Relation between structural properties and electron transport in Si nanowires

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One-dimensional medium-sized nano-structured systems such as nanowires are believed to be the most important building blocks for the next generation of electronic devices, due to the possibility to control the dimensionality, potentially affecting its physical properties. In particular, Silicon nanowires are attractive candidates due to their compatibility and ideal interface with the existing Si technology.

The electronic properties of Silicon nanowires can be modified by varying their diameter or by passivating the surface with different chemical species. Theoretical studies on the electronic properties of this systems have shown that the electronic structure depends on the growth orientation and the diameter. The band gap is strongly anisotropic and follows the order $E_g^{\langle 100\rangle} > E_g^{\langle 111\rangle} > E_g^{\langle 110\rangle}$ for wires of comparable diameter. Additionally, the gap strongly depends on the diameter. Bulk-Si has an indirect band gap, and Silicon nanowires have a direct gap. This property enables the use as optically active materials for photonics applications.

We investigate Silicon nanowire systems with different diameters. The electronic properties are modeled with density functional theory with the SIESTA package [1]. Electron transport calculations are performed using the non-equilibrium Green function approach as implemented in the SMEAGOL package [2], which is interfaced with SIESTA. We adopt different configurations: First we consider the leads as pure nanowires, obtaining a semi-infinite system, then we investigate the transport using metallic leads, Au$\langle 111\rangle$ and Fe$\langle 111\rangle$ electrodes are considered. Using density functional theory we relax the system and obtain the optimal configuration of the wire in contact with the metal electrodes. The distance between nanowire and metal and the nanowire length are optimized. For Au-electrodes we investigate how the symmetry of the orientations of the nanowires affects the transport properties by using transmission and complex band structure calculations. The results show a high symmetry of the $\langle 110\rangle$ growth orientation, as illustrated by a wave function isosurface plot.

For Fe-electrodes we analyze the transport considering different mutual alignments between the magnetization vectors of the electrodes. The magneto-resistance is calculated for the different orientations, showing a clear relationship between the symmetry of the wave function and the magnetic properties.

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