

LA-UR-01-5228

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*Submitted to:*

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# Image Simulations of Quantum Dots

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**ABSTRACT:** An image simulation method for quantum dots based on a Bloch wave algorithm is described and applied to the case of quantum dots in the InN/GaN system.

## 1. INTRODUCTION

Quantum dot (QD) nanostructures have drawn increased interest in recent years. Their small size leads to quantum confinement of the electrons, which is responsible for their unique electronic and optical properties. They promise to find use in a wide range of devices ranging from semiconductor lasers (Bimberg et al (2001), Ribbat et al (2001)) to quantum computing. The properties of QDs are also determined by their shape and composition. All three parameters (size, shape and composition) have a significant impact on their contrast in the transmission electron microscope (TEM), and consequently the possibility arises that these parameters can be extracted from the images. Zone axis plan view images are especially sensitive to the composition of QDs, and image simulation is an important way to understand how the composition determines the contrast. This paper outlines a method of image simulation of QDs developed by Liao et. al. (1999) and presents an application of the method to QDs in wurtzite InN/GaN.

## 2. THE FORM OF THE IMAGE

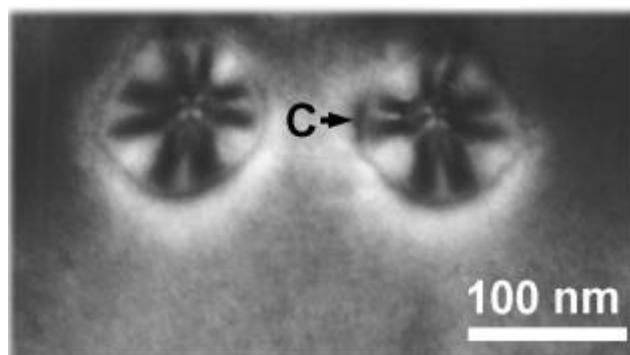


Fig. 1 Two Ge/Si QDs. The angle of the spreading of the Maltese cross like bars is related to the composition of the dots (Liao et. al. 1999, 2001a, 2001b).

Fig. 1. shows a bright field on-zone axis TEM image of a Ge/Si QD. This contrast has been shown to be related not to any particular physical shape of the dot but to the

crystallography and the composition (Liao et. al. 1999, 2001a, 2001b ). To be able to interpret such an image, image simulation is essential. Therefore a method that is able to test different models of the physical properties of the QD is necessary.

### 3. METHOD FOR IMAGE SIMULATIONS

The method used for image calculation consists of two main steps. In the first step, the displacement field of the QD is calculated. This is done using finite element analysis (FEA). To facilitate the process, the commercial package Strand7 (<http://www.aust.strand.com>) is used which provides a graphical interface that assists in the creation of the mesh of nodes (Fig. 2) and the generation of a plot of the displacement and strain field. In this case, the dot is modelled as a spherical cap with a height to width ratio of 1 : 3. The elastic constants of the substrate material and the material of the QD enter the calculation as a 6 x 6 stiffness matrix. A thermal expansion that resembles the magnitude of the lattice mismatch between the dot material and the substrate material creates the stress at the interface between dot and substrate. The displacements and positions of the nodes are then exported to a file, which is read in by the main image simulation program.

The Bloch-wave theory is used in the image simulations. A program for image simulations is based on a program provided by S. Matsumura. Fig. 3 shows the steps performed by the program.

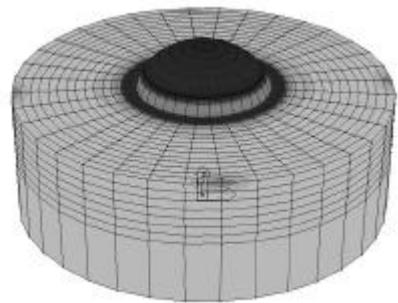


Fig. 2 Finite Element mesh of a QD and the substrate.

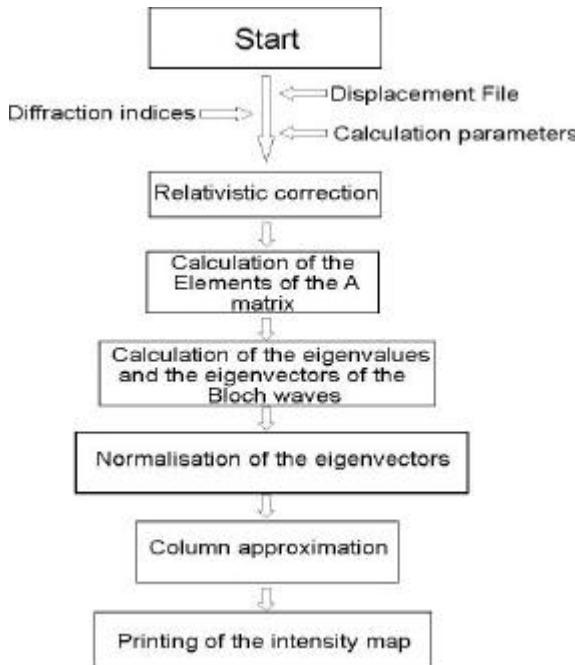


Fig. 3. The steps performed by the image simulation program used to calculate the contrast of QDs.

The  $A$  matrix has diagonal elements  $A_{00}=0$ ,  $A_{gg} = 2Ks_g$  where  $\mathbf{K} = \mathbf{k} + \mathbf{g}$  and  $s_g$  is the deviation parameter and off diagonal elements  $A_{gh} = 1/(2?_{g-h})$ , where  $?_g$  is the extinction distance of diffraction vector  $\mathbf{g}$ .

During the column approximation the specimen is divided into two parts, with the dot being on the exit surface of the sample (see below and fig. 4). The first part is regarded as a 'perfect' area where the crystal lattice has no distortion. The second part is a strained area in which the film is further divided into many slices with each slice assumed to have a constant displacement in each column. Usually the QD and a part of the substrate area are regarded as the strained region. The QD is placed on the exit of the sample and this configuration should also be used in any experiment in which comparisons with simulated images are made. In this way the electron beam will enter into the thin film simultaneously for all column positions, and leave the film at a different 'time' depending on the column position.

At the end of the column approximation, the intensity of the transmitted beam is calculated and the intensity map is saved as a postscript file.



Fig. 4 The dot is put into the calculation upside down.

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#### 4. APPLICATION: IMAGE SIMULATION OF A WURTZITE InN/GaN QD

A field that has attracted considerable attention recently is the growth and application of III-nitride semiconductors. Blue light emitting diodes based on single quantum wells have been designed and put into practice. One of the most prominent materials is InN/GaN. InN and GaN have a lattice mismatch of 9% and are therefore expected to grow QDs by the Stranski – Krastanov growth mechanism. It is thought that QDs in this material system will be used in quantum computers. However, as for most III-nitride semiconductors, InN/GaN is only stable in the wurzite structure although it has a metastable cubic phase. Furthermore the lattice mismatch in the InN/GaN system is considerably larger than in Ge/Si, for which there have been many TEM studies. Therefore it is

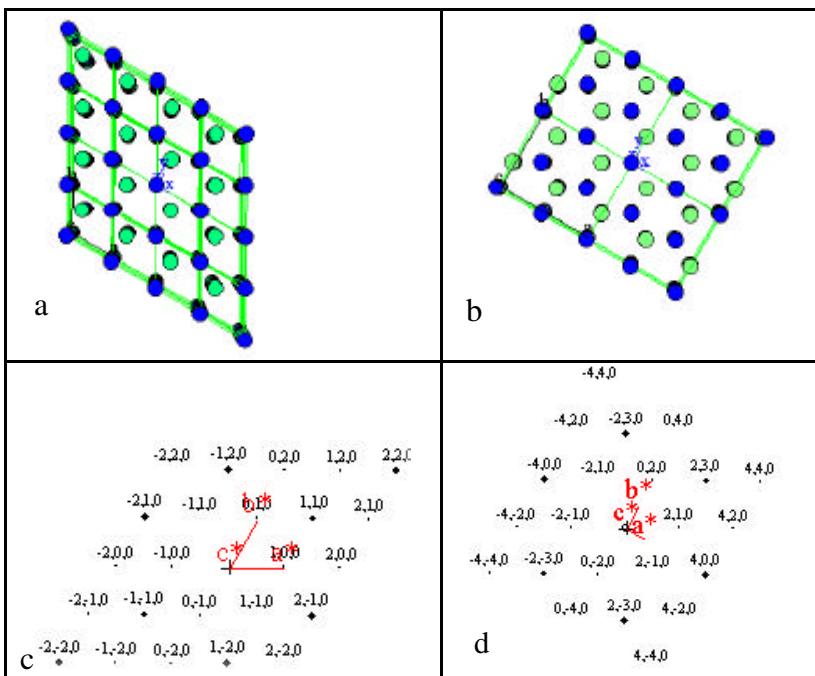


Fig. 5 The original wurtzite crystals and the crystal built from the orthogonal unit cell (a, b) and the corresponding diffraction patterns (c,d).

important to investigate their growth in detail, determine whether the basic characteristics of images deduced for QDs in cubic crystals still hold, and in what way they are influenced by the hexagonal symmetry of the crystal.

The image simulation program described in the previous section was adapted for non-cubic crystals, including describing the InN/GaN structure as a unit cell with orthogonal axis. In the InN/GaN wurtzite structure the atoms of Ga (In) are in (0,0,0) and (1/3,2/3,1/2) and the N atoms are at (0,0,3/8) and (1/3,2/3,7/8). In the redefined orthogonal cell the Ga (In) atoms are at (0,0,0), (1/4,1/2,0), (1/2,0,0), (3/4,1/2, 0), (0, 1/3,1/2), (1/2,1/3,1/2), (1/4,5/6,1/2), (3/4,5/6,1/2) and the nitrogen atoms are at (0,0,3/8), (1/4,1/2,3/8), (1/2,0,3/8), (3/4,1/2,3/8), (0,1/3,7/8), (1/2,1/3,7/8), (1/4,5/6,7/8), and (3/4,5/6,7/8).

A series of bright field on-zone [001] image simulations was carried out for spherical cap shaped QDs of diameter 60 nm. The substrate was assumed to be Ga and the dot pure In (no segregation). An example is shown in fig. 6. Compared with fig. 1 for Ge/Si, it is seen that fig. 6 has six fold symmetry showing six dark bars meeting in the centre. This is a clear indication that the features of the contrast of QDs in a TEM are closely related to the crystal symmetry. No spreading of the bars is observed. This is in agreement with the earlier studies of InGaAs/GaAs and of Ge/Si where spreading was only observed when segregation in the QD was included (Zou et al 1999). The model of InN/GaN has no segregation. It is also noted that the boundary of the dot is approximately circular, in agreement with the projected shape of the dot in the FEA. The diameter of the contrast of the dot is within 5% of the diameter of the dot in the FEA. Since the contrast in the InN/GaN QD image has features (e.g. dark bars) similar to those observed in the Ge/Si and InGaAs/GaAs systems, and since in these systems these features have been shown to give composition and segregation information, it is likely that the images of InN/GaN can be used for the same purpose.

Support from the EPSRC is acknowledged.

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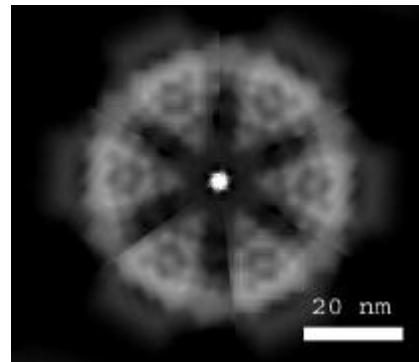


Fig. 6 Multiple beam [001] zone axis calculation of a InN/GaN QD . The image shows the six fold symmetry of the dot. There is no spreading of the bars since the model of the dot does not incorporate segregation.

FEA. The diameter of the contrast of the dot is within 5% of the diameter of the dot in the FEA. Since the contrast in the InN/GaN QD image has features (e.g. dark bars) similar to those observed in the Ge/Si and InGaAs/GaAs systems, and since in these systems these features have been shown to give composition and segregation information, it is likely that the images of InN/GaN can be used for the same purpose.