Modelling GaAs nanowire growth: insights from ab-initio calculations

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The talk will give a theoretical perspective on the pros and cons of using a gold catalyst in III-V semiconductor nanowire growth. While e.g. size-selected Au nanoparticles allow one to control the nanometer diameter, potential incorporation of Au impurities could be a major drawback. Our approach to these issues combines an atomistic description of the energetics with concepts from macroscopic thermodynamics. Using judiciously chosen periodic supercells, we obtain from our density functional theory (DFT) calculations not only the formation energies of point defects, but also the surface energies of the catalyst particle and the nanowire side facets, as well the energy of the interface between the GaAs nanowire tip and the Au catalyst particle.

While the driving force for nanowire growth is the *chemical non-equilibrium* between the gas phase, the liquid Au-alloy particle and the solid GaAs wire, it is mostly the *mechanical equilibrium* at the boundary between these three phases that determines the geometrical shape of the nanowire-catalyst interface. Our atomistic interface model puts us in position to calculate the contact angle of wetting and the thermodynamically determined 'neck' radius of the nanowire that grows out of a catalyst particle of given volume.[1]

Moreover, we studied theoretically the formation energy of Au impurities at the interface [2], as well as in bulk GaAs in both zincblende and wurtzite structure. [3] The results show that Au impurities are easily formed at the interface, but as a consequence of their somewhat larger formation energies in GaAs bulk (several tenth of eV), most of the Au point defects will travel with the growth zone, and thus stay near the interface. Since the Au_{Ga} impurity is formed more easily than the Au_{As} impurity in *n*-type GaAs, gallium-rich growth conditions are recommendable to suppress bulk Au_{Ga} impurities, whereas arsenic-rich conditions help to stabilize a smooth and sharp Au-GaAs interface. Once formed, however, the Au impurities are predicted to act as deep centers with several charge transfer levels, ranging from the 2+ to the 2- charge state.[3]

[1] S. Sakong, Y. Du, and P. Kratzer, submitted to Phys. Rev. B
[2] S. Sakong, Y. A. Du, and P. Kratzer, Phys. Stat. Solidi, DOI: 10.1002/pssr.201307210 (2013).
[3] Y. A. Du, S. Sakong, and P. Kratzer, Phys. Rev. B **87**, 075308 (2013).