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Ab INITIO STUDY OF POINT-LIKE DEFECTS INFLUENCE ON CHARGE TRANSPORT IN AlN NANOWIRES

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The influence of intrinsic and some extrinsic point-like defects on the charge transport properties of atomic-sized würtzite AlN wires coupled to nanoscopic wire contacts and Al (111) bulk contacts is investigated at low temperatures using Green-Keldysh formalism. The AlN wires under investigation exhibit a stress induced phase transition from the native würtzite bulk structure to a graphite-like configuration. We find that the conduction of the wide band-gap semiconductor wire in each phase is essentially enhanced by the presence of surface states, which are further influenced by the point-like defects.

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1. Introduction

The current attention devoted to molecular electronics stems from the possibility to achieve the ultimate device scaling. Such structures exhibit peculiar effects such as negative differential conductance, Coulomb blockade and other features specific to the resonant coherent transport. These properties confer them the status of strong candidates for future quantum information technology, where the construction of quantum gates and qubit manipulation is essential.

A multitude of single molecule, atomic chain and break-junction devices have received a lot of interest lately, from both experimental and theoretical point of view. Mono-atomic chains are usually fabricated by mechanically controlled break-junction techniques or, alternatively, the patterned structures and organic molecules are investigated using the scanning tunneling microscope. Most theoretical works which concern atomistic transport calculations include the simulation of nanowires [1] and tubes [2] with linear sizes of a few lattice constants, or atomic chains [3] and molecules [4] contacted to nano- or bulk electrodes. Recent studies are mainly focused on mono-atomic wires where a series of aspects were analyzed, such as for example the conductance oscillations in metallic wires [5-8]. Substrate tunneling [9] or the effects of water molecules as an external environment [10]

Besides the issues mentioned above, attention must be also directed to the changes in the conduction properties produced by intrinsic or extrinsic defects which are likely to appear in structures more complex then the mono-atomic chains, i.e. wires with a cross section of one or more lattice constants. At this system sizes, the coordination effects induced by atoms near the boundaries, the orbital coupling between the wire and the electrodes and the presence of dangling bonds play a major role in the transport properties, which may turn to be completely different from

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the bulk. Examples of such materials can be found in the category of group-III nitrides which are low conductive, *wide* band gap semiconductors in their native bulk configuration. When casted into atomic sized nanowires, the electrical properties are dramatically influenced by the presence of surface states inside the band gap.

In this regard, structural and electronic characteristics of the AlN nanowires have been recently studied [11, 12]. It is known that small diameter nanowires possess peculiar properties. For small non-passivated nanowires, with a high surface-to-volume ratio the effects of the surface states are significant [12] effectively reducing the band gap, which has consequences in the optical absorption and electronic transport.

Moreover, the AlN nanowires experience a size-dependent phase transition [13] from their würtzite (WZ, space group $P6_3/mc$) configuration with [001] orientation along the nanowire axis to a graphite-like (GL, space group $P6_3/mmc$) structure with stacked hexagonal planes.

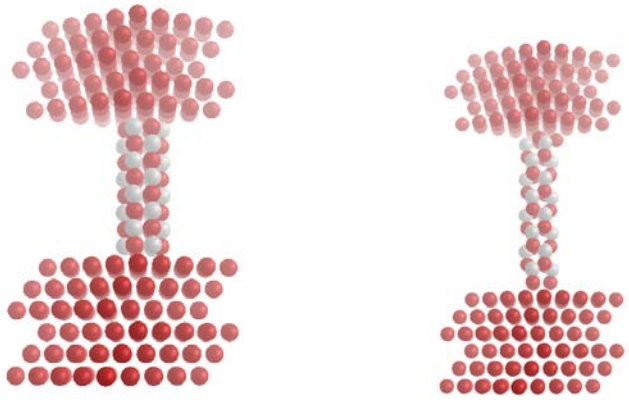

Fig. 1. AlN wires connected to Al bulk electrodes, in the two structural configurations, GL (left) and WZ (right) phase.

In this paper we investigate the effects of intrinsic and extrinsic defects on the electronic transport in AlN nanowires. The analysis includes the presence of different add-atoms (Al and Si impurities), placed on the surface and inside the wire, showing a different behavior in the two structural configurations, WZ and GL. Results corresponding to bulk- and nano-contacts are also presented comparatively. Our *ab initio* study reveals key aspects regarding the tunnability of the surface states, which has important consequences in the conduction properties.

2. Simulation model and method

We analyzed AlN nanowires placed between nanoscopic wire contacts and fcc-Al(111) bulk electrodes in the two structural configurations, WZ and GL (see Fig. 1). In the WZ phase there are three atoms in each of the Al/N alternating layers, while in the GL phase each layer contains six atoms, obtained by contracting two adjacent planes of Al and N in a single layer. For the DFT calculations we use the SIESTA package [14], in the LDA approximation. It makes use of finite-support (localized) basis sets, which is key to achieving linear scaling of computational time with the number of atoms involved. For the structural relaxation we consider as initial input the experimental values for the bulk lattice constants, $a_{Al} = 4.05$ Å, for fcc Al, and $a_{AlN} = 3.112$ Å, $c_{AlN} = 4.982$ Å AlN. The shift between Al/N planes is u = 0.375. We consider wires which are four unit cells in length, i.e. $4c_{AlN}$. The relaxations are performed until the inter-atomic forces are less than 0.01 eV/Å. In case of the bulk Al electrodes, the hexagonal lattice structure of each layer in the ABC stacking of the fcc-Al (111) ensures a natural coupling to the AlN wire, not only from the symmetry point of view but also from the small lattice mismatch ($a_{AlN} \approx a_{Al}/\sqrt{2}$). The distance between the A-B-C planes of fcc-Al is $z_{Al} = 2.34$ Å. The WZ wire has at both ends Al atoms in stacking-position A, which couple to the lower electrode by the layer of type C, and to the upper

electrode by a layer of type B. The transmission function is subsequently calculated using the additional TRANSIESTA package, which employs the Keldysh formalism to simulate electrical transport in molecular devices.

3. Results and discussion

This paper is focused on the study of defects induced changes in the AlN nanowires transmission for the two distinct crystalline phases, WZ and GL. AlN is native WZ in the bulk configuration. However, it was established [13,15] that the free standing wire of this size suffers a phase transition to the GL phase and only by applying enough pulling stress F= - 0.2 nN it retains the WZ configuration.

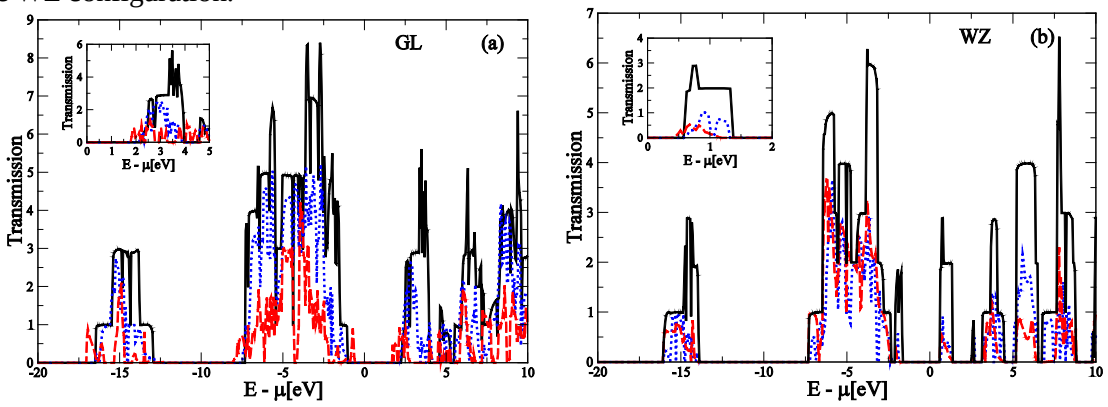

Fig. 2: Transmission for graphite-like (GL) phase (a) and würtizite (WZ) phase (b) for the following systems: ideal (solid/black) and wires with impurities Al-s (dotted-blue), Al-c (dashed-red) with wire nano-contacts. The inset contains similar data for ideal, Si-s, Si-c wires

We first analyze comparatively in Fig. 2 the transmissions in the two phases, for the ideal structures and for wires with extra atoms. In this case, the contacts are nanoscopic and they correspond to a translation in space of the undisturbed wires, in either GL or WZ configurations. As expected, for the ideal infinite systems one obtains a unit plateau for each propagating perpendicular mode. The surface states are located in each case inside the band gap, above the Fermi level (E-μ = 0) at about 2eV (GL) and 0.5 eV (WZ). Note that although the notion of surface state is well defined for wires with larger diameters, the structure of the bands is remarkably similar even in the case of the thinest wire [12]. Next, by introducing intrinsic (Al) and extrinsic (Si) impurities, placed in the center of the nanowire (Al-c) and on its surface (Al-s), the transmission is overall reduced. For the GL nanowire, the transmission is visibly smaller when the impurity, either Al or Si, is placed in the center of the nanowire, compared with the case where the impurity is located on the surface. By contrast, for the nanowire under stress (WZ) one finds a relatively similar disturbance of the ideal transmission for both locations of the add-atom, suggesting a more robust behavior at defect engineering.

We now focus on the energy range in the proximity of the Fermi energy, which is relevant for the linear regime, i.e. small biases, for similar systems connected to bulk Al contacts. In order to gain more insight about the role played by the bulk Al electrodes, we plotted in Fig. 3(a) the density of states (DOS) for the bulk Al and bulk AlN, together with similar data for the defect-free WZ and GL wires. One can notice that, even if the radius of the nanowires is very small, there is still a good resemblance to the bulk-DOS. The overlap between the two densities of states (Al and AlN) gives reliable qualitative information about the overall transmission. In our case one may notice that the first group of states of the AlN systems will not bring contribution to the transport. Next, in Fig. 3 (b) and (c) is depicted the transmission for the same sequence of systems as in Fig. 2, except the wire nano-contacts are replaced by bulk Al electrodes.

For the ideal wire, the plateaus are replaced by oscillations which correspond to the overlap between the density of states in the wire and in the bulk contacts. One interesting feature exhibited by the wires in the GL phase is a peak in the vicinity of the Fermi energy. The peaks are artifacts of the perturbations introduced by the extra atoms. Similar to the systems with wire nano-contacts, the location of the impurities has consequences in the transmission, i.e. the add-atoms placed inside the nanowire introduce a larger decrease. The perturbed GL structure indicated sharp peaks in the middle of the band gap. As a consequence, the otherwise non-conductive wire changes its behavior. The surface states are located, in this case, well above the Fermi level (~ 2 eV, see Fig. 2) and they do not have a major contribution to the charge transport in linear regime.

In the case of the WZ system, the peaks are smaller and they are followed by broader structures which correspond to the surface states. By comparing the obtained data with the defect-free transmission function (black solid line), one can observe that the extra atoms merely shift the location of the surface states, closer to the Fermi level. In both cases, by introducing point defects, the conductivity is enhanced for the case of small applied biases.

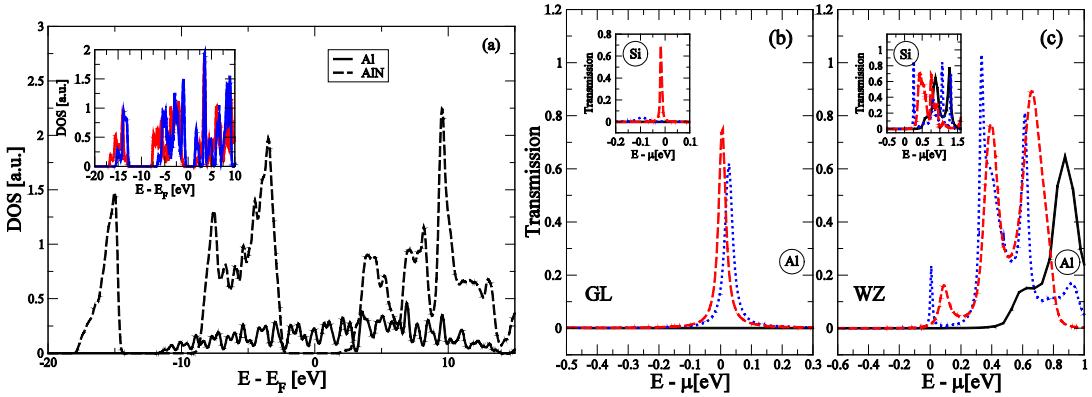

Fig. 3: (a) Density of states for bulk Al (main plot) and for the AlN wires in the two structural configurations inset, WZ (red) and GL (blue). (b) Transmission around the Fermi energy for GL wire connected to bulk electrodes: defect-free wire (black), wire with extra atoms Al-s (dotted blue), Al-c (dashed-red). The inset contains similar data for Si impurities. (c) Same as (b), for WZ wire

4. Conclusion

The transport properties of AlN nanowires with point defects, in both GL and WZ structural configurations, have been investigated. We found that the extra atoms reduce drastically the overall transmission and the effect is larger when the add-atom location is inside the wire. However, when focusing on the energy range around the Fermi energy - which is relevant for small applied biases - we observed the conduction is enhanced. The structural deformations introduced by the extra atoms are able to influence the surface states strong enough and peaks become visible in the transmission.

The results also indicate that the WZ wire is more reliable at defect engineering than the closely packed GL structure.

Acknowledgments

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