Theory of defect formation energies in one-dimensional systems: dopant activation in Si nanowires

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The formation energy of a defect [1] is a quantity of paramount technological importance; it determines the structural configuration and the charge state that a given set of impurities will favor, and it is used in the computation of impurity equilibrium concentrations, solubilities, diffusivities, dopant compensation mechanisms, etc. In addition, the calculation of the formation energy is required whenever a comparison between configurations with different number of atoms/chemical species is wanted.

In bulk host materials the study of the energetics of the formation of defects is a very well-developed topic, [2–4] 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. Additionally, the most stable configuration of a defect in a semiconductor may have a charge state different from zero, depending on the doping condition of the material. In a periodic boundary condition (PBC) formalism, a finite net charge in the simulation cell would give rise to a divergent Coulomb energy because of the monopole-monopole interaction with its periodic images. While the correct procedure for the removal of this contribution to the total energy is still a matter of debate, recent reports [5] indicate that the uniform background charge [6, 7] and the local-moment counter charge [8] yield similar results for bulk materials. However, a treatment for charged defects in one-dimensional systems is lacking so far.

We will present a recently proposed [9] framework for the calculation of formation energies of neutral and charged point defects in 1D systems. 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 (Fig. 1), and a derivation of the Madelung correction for systems with a dielectric *tensor* as opposed to a dielectric constant.

As a case study of technological significance, we have investigated the energetics of dopant incorporation into SiNWs, focusing on the case of Al, which can also be found as a contaminant from Al-catalyzed growth process [10]. Specifically, we deal with substitutional and interstitial defects at different radial positions in $\langle 110 \rangle$ and $\langle 111 \rangle$ SiNWs of 1.0 (Fig. 2) and 1.5 nm diameter, finding that, as in bulk, substitutionals are preferred over interstitials. However, although Al continues to behave as an acceptor in the SiNWs (ie. there is a 0/- transition as the Fermi level is increased), 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. We stress that these calculations are made possible only thanks to the use of the dielectric tensor-enabled Madelung correction that we have derived, which provides a strong convergence with respect to the unit cell lateral size (Fig. 3), with previous calculations [11] not performing the necessary correction.

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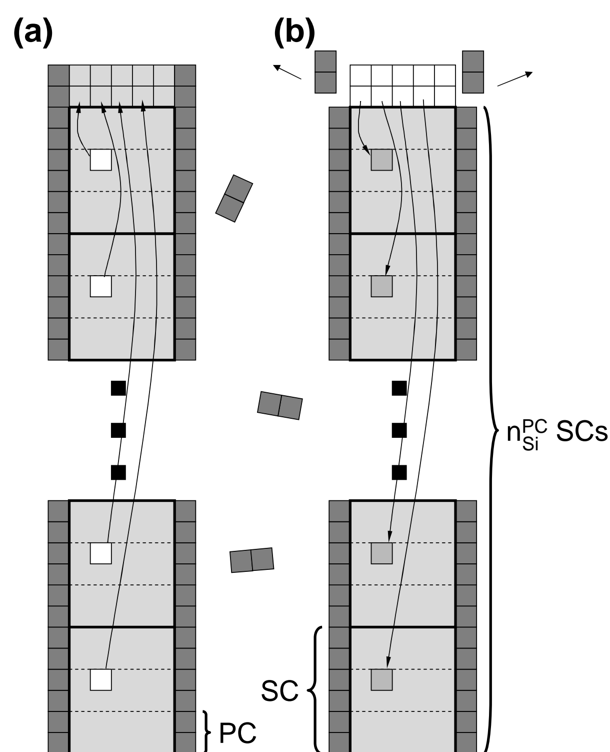

FIG. 1: Construction for dealing with defects in 1D semiconductor structures. (a) Vacancies and substitutionals: we create as many defects as necessary for adding an extra primitive cell to the wire. (b) Self-interstitials: we create as many defects as necessary for removing a primitive cell from the wire.

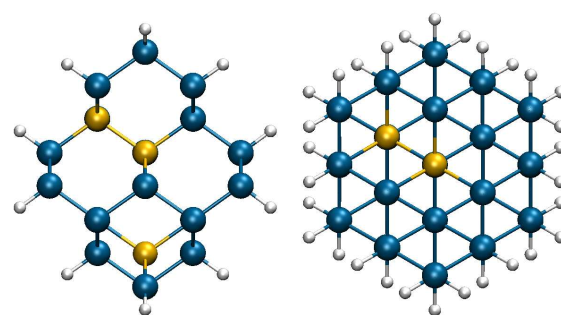

FIG. 2: 1.0 nm ⟨110⟩ and ⟨111⟩ nanowires with several Al positions marked.

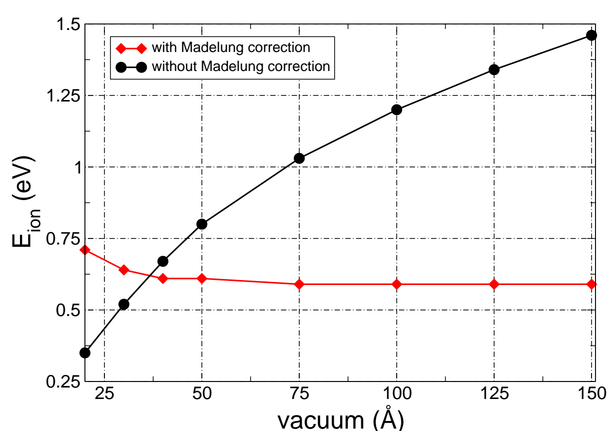

FIG. 3: Activation energy of an Al donor in a 1.0nm ⟨110⟩ SiNW host as a function of the lateral separation between the nanowire instances, with and without the dielectric tensor-enabled Madelung correction.