First-Principles Study of Doped GaAs nanowires

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The problem of doping of nanowires (NWs) has become recently one of the major challenges to the growers of one-dimensional III-V semiconductor structures. GaAs NWs are considered as one of the most interesting structures for nanoelectronics and nanophotonics. Their potential application in novel electronic devices requires, however, controllable p-type and n-type conductivity. The specific growth conditions for NWs, their crystal structure and orientation of their side facets may lead to different incorporation behavior than known for planar layers.

To study theoretically the problem of doping the NWs, we consider GaAs wires, in which one cation/anion is substituted by a dopant atom. We consider several elements, which are usually used to obtain p- or n-type conductivity in GaAs, i.e., Si, Be and Sn. We study also the distribution of Au and O atoms, which can be unintentionally incorporated during the growth of these wires. Since the III-V semiconductor NWs can grow in both, zinc-blende (ZB) and wurtzite (WZ) structures, we check whether the crystal structure of the wire has an impact on the doping level and the distribution of impurities in GaAs NWs and, most important, on the electronic properties of the doped nanowires. The studied ZB NWs are oriented along (111) axis and WZ NWs along (0001) axis. These growth directions were shown to be the most energetically preferred for GaAs nanowires [1]. Using ab initio methods based on the density functional theory we have calculated the segregation energies for the studied impurities. The segregation energy is defined as the energy difference between the NW with a dopant in a given site and with this impurity situated in the center of the wire.

The calculations have shown that the distribution of impurities in the wires depends crucially on the crystal structure [2]. In NWs of ZB structure the segregation for the studied dopants is high, suggesting that the most common impurities should accumulate at the side surfaces of such wires – for Au, O and Be the lowest energy has been obtained when the dopants substitute the atom with extra dangling bond, at the corner of the wire's cross-section. This result is analogous to the result obtained before for ZB (Ga,Mn)As NWs [3]. Also Sn should be trapped in the outer shell of the wire, but at the subsurface, still in the vicinity of the surface atom with additional dangling bond. The energies of ZB GaAs NWs with the impurity in these positions are lower than in the core of the wire by ca 0.4 eV for beryllium, but by even 1.5-3 eV for gold and oxygen. For gold and oxygen in WZ wires the results are similar to those obtained for ZB structure but with lower, however still high, segregation. In contrast, all other studied impurities distribute much more homogeneously across the WZ wire and Be even prefers to substitute the Ga ion at the center of the wire.

Thus, our calculations suggest that growth conditions leading to WZ structure should be chosen in order to avoid accumulation of impurity atoms at the surface during the growth of doped III–V wires and that using Be seems to be the best choice for effective p-type doping of GaAs NWs. On the other hand, the results show segregation of Au atoms to lateral surfaces, in perfect agreement with the experimental observation [4]. According to our results the same should be also observed for oxygen. Finally, the formation energies for Si in GaAs NWs, calculated for various sets of chemical potentials suggest that the energy needed for substituting the anion and the cation, and thus the type of conductivity obtained by Si-doping, can be also different in ZB and WZ wires.

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References

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