HL 34: Quantum dots and wires: Theory

Time: Tuesday 9:30–10:45 Location: H15

HL 34.1 Tue 9:30 H15

Bulk and interface defects and impurities in Au-catalyzed GaAs nanowire growth: First principles study — Sung Sakong, Yaojun Du, and •Peter Kratzer — Fakultät für Physik and Center for Nanointegration (CENIDE), Universität Duisburg-Essen, Duisburg, Germany

For the growth of GaAs nanowires, often an Au nanoparticle is used as catalyst, which allows for generating co-existing zincblende and wurtzite polytypes of GaAs, but may also introduce Au impurities in the nanowire. We use density functional theory to calculate the formation energy of various growth-related defects and impurities in both GaAs polytypes and at the Au(111)/GaAs(111)B interface. Defects whose formation energy in bulk is much larger than at the interface, e.g., an As vacancy or a substitutional Au impurity at the As site will travel with the growth zone and hence are less harmful. However, the energetics of the Ga_{As} antisite defect and the substitutional Au impurity at the Ga site are comparable in bulk and at the interface. Especially, the formation of the Au impurity at the Ga site costs relatively low energy. Thus, we predict that the most abundant defect in the GaAs nanowire will be the Au impurity at the Ga site, in good agreement with the recent experimental findings by Bar-Sadan *et al.* [Nano Lett. 12, 2352 (2012)]. In conclusion, we suggest that an As-rich growth regime could reduce the defects and impurities in the nanowire by avoiding the Ga-termination of GaAs at the growth zone which could act as a source of defects at the Ga site.

HL 34.2 Tue 9:45 H15

Modeling the interface between GaAs nanowire and Au capping: First principles study — •Sung Sakong, Yaojun A. Du, and Peter Kratzer — Fakultät für Physik and Center for Nanointegration (CENIDE), Universität Duisburg-Essen, Duisburg, Germany

We present first-principles calculations of the interface between a Au nanoparticle and a GaAs nanowire. The interfaces are modeled with Au ad-layers on a GaAs(111)B substrate. The GaAs surface can be terminated with As or Ga which reflects the two extreme cases in the growth process. The interface energies of As- and Ga-terminated interfaces are expressed as a function of As chemical potential μ_{As}. Under Ga(As) rich growth, the Ga(As)-terminated interface becomes more stable than the other. We note that under a specific μ_{As} the two interface energies become equal, i.e. the two terminations are energetically competing configurations and a layer-by-layer growth of the GaAs nanowire is possible. When one interface is dominantly more stable than the other, then a bilayer growth mode is preferred. The layer-by-layer growth of GaAs nanowire is at $\mu_{As} - \mu_{As}^{bulk} = -0.28$ eV in LDA density functional. Using the estimated interface energy of 47 meV/Å^2, we explore the optimal geometric structures of a Au capped GaAs nanowire with minimizing the surface free energy under near-equilibrium growth. With replacing the pure Au layers with a Au_7Ga_2 alloy, we are able to simulate an interface to a more Ga-rich nanoparticle. The interface energy of the Au-Ga alloy interface is smaller than the pure Au interface, which results in a more flat nanoparticle geometry due to the Gibbs-Thompson effect.

HL 34.3 Tue 10:00 H15

Topological phase transitions in α-Sn Nanocrystals: a first-principle approach — •Küfner Sebastian, Jürgen Furthmüller, Martin Fitzner, Lars Matthes, and Friedhelm Bechstedt — Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, D-07743 Jena

Nanostucturing significantly changes the properties of materials. This especially holds for nanocrystals (NCs). The increased surface to volume ratio influences the electronic structure. There is a strong dependence of the electronic properties on the geometry, the size, and the surface passivation of the nanoscale objects. α-Sn is a zero-gap semiconductor with an inverted band structure at the Γ-point with respect to other group-IV semiconductors. Using density-functional theory within local XC-functionals we show that the level-ordering of s- and p- like states at Γ is inverted in nanocrystals with respect to the bulk. Since the fundamental energy gap decreases for increased nanodot-diameter, we show that there has to be a phase transition for a diameter of about 13 nm where the level odering changes. We determine this critical dot-size by tight-binding calculations. Furthermore, we prove that our results for the fundamental energy gaps of the NCs agree perfectly with methods taking many-body effects and screened Coulomb-interaction into account.

HL 34.4 Tue 10:15 H15

Fast kinetic Monte Carlo simulations of quantum dots — Petar Petrov and •Wolfram Miller — Leibniz-Institut für Kristallzüchtung (IKZ), Max-Born-Str. 2, 12489 Berlin

We present a new three-dimensional heteroepitaxial kinetic Monte Carlo method (KMC) for fast simulation of self-assembled quantom dot arrays. The incorporation of elastic effects due to misfit strained are based on a ball-and-spring model [1]. In contrary to our previous work [2] we simplify the computation of the corrections to the hopping barriers because of the elastic strain in order to accelerate the computation. As an application we studied the system $In_{1-x}Ga_xAs/GaAs$ and analysed wetting layer formation, uniformity of quantum dots in size, distance, and aspect ratio, and others as a function of deposition rate and substrate temperature.

[1] G. Russo and P. Smereka, J. Comput. Phys. 214 (2006), 809
[2] P. Petrov and W. Miller, Comput. Mater. Sci. 60 (2012), 176

HL 34.5 Tue 10:30 H15

Limit Cycles and Chaos in the Current Through a Quantum Dot — •Carlos López-Monís[1,2], Clive Emary[3], Gerold Kiesslich[3], Gloria Platero[2], and Tobias Brandes[3] — [1]Institute für Theoretische Physik, Universität Regensburg, 93040 Regensburg, Germany — [2]Institute für Theoretische Physik, TU Berlin, DE-10623 Berlin, Germany — [3]Instituto de Ciencia de Materiales de Madrid, CSIC, ES-28049 Madrid, Spain

In this talk I shall discuss, nonlinear magnetotransport through a single-level quantum dot coupled to ferromagnetic leads, where the electron spin is coupled to a large, external (pseudo)spin via an anisotropic exchange interaction. We find regimes where the average current through the dot displays self-sustained oscillations that reflect the limit cycles and chaos and map the dependence of this behavior on magnetic field strength and the tunnel coupling to the external leads.

C. López-Monís, C. Emary, G. Kiesslich, G. Platero and T. Brandes, Phys. Rev. B. **85**, 045301 (2012).