Electronic properties of strained nanowire heterostructures

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Semiconducting nanowires grown from metal catalysts have attracted a lot of interest in the past few years [1]. They provide new insights into the physics of one-dimensional systems, and are promising building blocks for opto- and nanoelectronics. These nanowires are very versatile. Their composition can be modulated along the growth axis, which allows the synthesis of high-quality heterostructures with embedded quantum dots or tunnel barriers. GaAs/GaP [2], InAs/InP [3], or InAs/GaAs [4] nanowires for example have shown remarkable optical and electrical properties. Nanowire-based devices such as resonant tunneling diodes [5] or single-electron transistors [6] have been sucessfully realized.

Strain is a fundamental issue in semiconductor heterostructures. The lattice mismatch between the different materials indeed limits the design of conventional, quantum well systems. The coherent epitaxy of thick lattice mismatched layers has however been demonstrated in nanowires. Their surface can actually bend to help relieving the strains. The relaxed strain distribution might however be very inhomogeneous. Moreover, the actual effect of strain relaxation on the electronic properties of the nanowires is largely unknown. Previous studies on etched nanowires suggest that the carriers might be localized (in compressed layers) near the surface where strong relaxation takes place [7,8]. This, of course, is not desirable for most experiments and applications.

In this work, we compute the structural and electronic properties of InAs/GaAs and InAs/InP nanowire superlattices, using a semi-empirical $sp^3d^5s^*$ tight-binding model. We take strains and piezoelectric fields into account. The effects of the image charges, that arise from the dielectric mismatch between the nanowire and vacuum, and of the electron-hole interaction are also included in the calculation. We show that strain relaxation is indeed efficient in nanowire heterostructures. It is, however, very inhomogeneous if the thickness of the InAs layers is much smaller than the radius of the nanowire. Strain relaxation then digs a well in the conduction band that traps the electrons at the surface (see Fig .1). This decreases the oscillator strength and might ease the capture of the electrons by nearby surface defects. We discuss in detail the electron and hole localizations as a function of the geometry of the nanowire.

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Figures:

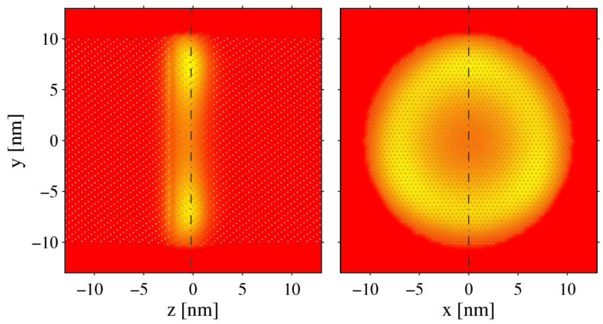

Fig. 1 : Square of the lowest electron wavefunction in an InAs/GaAs nanowire superlattice with radius R = 10 nm. The thickness of the InAs layer is t = 4 nm. It extends from z = -2 nm to z = +2 nm. The wavefunction is plotted in a plane containing the axis of the nanowire (left), and in the z = 0 plane (right). The dots are the In/Ga atoms in the plane of the plots.