ON THE PROPERTIES OF SURFACE RECONSTRUCTED SILICON NANOWIRES

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One-dimensional nanostructures are attracting great interest for their potentially high impact in future molecular electronics applications, such as nanoswitches and nanocontacts [1]. Silicon nanowires (SiNWs) appear to be a special appealing alternative, due to the ideal interface compatibility with conventional Si-based technology and to the possibility to tune their conductive properties by means of electrical doping. Moreover, SiNW have exhibited remarkable properties as real-time label-free chemical sensors for NH_3 [2] and for biological macromolecules [3,4], virtually reaching the single-molecule detection limit.

For these reasons, a detailed understanding of the structural, electrical and mechanical properties of SiNW is required. While it has been extensively demonstrated that in H-terminated SiNW quantum confinement induces a gap-broadening effect, very little is known about surface reconstruction of non-passivate wires and their electronic structure features. In this paper, we present a theoretical study based on Density Functional Theory (DFT) of realistic <100 > SiNW, with a bulk Si core and a diameter of ~ 1.5 nm. Particularly, we focus our attention on the features of the electronic properties of the wire as determined by the different possible lateral surface reconstruction.

The faceting geometry adopted by the wire is given by thermodynamical considerations and is dominated by {100} facets. We have found two competing geometries for the {100} facets: a symmetric reconstruction with the bulk lattice vector along the wire-axis and an asymmetric reconstruction with double lattice vector. The symmetric reconstruction is 3 meV/atom more favourable. The asymmetric reconstruction shows a semi-metallic behaviour with one state approaching the Fermi level at the zone boundary, while the symmetric wire has four metallic states. These states show a great degree of surface localisation. Therefore, current flow is almost entirely sustained by the outer layers of the SiNW. We have also studied the response to axial stress with tight-binding, finding a Young's modulus of ~ 137 GPa and a Poisson ratio of ~ 0.35, values that support the mechanical robustness of these wires.

The possibility to obtain one-dimensional metallic Si nanostructures opens up the way to a wide range of novel nanoscience applications that require stout and atomic-scale contacts. Metallic SiNW are a promising path to usher Si in nanotechnology applications.

References:

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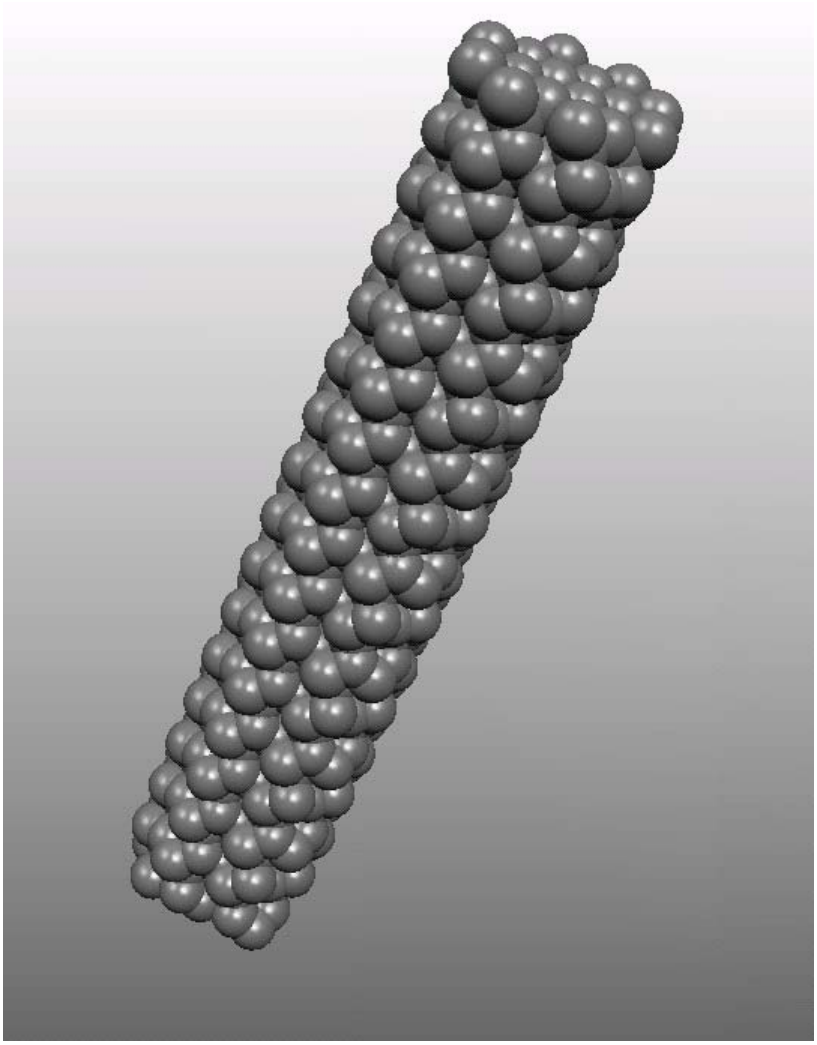
Figures:



The metallic reconstruction of the <100> Si nanowire.