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## Structural and electronic properties of Si (111) and (001) nanowires: A theoretical study

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### Abstract

In this work, our preliminary theoretical results for the structural and electronic properties of both Si (111) and (100) nanowires, with their lateral surfaces saturated with H or not, are shown. Our results show that, without the saturators, there is the formation of {110} facets to partly release the stress accumulated at lateral surfaces of the nanowires. These facets give rise to states close to the top of valence band and to the bottom of the conduction band that have character arising from both the occupied and empty Si-derived dangling bonds, respectively. Moreover, while the (111) nanowires have a direct band gap, with values within the visible range of the electromagnetic spectra, the (100) ones have an indirect band gap.

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### 1. Introduction

In last years, silicon nanowires (NW) were considered as systems of great importance for the future development of silicon-based optoelectronics, in particular as in the active media in high-efficient photovoltaic devices. This is due to the fact that these nanostructures show direct gap instead of the indirect gap observed in bulk silicon. However, despite the fact that the electronic structure of these nanostructures have been extensively studied by applying hydrogen saturators to avoid surface effects in the calculations, little is known about how this system behaves when these hydrogen saturators are absent, i.e, how are the effect of the surface states on both the structural properties and the electronic structure of these nanostructures [1-4].

In order to complete these missing informations, we have show in this work, by using the Density Functional Theory within the Local Density Approximation, gradient conjugated techniques, the Tight-Binding method (DFTB) [5], together with the supercell models, our preliminary results of both the structural and electronic properties of both the Si (111) and Si (100) NWs with several diameters. Our calculations started with the optimization of the atomic structure of the Si NWs saturated by H atoms, and finished by repeating the optimization procedure for the Si

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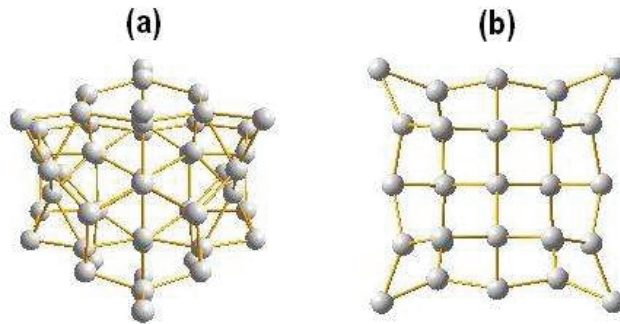
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NWs without these H atoms. We have, then, analyzed the changes in the bond-lengths, bond-angles, as well as in its electronic structure, before and after the absence of the H saturators.

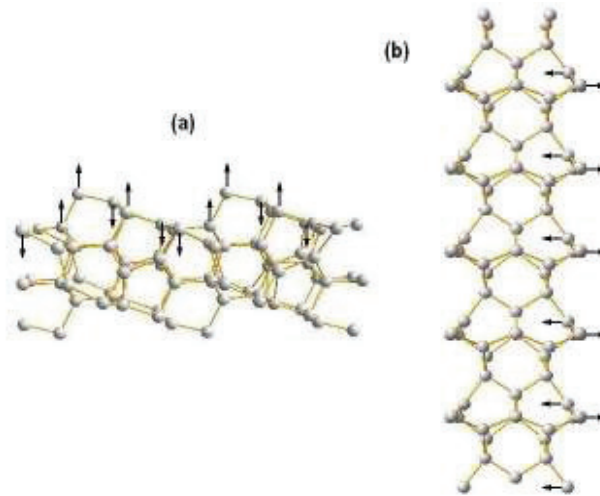
## 2. Results

We show in Fig. 1, the top view of the relaxed Si NWs grown in both (111) and (100) directions, which illustrates the observed features found in all considered Si NWs in our calculations. From Fig. 1(a), we have observed the atoms of the lateral surfaces relax in such way that induces the formation of {110} facets to partly release the stress accumulated at outermost surfaces, similar to those described in previous theoretical work [6]. In Fig. 1(b), for the Si (100) NWs, also the formation of the {110} facets prevail and, also, the four Si atoms at the vertices make a bond angle of  $52.0^\circ$  with its neighbours. This same feature is found in Fig. 1(a), which these four Si atom make a bond angle of  $61.0^\circ$ , but the plane that contain these four atoms is tilted of  $46.6^\circ$  from the plane of the top view, i.e., the (111) plane of the NW. As described by Rurali and Lorente [6], these facets are described as the contraction of the Si-Si bonds at the lateral surface to release the stress accumulated, pushing the Si atoms at the vertices away from the {110} facet. Moreover, we have noted that the Si atoms of this surface relax in a similar way to that verified in the Si (110) surfaces [7,8]: one Si atom relaxes outward and the other inwards the lateral surface, as indicated by the arrows in Fig. 2, which the side view of the Si NWs depicted in Fig.1. This relaxation gives rise to a tilt angle of around  $34.9^\circ$ , in the case of the (111) NWs, and  $36.4^\circ$ , for the (100) ones, which is close to that inferred from the published Si (110) surfaces,  $42.9^\circ$  [7].

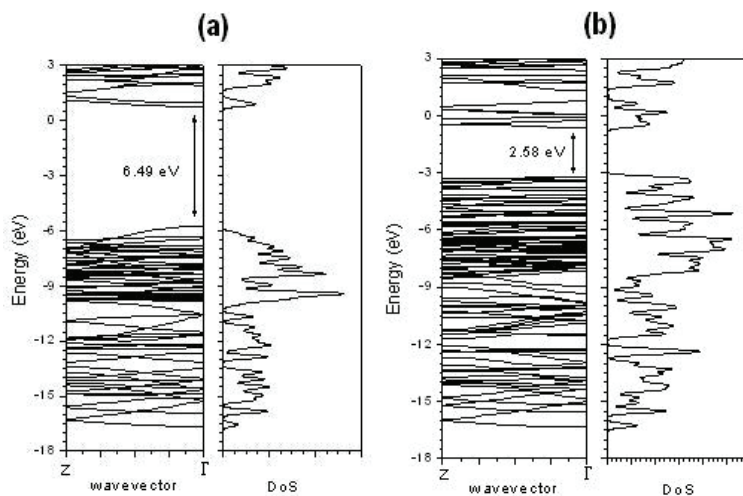


**Figure 1:** Top view of the relaxed Si NWs with: (a) (111) direction with diameter 8.48 Å; (b) (100) direction with diameter 10.38 Å.

In order to check the tilt angle observed in the Si (110) (1×1) surfaces, we also have performed slab supercell calculations on these surfaces as described in our previous work on III-Nitrides [9]. It is well known that both the Si and Ge (110) surfaces do not relax like the III-V and II-VI (110) ones: they prefer, instead, to rearrange their atoms in a complex (16×2) reconstruction pattern [8]. However, our results for the (1×1) reconstruction pattern, in good agreement with the previous theoretical calculations [7,8], show that this tilt angle is  $35.7^\circ$ , which is very close to the observed tilt angle in the Si NWs, and thus, supporting our remarks described above.

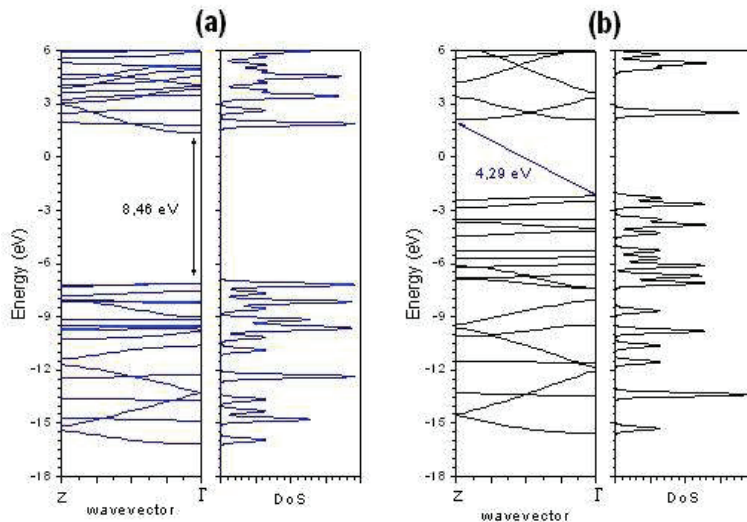


**Figure 2:** Same as Fig. 1 for the side view of the relaxed Si NWs: (a) (111) NW and; (b) (110) NW. The arrows show the atomic displacement of the Si atoms at the facets, and they are not repeated at the other side of the wire for a clear view of the relaxation.



**Figure 3:** Calculated band structures and density of states for the Si (111) NW depicted in Fig. 1, which: (a) the lateral surfaces were saturated with H atoms, and (b) the lateral surfaces were not saturated.

In Fig. 3, we show both the band structure and density of states (DOS) for the Si (111) NW described in Fig. 1, where we compare, side-by-side, the case which the lateral surfaces were saturated by H atoms (Fig. 3a), with that which these surfaces were not saturated (Fig. 3b). We would like to remark that the obtained band structures of all H-saturated NWs considered in this work are in good agreement with other theoretical calculations [3]. And, for the non-saturated NWs, to our knowledge, this is the first time that both the band structures and the DOS are presented. It is clear, from Fig. 3a, that the presence of the H atoms cleanup the band gap. As a consequence, both the top of the valence band and the bottom of the conduction band have a bulk-like-state character, as described in [3]. From Fig. 3b, we have remarked that the states close to the top of valence band and to the bottom of the conduction band have surface character arising from both the occupied Si dangling bond and the empty one, respectively.



**Figure 4:** Same as Fig. 3 for the Si (110) NW, with diameter of 5.19 Å.

Concerning the nature of the calculated band gap, all the band structures calculated for the Si (111) NWs considered in this work (with diameters  $\leq 20$  Å) show direct gap, in contradiction to the previous simple tight-binding results of Harris and O'Reilly [10]. Moreover, we would like to remark that, in Fig. 3, when we remove the H atoms, the band gap value diminishes from 6.49 eV to 2.58 eV. This value remains rather constant with the increasing of the NW diameter, and lies in the visible range of the electromagnetic spectra, which is good for light-emitting and photovoltaic devices [11].

In Fig. 4, we show both the band structure and DOS for the Si (100) NW with diameter of 5.19 Å. Concerning the character of both the top of the valence band and the bottom of the conduction band states, the same features observed for (111) NWs are reproduced in this case. However, after removing the H atoms, the band structure of the Si (100) NWs show an indirect band gap, with values greater than that observed in the (111) ones. For instance, in the NW considered in Fig. 4, the band gap value diminishes from 8.46 eV to 4.29 eV, which is well above of the obtained values for (111) NWs,  $\sim 2.58$  eV. Moreover, as verified for the (111) NWs, without the presence of the H saturators, the band gap value remains rather constant with the increasing of the NW diameter.

In summary, we have presented in this work our preliminary results for the structural and electronic properties of both Si (111) and (100) NWs, varying their diameters from 3.7 to 17.0 Å. The calculations were done with and without the presence of the H saturators in the lateral surfaces of the NW. From the obtained results, we have observed that, without the saturators, there is the formation of {110} facets to partly release the stress accumulated at outermost surfaces of the NWs. In these facets, the atoms relax as observed in the Si (110) surfaces: one Si atom

relaxes outward and the other inwards the lateral surface, giving rise to states close to the top of valence band and to the bottom of the conduction band that have character arising from both the occupied and empty Si-derived dangling bonds, respectively. Moreover, we found that, while the (111) NWs have a direct band gap, the (100) ones have an indirect band gap. A complete description of our obtained results will be published elsewhere.

### 3. Acknowledgements

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### 4. References

- [1] H. Scheel, *et al.*, *phys. stat. sol (b)* **242**, 2474 (2005).
- [2] B. Aradi, *et al.*, *Phys. Rev. B* **76**, 035305 (2007).
- [3] R. Q. Zhang, *et al.*, *J. Chem. Phys.* **123**, 144703 (2005); *J. Appl. Phys.* **109**, 083106 (2011).
- [4] D. Yao, G. Zhang and B. Li, *Nano Lett.* **8**, 4557 (2008).
- [5] M. Elstner, *et al.*, *J. Chem. Phys.* **114**, 5149 (2001).
- [6] R. Rurali and N. Lorente, *Nanotechnology* **16**, S250 (2005).
- [7] N. Takeuchi, *Surf. Sci.* **494**, 21 (2001).
- [8] A. A. Stekolnikov, J. Furthmüller, and F. Bechstedt, *Phys. Rev. B* **70**, 045305 (2004).
- [9] H. W. Leite Alves, *et al.*, *Braz. J. Phys.* **29**, 817 (1999).
- [10] C. Harris and E. P. O'Reilly, *Physica E* **32**, 341 (2006).
- [11] L. Tsakalacos, *et al.*, *Appl. Phys. Lett.* **91**, 233117 (2007).