Theory of Doping in Silicon Nanowires

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In bulk host materials the study of the energetics of the formation of defects is a very well-developed topic, and formation energies are calculated according to the well-established expression due to Zhang and Northrup [1], where they are formulated in terms of the chemical potentials of the constituent species and the total energy of the system with the impurities.

On the other hand, for one-dimensional (1D) semiconductor systems the nonequivalence of the different constituent atoms in, say, a silicon nanowire (SiNW), in addition to the possible presence of surface passivation and the proper treatment of the defect charge state, render the straightforward application of the Zhang-Northrup formalism troublesome. In particular, the choice of the chemical potential of the atomic species involved is ill-defined, preventing calculations of the formation energy of self-interstitials, vacancies or substitutionals for semiconductor nanowires.

We will present a recently proposed framework for the calculation of formation energies of neutral and charged point defects in 1D systems [2]. The difficulties mentioned above are overcome thanks to the use of a construction involving as many unit cells as necessary to form a new *layer* of NW, and a derivation of the Madelung correction for systems with a dielectric *tensor* as opposed to a dielectric constant. We apply this formalism to two 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 (see Figure 1) 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. Also, we predict a solubility of Al in the studied NWs at least an order of magnitude larger than in bulk.

References:

[1] S. B. Zhang and J. E. Northrup, Phys. Rev. Lett. **67** (1991) 2339.
[2] R. Rurali and X. Cartoixà, Nano Lett., **9** (2009) 975–979.
[3] M. V. Fernández-Serra, Ch. Adessi, and X. Blase, Phys. Rev. Lett., **96** (2006) 166805.
[4] H. Haick, P. T. Hurley, A. I. Hochbaum, P. Yang, and N. S. Lewis, J. Am. Chem. Soc., **128** (2006) 8990.
[5] E. Durgun, N. Akman, C. Ataca, and S. Ciraci, Phys. Rev. B, **76** (2007) 245323.
[6] Y. Wang, V. Schmidt, S. Senz, S. and U. Gösele, Nat. Nanotechnol., **1** (2006) 186.

Figures:

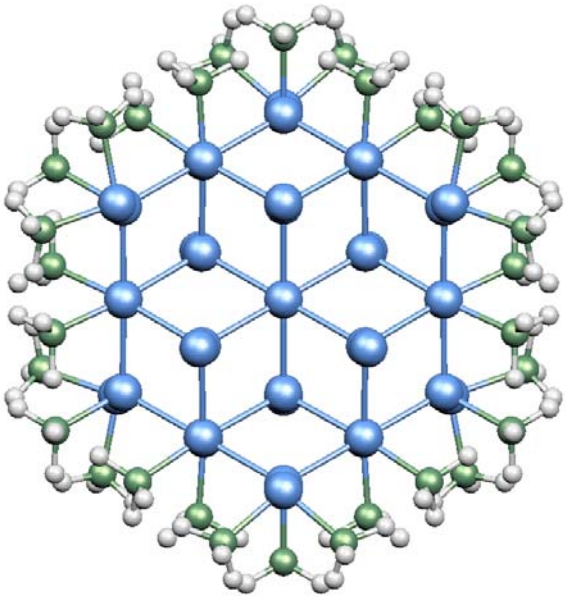

Figure 1 Cross-section view of a 1.0 nm <111> SiNW with CH_3 passivation (see Ref. [4]).