Doping and sensing in silicon nanowires

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The theoretical study of dopant properties in one-dimensional (1D) semiconductor systems, such as passivated nanowires (NWs), is hindered by the inadequacy of the well-established Zhang-Northrup formalism [1] to deal with cases where the chemical potential of the NW constituents is not well defined. In addition, dopant properties demand the computation of total energies of systems with a net charge, which have to be compensated by a background jellium when using periodic boundary conditions, and corrected after that for spurious electrostatic interactions. Again, the procedure to make that correction—well established in bulk—is ill-defined for 1D systems.

We will present a recently proposed framework for the calculation of formation energies of neutral and charged point defects in 1D systems [2] which successfully overcomes the aforementioned difficulties. We apply this formalism to three case studies with potential high impact for future nanoelectronics applications.

Surface segregation of dopants in CH_3 passivated SiNWs — It was soon recognized that surface segregation was one of the most important limiting factors in the doping efficiency of thin SiNWs [3]. In presence of dangling bonds, dopant impurities are driven to the surface where they form electrical inactive complexes with the surface defects. We revise this scenario in the case of the novel methyl-passivated SiNWs (Fig. 2) that have been demonstrated experimentally recently [4], whose stability in air is believed to be superior with respect to more conventional H passivated wires.

Al solubility — We have studied Al point defects in 1 and 1.5 nm SiNWs grown along the <110> and <111> axes. Two reasons make Al impurities a very interesting case study: (i) group III elements can be efficient p-type dopants for Si, and the use of Al for doping in nanowires has indeed been proposed [5]; (ii) Al has proven to be a feasible alternative to Au as a catalyst for the epitaxial growth of SiNWs [6], having the considerable advantage of not introducing undesired midgap states that can act as traps and requiring lower growth temperatures. We find that, as in bulk, substitutionals are preferred over interstitials. However, although Al continues to behave as an acceptor in the SiNWs, the activation energy is strongly increased due to the quantum confinement effect (Fig. 3). Also, we predict that substrate bias can control the solubility of the Al impurity.

Molecular doping and gas sensing — As traditional substitutional dopants are ineffective in thin NWs due to dielectric and quantum confinement effects, we must look for alternative avenues. Surface adsorption by select molecular species can provide the necessary charge transfer (Fig. 1), as we have recently shown [7]. This will also be used to explain the observed gas sensing properties of porous Si [8].

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Figures:

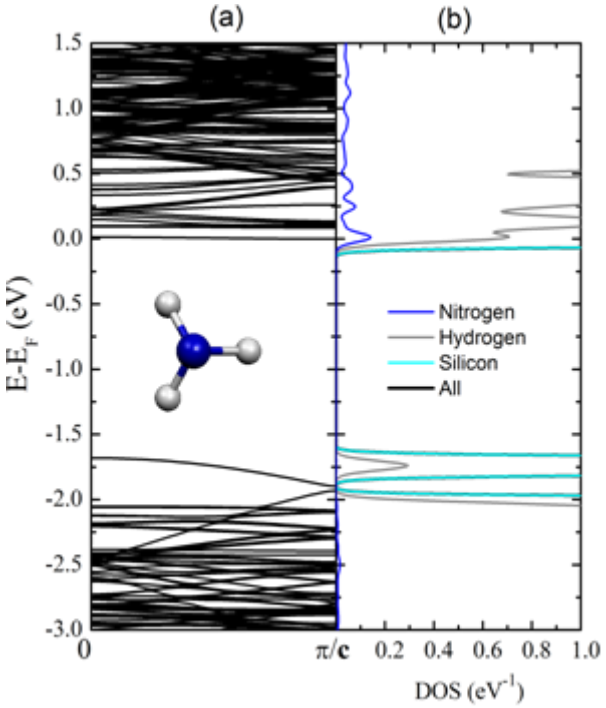

Figure 1 Band structure and projected density of states for a 1.5 nm SiNW with an adsorbed ammonia molecule.

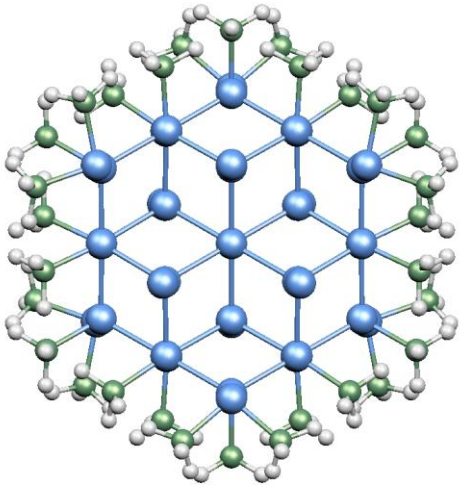

Figure 2 Cross-section view of a 1.0 nm <111> SiNW with CH_3 passivation (see Ref. [4])

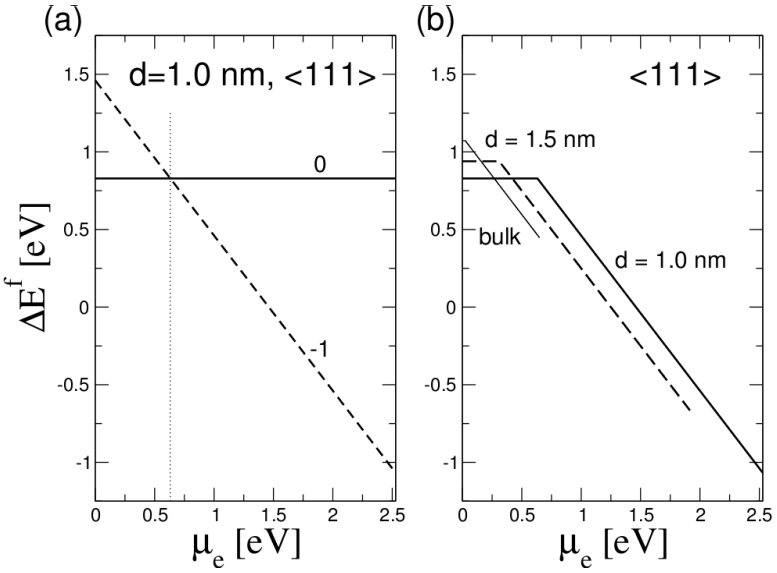

Figure 3 (a) Formation energy of the neutral (0) and the negatively charged (-1) Al substitutional in a ⟨111⟩ SiNW. The crossing μ_e signals the ionization energy. (b) Formation energy diagram for three different SiNW diameters.