Strain field calculations of quantum dots — a comparison study of two methods

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Abstract. The elastic strain field plays a crucial role during the self-organized growth of semiconductor quantum dot structures in the Stranski-Krastanov growth mode. Several theoretical methods have been developed for calculating the strain field of these lattice-mismatched systems. In this report we present a study exemplarily comparing an atomistic approach and calculations using elasticity theory. Features, limitations and selected possible applications of both approaches are discussed.

Keywords: strain field, quantum dots, self-assembly
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The concepts of self-assembly and self-organization are essential to understand the growth of quantum dots (QDs) in the Stranski-Krastanov mode [1, 2, 3]. The detailed knowledge of the strain fields that arise from the lattice mismatch between substrate and deposited material is needed for a thorough understanding of the experimentally observed growth properties of QDs. Atomistic approaches of calculating the strain fields, such as classical many-body potentials (MBP) or *ab-initio* methods, provide atomic resolution but are often limited by the numerical effort. Approaches based on continuum elasticity theory (CET), however, are hardly limited by the system size and can describe elastic properties on a mesoscopic length scale. In this work, we compare the strain tensor of characteristic structures as obtained with MBP and CET calculations.

In the first approach we use an MBP of the Abell-Tersoff type that was carefully parameterized recently [4]. It reproduces many properties of Ga, As, In, GaAs, and InAs bulk structures, and of GaAs and InAs surfaces with good overall accuracy. A detailed investigation of the elastic response of InAs and GaAs upon biaxial strain in different planes confirms its applicability to InAs/GaAs nanostructures. The strain tensor in this atomistic approach is determined by a structural relaxation that minimizes the total energy with respect to the atomic coordinates, followed by a comparison with a topologically equivalent, but undistorted configuration [5]. The resulting strain tensor for overgrown QDs is shown in Fig. 1. The atomistic strain tensor is interpolated to a cubic grid and compared with the CET approach for spatial positions that are 1 monolayer (ML) below the surface layer. This avoids potential inconsistencies due to the different treatment of the surface in the MBP and the CET approach.

The second approach developed in the framework of CET enables us to calculate the full three-dimensional strain field of arbitrarily shaped QDs taking into account the anisotropic elastic properties of the material. In our approach we model the multi-sheet array of QDs by inclusions of material A in a matrix of a host material B by solving the equilibrium equation of elasticity theory [6, 7, 9] under stress-free boundary conditions on the surface and using the homogeneous moduli approximation [6]. Further we express the elastic energy of interacting inclusions in terms of the Fourier transform of the static Green's tensor of elasticity theory [8].

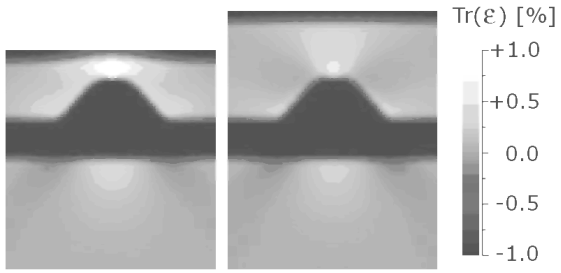

FIGURE 1. Trace of the strain tensor as obtained with the MBP approach for an InAs QD overgrown by 10 ML (left) and 15 ML GaAs (right). (Only values up to 1 % are shown.) In the comparison with the CET approach we refer to values of 1 ML below the surface.

A previous comparison of a (numerical) CET approach and a less accurate MBP [5] found good agreement for relatively small strain, but discrepancies for large strain, namely inside QDs and around its interfaces. In the following, we contrast the results of our (semianalytic) CET approach with those of a more reliable MBP: In Fig. 2 the trace of the strain tensor $[Tr(\varepsilon)]$ of a platelike circular QD with a radius of 10 l.s. is shown. Both methods yield a tensile strain of the central GaAs region

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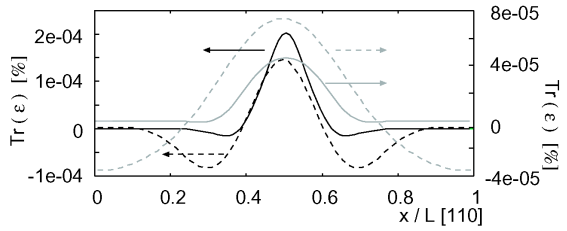

FIGURE 2. Trace of the strain tensor computed with elasticity theory (solid lines) and the atomistic approach (dashed lines): Strain at the relaxed surface of a circular monolayer QD with a radius of 10 lattice sites (l.s.). Distance between the surface and the buried sample structure is $d = 9$ l.s. (black) and $d = 17$ l.s. (grey). System size: $L \times L = 100 \times 100$ l.s. Host material: GaAs. Lattice constant $a_{GaAs} = 0.565$ nm$= 1$ l.s.

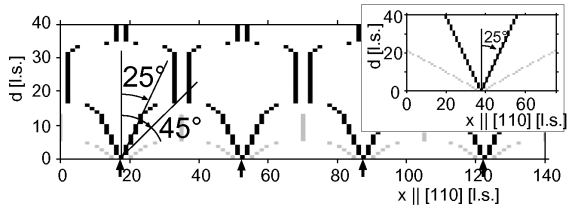

FIGURE 3. Elastic strain field of a periodic array of QDs and of a single QD (inset) calculated from elasticity theory. Minima ($E < 0$, black) and Maxima ($E > 0$, grey) of the elastic interaction energy E in the relaxed surface at d are shown. Arrows: QDs (lateral spacing 25 l.s.).

that is directly above the InAs QD, and a similar range of values of $Tr(\varepsilon)$ for both investigated heights. The lateral extension of the region with $Tr(\varepsilon) > 0$ obtained by the two methods is in good agreement at a height of $d = 9$ ML and still reasonable for the weakly strained layers at a height of 17 ML. At the GaAs border regions surrounding this tensile central area, both methods yield vanishing strain at small height, but show some discrepancy in the description of the weakly strained GaAs regions at larger height, namely an opposite sign of $Tr(\varepsilon)$ in the border regions. This effect is due to the periodic boundary conditions that were used in the MBP calculations, in contrast to the semi-infinite treatment of the same structure in the CET calculations. The Green's tensor approach furthermore yields a weaker compression of the intermediate GaAs region above the corner of the InAs inset as compared to the many-body potential that exhibits two distinct minima of $Tr(\varepsilon)$.

Using CET it is possible to calculate strain fields for large arrays of QDs. In Fig. 3 the vertical propagation of the minima and maxima of the elastic interaction energy in the relaxed surface at spacer thickness d are shown for a single point-like QD (inset) and for a periodic array of point-like QDs with GaAs as host material [9] The interaction energy minima (maxima) correspond to maximum tensile (compressive) strain and give rise to an attractive (repulsive) potential. Minima form preferred sites for nucleation [11]. For a single QD the inclination angle of the strain field minima against the vertical agrees with previous theoretical findings [12], but seriously contradicts the experimental observation [13]. However, if a whole array of QDs is considered, with increasing d the inclination angle increases more and more until at $d = 17$ ML the strain fields of two QDs meet and form a double minimum exactly in the middle between these QDs. The transition from vertically correlated to anticorrelated growth occurs at an inclination angle of 45° for GaAs (Fig. 3), in close agreement with experiment, where a value of 50° was found [13]. The small remaining discrepancy might result from modulations in chemical composition or morphological changes in the spacer layer.

In conclusion, we have presented two complementary approaches to self-assembled QDs: Classical many-body potentials can give detailed microscopic insight into their shape and structure, while continuum elasticity theory can explain correlation and anticorrelation effects in large arrays of QDs.

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