

Role of strain relaxation during different stages of InAs quantum dot growth

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Abstract. Recent experiments suggest that InAs quantum dots grown on GaAs (001) undergo a shape transition during growth from 'hut' to 'dome'-like shapes, similar to Ge quantum dots on Si. From a thermodynamic point of view, quantum dot formation is governed by the energetic balance between the energy gain due to strain relief and the energy cost due to formation of quantum dot side facets and edges. In order to account for both contributions, we have developed a carefully parametrized bond-order potential. Its analytical form follows the previous suggestions by Abell and Tersoff, but the newly determined parameters have been fitted to reproduce the elastic constants as well as properties of both GaAs and InAs low-index surface reconstructions obtained from density-functional theory calculations. The potential describes the elastic constants with less than 10 % deviation and the considered surface energies within 10 meV/Å². The results of our calculations are helpful in analysing the energetics of different experimentally observed shapes, and of incomplete layer growth on the facets.

INTRODUCTION

While it is widely accepted that formation of self-assembled quantum dots (QDs) is mainly driven by strain relaxation, the exact route of strain relief during the different growth stages is still unclear. Recent experiments managed to identify the facets of InAs QDs with atomic resolution by STM [1], and suggested a QD shape transition during growth [2]: With increasing size the QD change their shape from a shape with mainly {137} facets ('hut' shape) to a shape dominated by {101} facets ('dome' shape). We analyse the changes in energy and the strain relief during QD growth using a hybrid approach, or alternatively by molecular mechanics employing an atomistic many-body potential.

METHODS

For not too small quantum dots, it has been shown that the energetics of dot formation can be described by a hybrid approach [3, 4]. However, in the limit of small QDs, a unified approach which allows to include atomistic details is required.

Hybrid approach

In the hybrid approach described previously [3, 4], the elastic strain relaxation due to the formation of QDs is obtained from continuum elasticity theory, as imple-

mented by the finite-element method, using experimental elastic constants as input. The energy cost associated with the formation of side facets of the QD is calculated using surface energies obtained with the help of first-principles density-functional theory (DFT) calculations. The hybrid approach describes the quantum dot as a geometrical shape without atomistic detail, but implicitly includes information about surface reconstructions through the surface energies.

Atomistic bond-order potential

Using previous works [5, 6] as a starting point, we derived a new analytical potential for InAs and GaAs based on the bond-order scheme of Tersoff [7] for covalently bonded materials. We developed a sophisticated fitting environment that allows to minimize the least-square deviations between the output generated by the potential and a set of reference data (Levenberg-Marquardt algorithm). The advantage of our approach lies in its flexibility, enabling us to easily optimize any desired system properties by varying a user-defined subset of potential parameters, to include additional reference data, and to assign weights to the requested system properties. Here, we optimize the potential parameters [8] for bulk phases and for reconstructed (001) surfaces of InAs and of GaAs especially with the aim to study QD growth. The experimental lattice constants, cohesive energies, bulk moduli and elastic constants of zincblende GaAs and InAs are reproduced within less than 2%

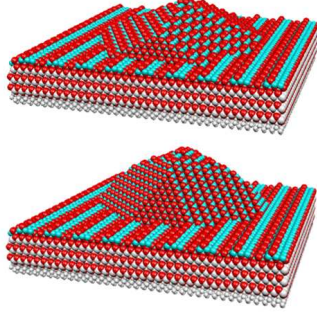


FIGURE 1. InAs QD in 'hut' shape (top) and 'dome' shape 110 (bottom). The substrate is GaAs(001) covered with two monolayers InAs in $\beta 2(2 \times 4)$ reconstruction.

error. The lattice constants and cohesive energies of hypothetical GaAs and InAs phases, as well as of realistic and hypothetical Ga, As and In bulk phases are captured within less than 10% error. The surface energies of several (001) facets of GaAs and InAs obtained from DFT calculations are reproduced within ± 10 meV/Å². Possible applications of this potential include the investigation of elastic strain in capped and uncapped QD's, of the total energies of free-standing QD with reconstructed facets, and of strain effects in surface diffusion.

RESULTS

We start from the detailed atomic structure of 'hut'- and a 'dome'-shaped InAs QD (Fig. 1 and Fig. 2), as observed in recent STM studies [1, 2]. These shapes are dominated by {137} facets and {110} facets, respectively. We determine the fully relaxed atomic structure of differently sized QDs of these two shapes, using our bond-order potential. Figure 2 shows the average cohesive energy per atom in the dot. We find that for small QD sizes, the hut shape is energetically favorable, in agreement with experiment. The same conclusion is obtained from calculations using the hybrid approach, which predict that 'dome' shapes become more favorable only for more than about 30.000 atoms in the QD, the precise number depending on the details of the shape. We propose that shape changes during growth occur due to growth of incomplete layers on the side facets of the QD. To put this idea to the test, we compare the cohesive energies per atom of hut-shaped QDs with partially completed InAs layers on the {137} facets. For all three QD sizes considered, we find that layer growth from the QD bottom is energetically favorable compared to layer growth from the top. This finding is in agreement with the idea that the shape transition is triggered by incomplete layer growth

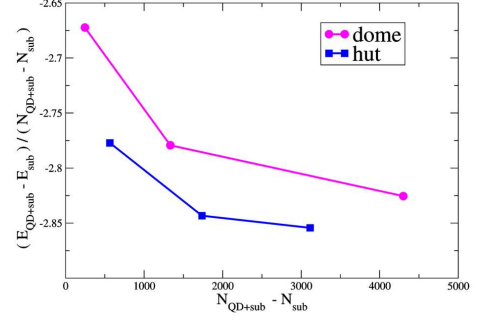


FIGURE 2. Average cohesive energy per atom in QDs in 'hut' or 'dome' shape, for three numbers of atoms $N_{QD} = N_{QD+sub} - N_{sub}$ in the dot, and a fixed number of substrate atoms N_{sub} , as obtained by relaxing the structures using the analytical many-body potential. For the rather small QDs considered here, the 'hut' shape, which is the experimentally observed shape in this regime, is found to be lower in energy.

from the top, but the QDs considered here are still below the critical size for the shape transition.

CONCLUSION AND OUTLOOK

We parametrized an analytic many-body potential that accurately captures bulk and elastic properties of GaAs, InAs, Ga, As and In, and, in addition, gives reasonable energies and geometries of several surface reconstructions. Using this potential, we find that the 'hut' shape is energetically lower for small QDs, in agreement with experiment. Moreover, we predict that layer growth on the facets from bottom to top is energetically preferred. We would like to acknowledge fruitful discussions with M. Scheffler and B. Lehner. This work was supported by the Deutsche Forschungsgemeinschaft, Sfb 296.

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