Conductance, surface traps and passivation in doped silicon nanowires

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Abstract

By means of *ab initio* simulations, we investigate the structural, electronic and transport properties of p- and n-type doped silicon nanowires. We find that impurities always segregate at the surface of unpassivated wires, reducing dramatically the conductance of the surface states. Upon passivation, we show that for wires as large as a few nanometers in diameter, a large proportion of dopants will be trapped and electrically neutralized at surface dangling bond defects, significantly reducing the density of carriers. Important differences between *p*- and *n*-type doping are observed[1]. Impurities located in the core of the wire induce a strong resonant backscattering at the impurity bound state energies. Upon trapping at such surface sites, impurities become electronically inactive, yielding neither a free carrier nor inducing a significant drop of conductance. This effect is also observed for isolated surface dangling bond defects.

References

[1] M. V. Fernández-Serra, Ch. Adessi and Xavier Blase, Phys. Rev. Lett. **96**, 166805 (2006).