On a Database of Simulated TEM Images for In(Ga)As/GaAs Quantum Dots with Various Shapes

Thomas Koprucki*, Anieza Maltsi*, Tore Niermann:†, Timo Streckenbach*, Karsten Tabelow*, Jörg Polzehl*
* Weierstrass Institute (WIAS), Mohrenstr. 39, 10117 Berlin, Germany
† Institut für Optik und Atomare Physik, Technische Universität Berlin, Straße des 17. Juni 135, 10623 Berlin, Germany

Email: thomas.koprucki@wias-berlin.de

***Abstract*—We present a database of simulated transmission electron microscopy (TEM) images for In(Ga)As quantum dots (QDs) embedded in bulk-like GaAs samples. The database contains series of TEM images for QDs with various shapes, e.g. pyramidal and lens-shaped, depending on the size and indium concentration as well as on the excitation conditions of the electron beam. This database is a key element of a novel concept for model-based geometry reconstruction (MBGR) of semiconductor QDs from TEM imaging and can be used to establish a statistical procedure for the estimation of QD properties and classification of QD types based on machine learning techniques.**

I. Introduction

The fabrication of semiconductor quantum dots (QDs) with desired electronic properties would highly benefit from the assessment of QD geometry, distribution, and strain profile in a feedback loop between epitaxial growth and analysis of their properties. To assist the optimization of QDs imaging by transmission electron microscopy (TEM) [1] can be used. However, a direct 3D geometry reconstruction from TEM of bulk-like samples (thickness 100-300 nm) by solving the tomography problem is not feasible due to its limited resolution (0.5-1 nm), the highly nonlinear behaviour of the dynamic electron scattering and strong stochastic influences in the images.

In [2], [3] we introduced a novel concept for 3D model-based geometry reconstruction (MBGR) of QDs from TEM imaging. The approach is based on (a) an appropriate model for the QD configuration in real space including a categorization of QD shapes (e.g., pyramidal or lens-shaped) and continuous parameters (e.g., size, height), (b) a database of simulated TEM images covering a large number of possible QD configurations and image acquisition parameters (e.g. bright field/dark field, sample tilt), as well as (c) a statistical procedure for the estimation of QD properties and classification of QD types based on acquired TEM image data. As a first step we developed a mathematical model for the numerical simulation of TEM images for semiconductor QDs, see [2], [3]. In this contribution we continue our effort towards MBGR by presenting a database of simulated TEM images.

II. Simulation of TEM images

The dynamic electron scattering in crystalline solids, e.g., semiconductor nanostructures, is influenced by spatial variations in the chemical composition and by local deformations of the lattice due to elastic strain [1]. By variation of the excitation conditions the sensitivity of the imaging can be tuned, e.g. to different components of the strain as shown in Figs. 1c and 1d. For the In(Ga)As QDs under consideration, the lattice-misfit between In(Ga)As and GaAs (surrounding matrix) induces mechanical stresses in the nanostructure. For the elastic relaxation of the misfit-induced strain we employ continuum mechanics and the concept of Eshelby's inclusion. For the numerical simulation of the TEM images we use the FEM-based elasticity solver from WIAS-pdelib [4] to obtain the strain profile, which enters the solver pyTEM [5] for the Darwin-Howie-Whelan equations describing propagation of the electron wave through the sample, see [2], [3].

III. Database of TEM images

For the generation of TEM images for the database we use a parametric geometry description of the QD shape, e.g. using base length and height of the QD, in combination with the mesh generator TetGen [6], see Fig. 1a. By variation of the geometrical parameters as well as the excitation conditions a database of TEM images is created. In the database the geometrical model, the computed strain profile, the multi-beam solution as obtained by the solution of the Darwin-Howie-Whelan equations and the resulting TEM images are stored together with necessary meta data. Snapshots from the database including pyramidal and lens-shaped QDs with different values of the vertical aspect ratio and two excitations conditions, respectively, are shown in Fig. 1. Our aim is a comprehensive database covering all the different types and shapes of QDs as introduced in [7].

IV. Outlook

The next step on our agenda towards MBGR is to analyse the resulting population of TEM images and to study if this database is large enough to train a convolutional neural network for the solution of the classification problem.

As a by-product the database can also serve as an extensive resource for benchmarking elasticity solvers for geometrically complex semiconductor nanostructures since we also store the corresponding strain profiles.

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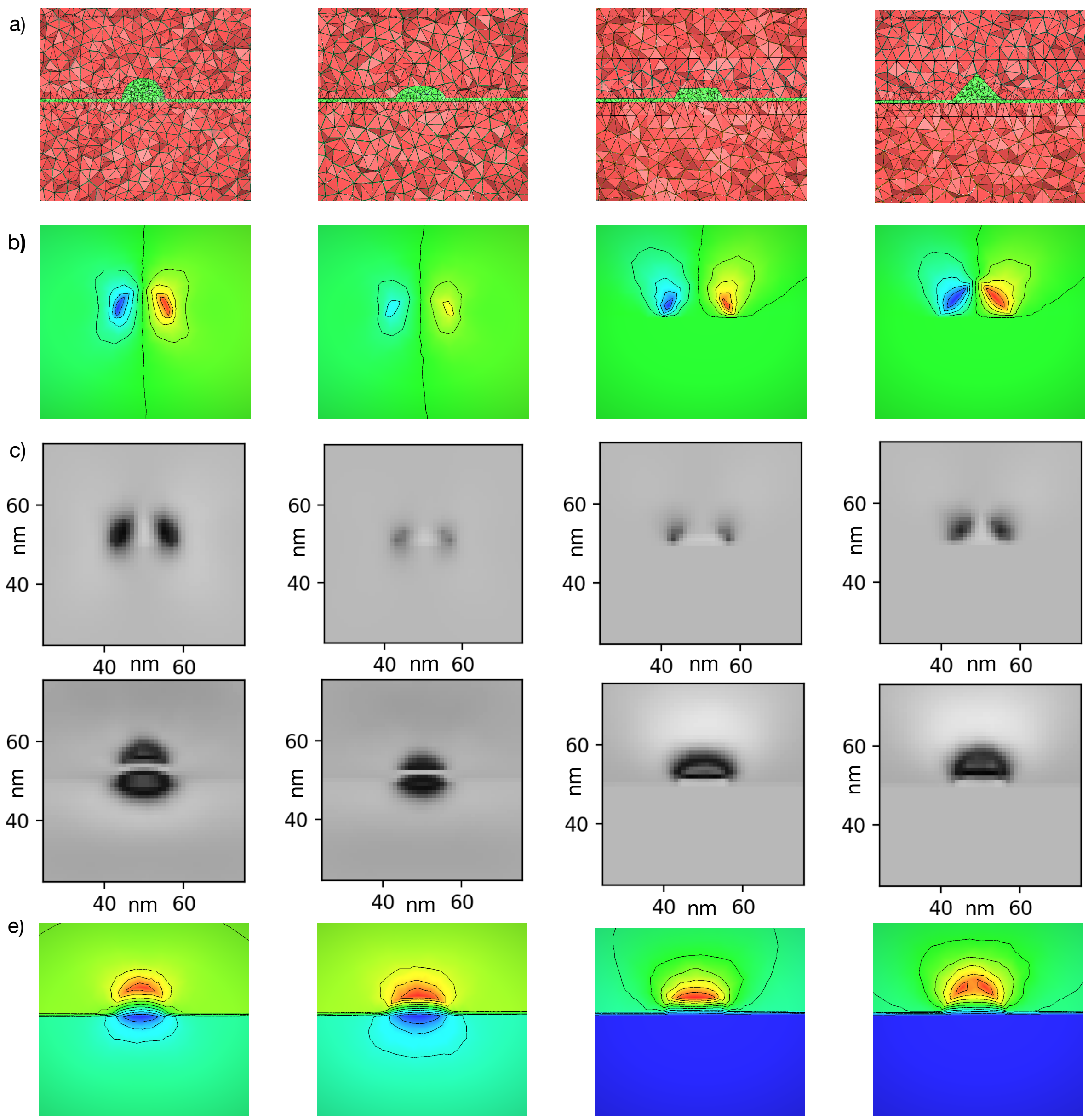

Fig. 1. InGaAs quantum dots (indium content 80%) embedded in a GaAs matrix with different shapes: lens-shaped QDs with circular base (two left columns) and pyramidal QDs (two right columns) with different vertical aspect ratios, respectively. FEM simulation of the elastic relaxation of the misfit induced strain: (a) geometry and FEM mesh (b) u_y component and (e) u_z component of the displacement field along a yz-cross-section through the center of the QDs. Simulated TEM images for two different excitations: (c) dark field for (040) reflection for excitation under (040) strong beam conditions and (d) dark field for (004) reflection for excitation under (004) strong beam conditions. Due to the excitation conditions, the image contrast (c) is sensitive to the [010]-component of the displacement field corresponding to u_y in (b) and the image contrast (d) is sensitive to the [001]-component of the displacement field corresponding to u_z in (e). In all cases a coffee-bean like contrast can be observed. The TEM images (c) and (d) have been simulated with pyTEM [5], using the displacement field obtained with the FEM-based elasticity solver of WIAS-PDELIB [4] assuming a sample thickness of 150 nm.

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