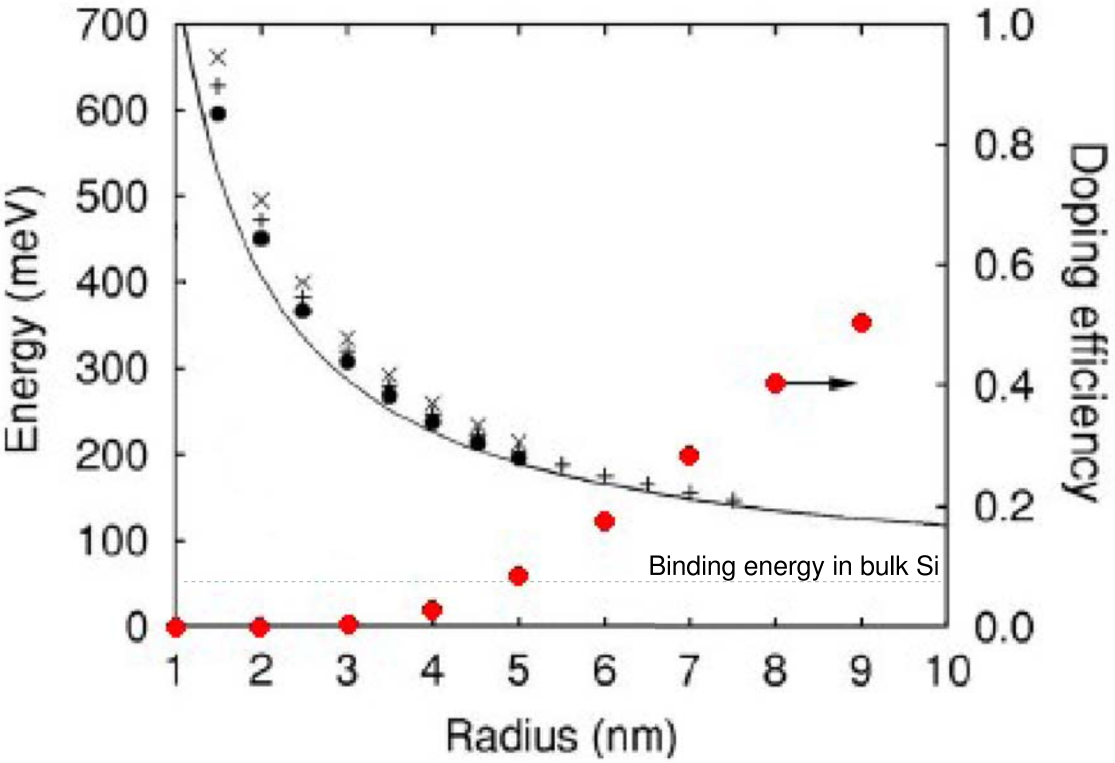


The electron is trapped around the donor by the impurity and its image charges.

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).

Doping the nanowires

<001>-oriented Si nanowires



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)

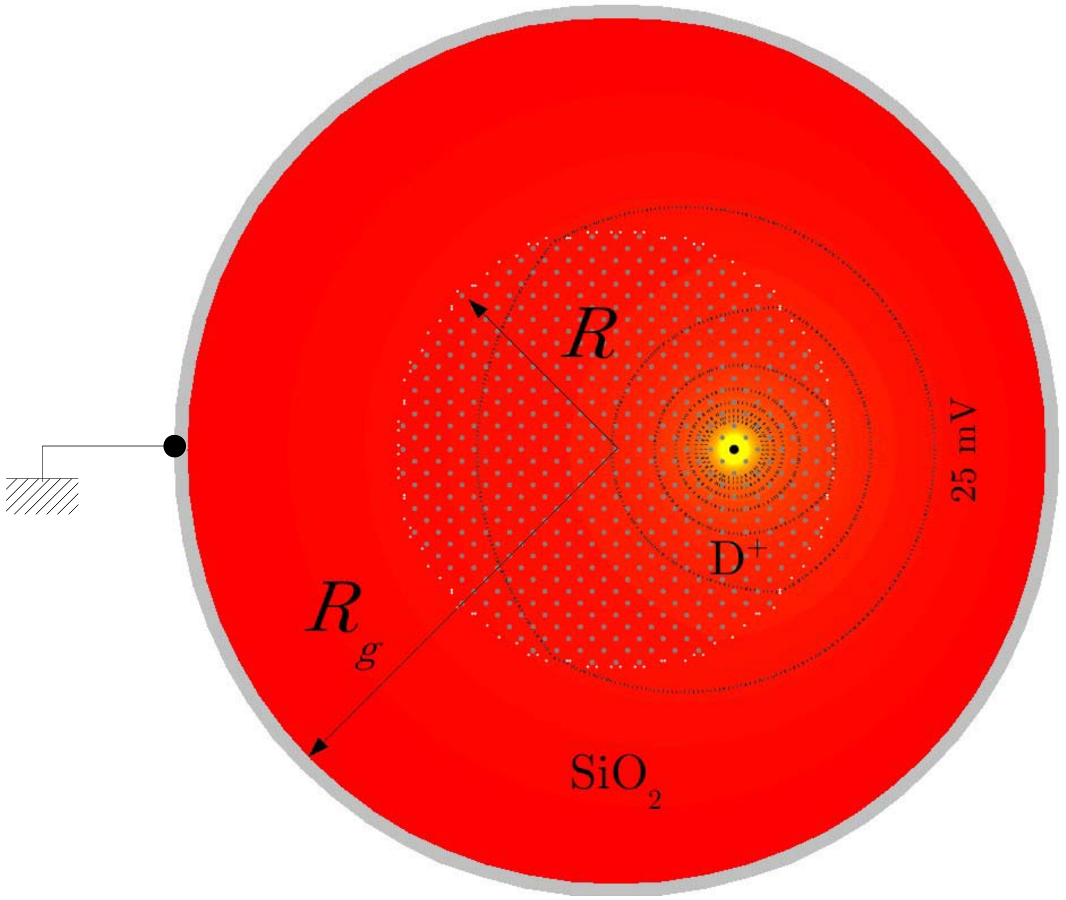
The binding energy of the impurities and the doping efficiency depend on the dielectric environment !

(E_0 ↘ if $\kappa_{\alpha t}$ ↗)

Electrostatic engineering of nanowire devices !!

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



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

⇒ **Decrease of the binding energy**

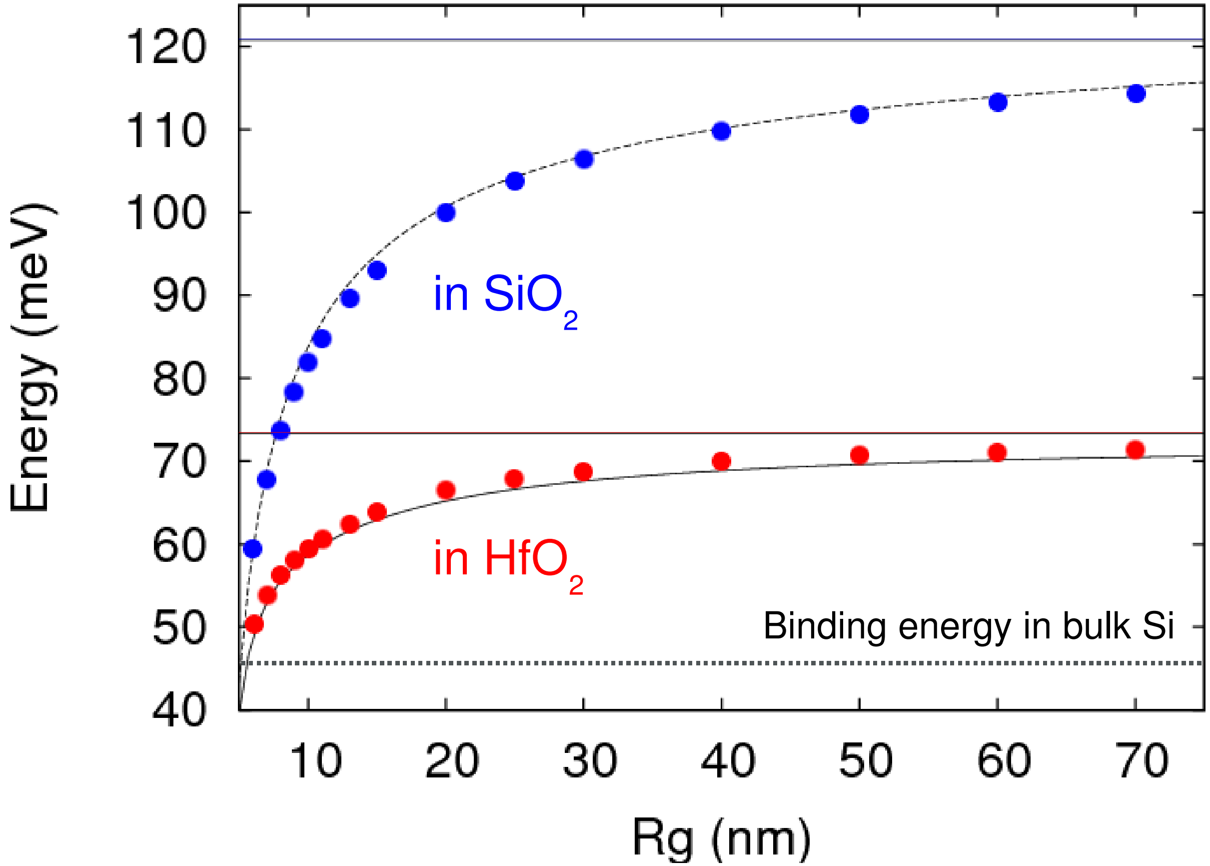
... BUT ...

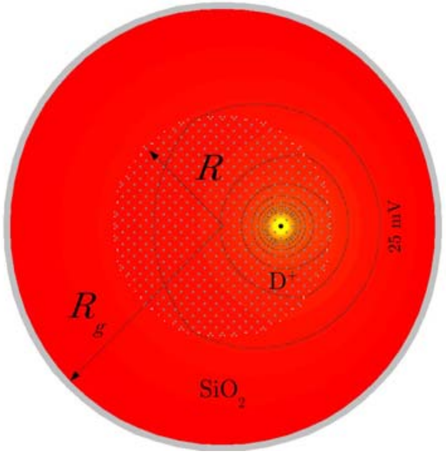
- The dielectric response of the oxydes is slow...

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

Effect of an « all-around » metallic gate

P impurities in <001>-oriented Si nanowires



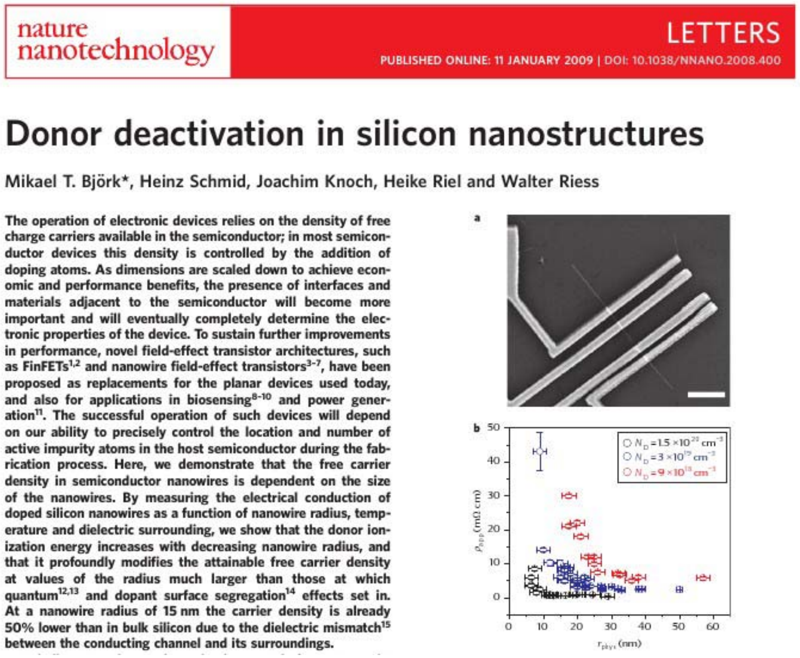


R = 5 nm

- 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, J. Appl. Phys. **103**, 073703 (2008).

Experimental evidences



nature nanotechnology

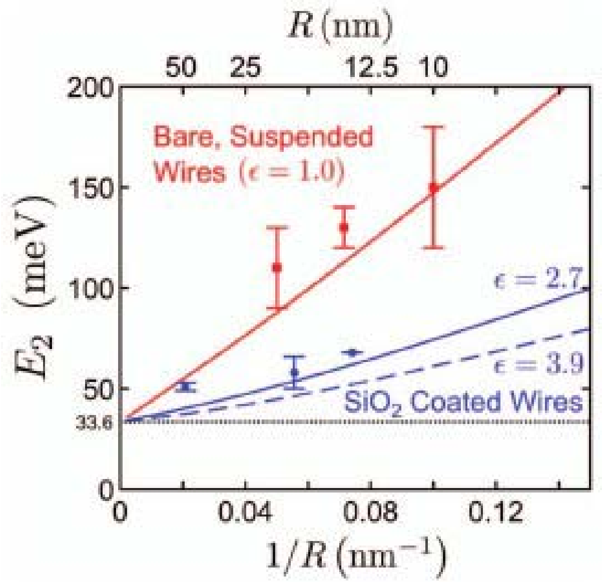
LETTERS

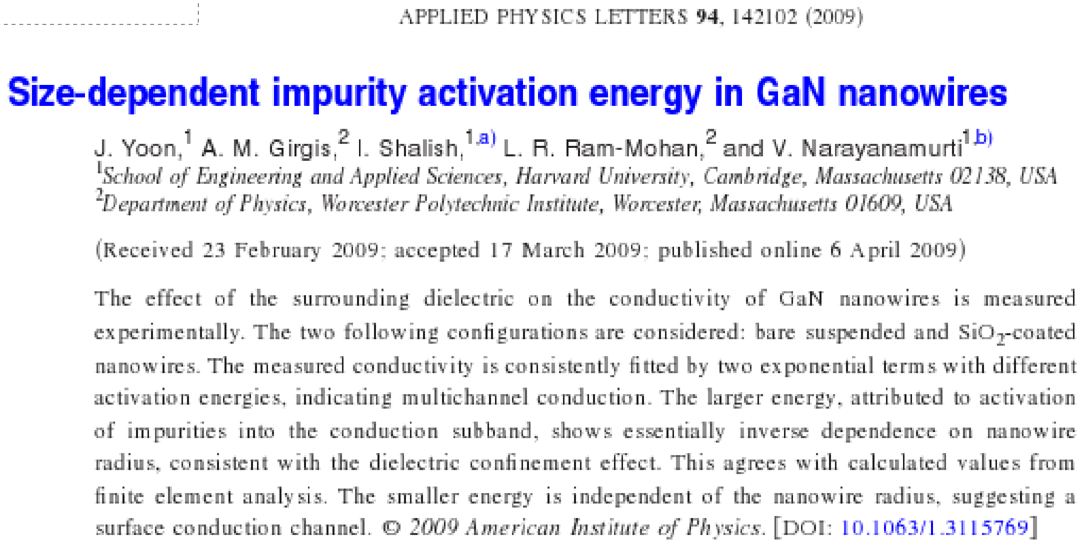
Donor deactivation in silicon nanostructures

Mikael T. Björk*, Heinz Schmid, Joachim Knoch, Heike Riel and Walter Riess

The operation of electronic devices relies on the density of free charge carriers available in the semiconductor; in most semiconductor devices this density is controlled by the addition of doping atoms. As dimensions are scaled down to achieve economic and performance benefits, the presence of interfaces and materials adjacent to the semiconductor will become more important and will eventually completely determine the electronic properties of the device. To sustain further improvements in performance, novel field-effect transistor architectures, such as FinFETs[1,2] and nanowire field-effect transistors[3-7], have been proposed as replacements for the planar devices used today, and also for applications in biosensing[8-10] and power generation[11]. The successful operation of such devices will depend on our ability to precisely control the location and number of active impurity atoms in the host semiconductor during the fabrication process. Here, we demonstrate that the free carrier density in semiconductor nanowires is dependent on the size of the nanowires. By measuring the electrical conduction of doped silicon nanowires as a function of nanowire radius, temperature and dielectric surrounding, we show that the donor ionization energy increases with decreasing nanowire radius, and that it profoundly modifies the attainable free carrier density at values of the radius much larger than those at which quantum[12,13] and dopant surface segregation[14] effects set in. At a nanowire radius of 15 nm the carrier density is already 50% lower than in bulk silicon due to the dielectric mismatch[15] between the conducting channel and its surroundings.

Nature Nanotechnology **4**, 103 (2009)





APPLIED PHYSICS LETTERS **94**, 142102 (2009)

Size-dependent impurity activation energy in GaN nanowires

J. Yoon,[1] A. M. Girgis,[2] I. Shalish,[1,a)] L. R. Ram-Mohan,[2] and V. Narayanamurti[1,b)]
[1]*School of Engineering and Applied Sciences, Harvard University, Cambridge, Massachusetts 02138, USA*
[2]*Department of Physics, Worcester Polytechnic Institute, Worcester, Massachusetts 01609, USA*

(Received 23 February 2009; accepted 17 March 2009; published online 6 April 2009)

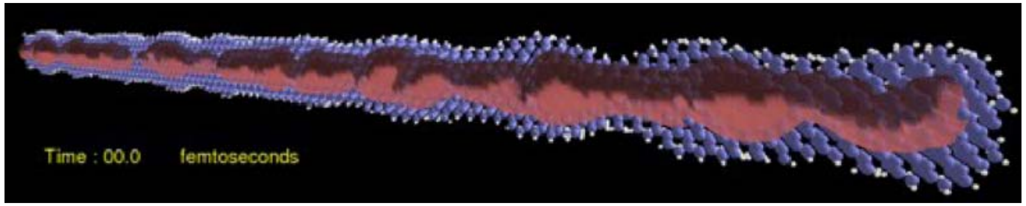
The effect of the surrounding dielectric on the conductivity of GaN nanowires is measured experimentally. The two following configurations are considered: bare suspended and SiO$_2$-coated nanowires. The measured conductivity is consistently fitted by two exponential terms with different activation energies, indicating multichannel conduction. The larger energy, attributed to activation of impurities into the conduction subband, shows essentially inverse dependence on nanowire radius, consistent with the dielectric confinement effect. This agrees with calculated values from finite element analysis. The smaller energy is independent of the nanowire radius, suggesting a surface conduction channel. © *2009 American Institute of Physics.* [DOI: 10.1063/1.3115769]

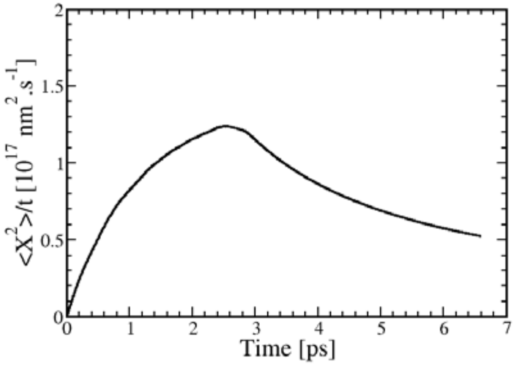
Part II :

Transport properties of semiconductor nanowires

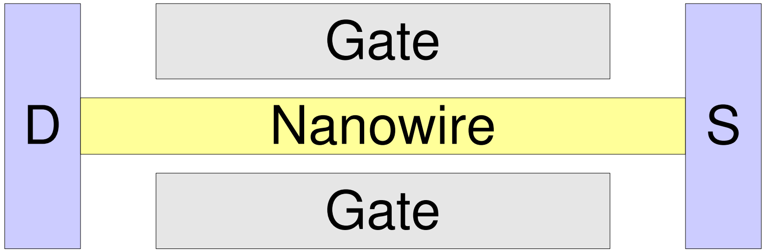
The Kubo and Landauer-Büttiker methods

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





- **Landauer-Büttiker method** : Green function method.
  - Yields the transmission/conductance through a nanowire connected to drain and source **electrodes**.



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

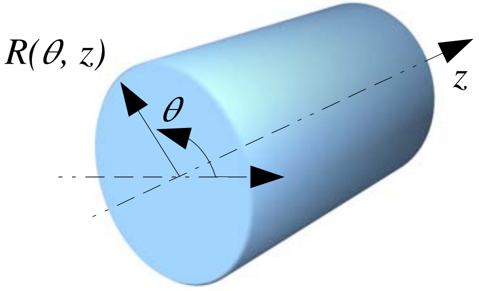
Application : Surface roughness

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

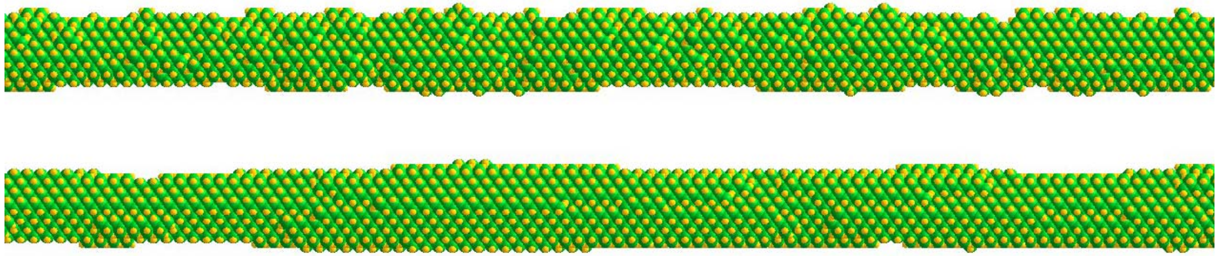
$$\langle \delta R(z,\theta)\delta R(z+\delta z,\theta+\delta\theta)\rangle \equiv \delta R_0^2 e^{-\sqrt{\delta z^2+R_0^2\delta\theta^2}/L_r}$$

Parameters :

- 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



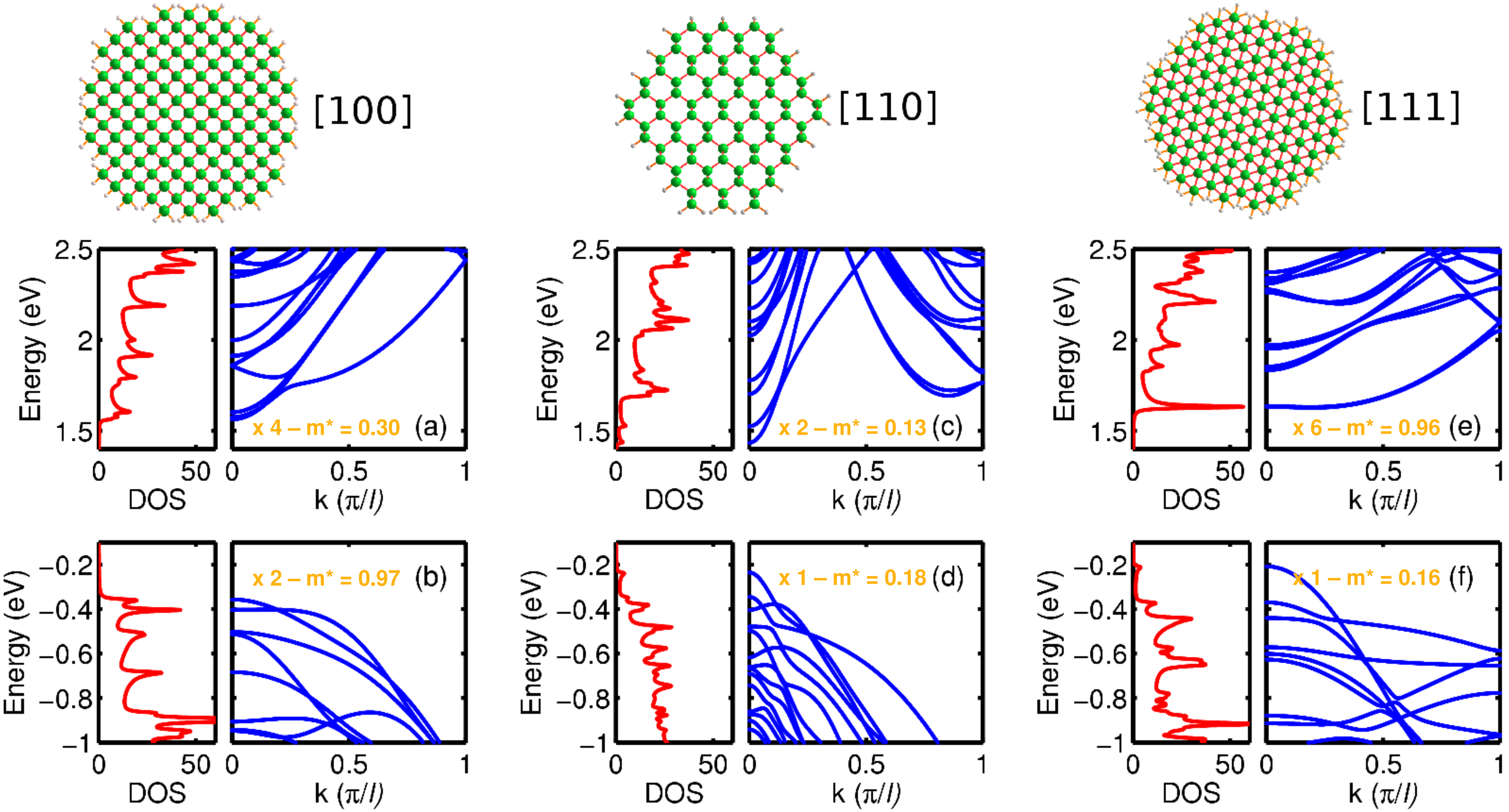
L_r = 5.4 Å

L_r = 21.7 Å

- **How does the conductance decrease with the wire length L ?**

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

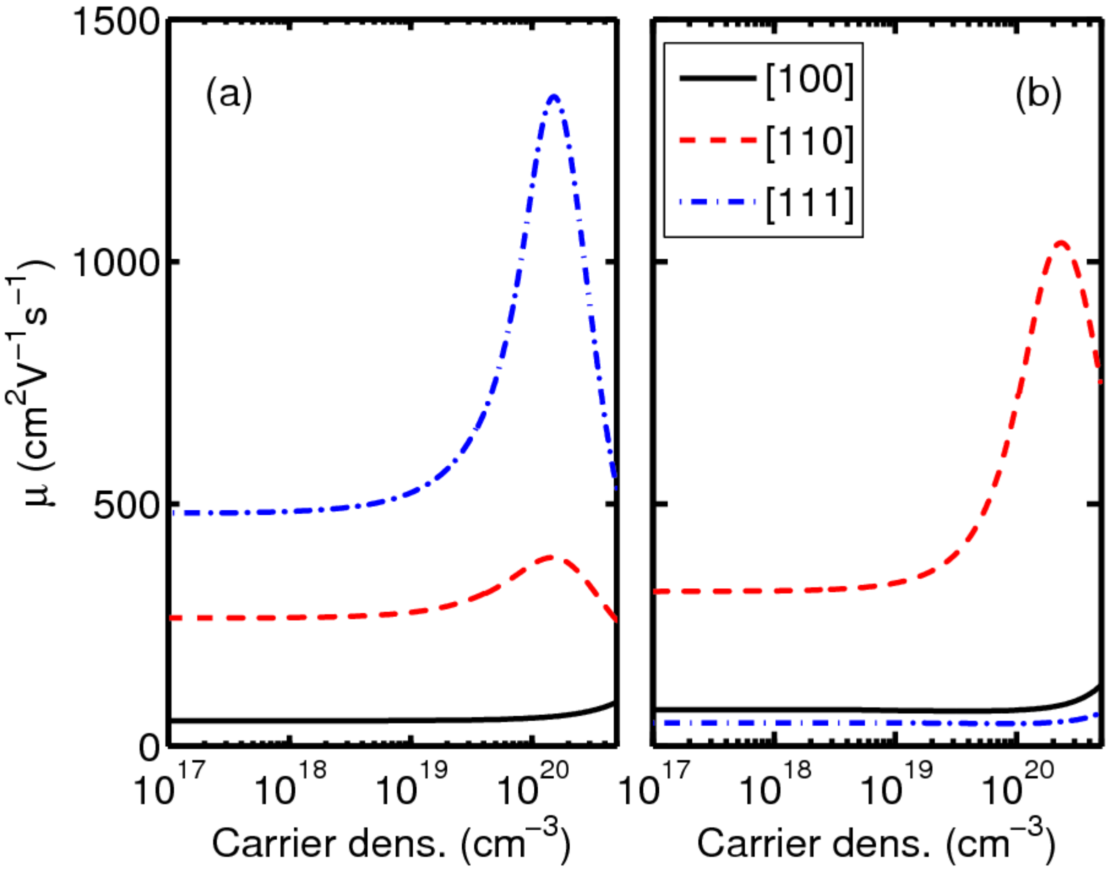
Band structure of silicon nanowires



- 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**.

Orientational dependence of charge transport in disordered silicon nanowires
M. Persson, A. Lherbier, Y. M. Niquet, F. Triozon and S. Roche, Nano Letters **8**, 4146 (2008).

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, Nano Letters **8**, 4146 (2008).

Conclusions

- The **electrostatics of semiconductor nanowires is very peculiar** and affects their properties even in the > 20 nm range where quantum confinement becomes negligible.

« **Electrostatic** » **engineering** of the environment of the NWs

(e.g. to decrease donor binding energies)

- The **[110]** direction is best for **electron** transport in ultimate Si nanowires, while the **[111]** direction is best for **hole** transport.