Features of microstructure of InSb quantum dots on InAs substrate

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Abstract. The properties of InSb/InAs quantum dots (QDs) were investigated by transmission electron microscopy (TEM). Specific features of diffraction contrast were discovered in plan-view TEM images of big (9–10 nm in height and 38–50 nm in diameter) InSb QDs. The simulation of image contrast from the InSb/InAs QD containing a partial Frank dislocation (FD) was carried out for the first time. The comparison of experimental and simulated data allowed us to explain the observed features of the moiré pattern in the image of big InSb QD by the presence of a misfit defect (FD) at the QD-substrate interface.

1. Introduction

Heterostructures with InSb QDs on GaSb or InAs substrates are potential for producing optoelectronic devices operating in the mid-infrared range (3–5 μm) [1]. For instance, mid-IR lasers are used in various fields – chemical process control, environmental monitoring, non-invasive medical diagnostics, leak detection and laser surgery.

The structural properties of InSb/InAs system are similar to those of the well studied InAs/GaAs system. Its crystal structure also forms the face-centered cubic (fcc) lattice. The InSb/InAs system has the lattice mismatch of 6.9 % which is quite close to that in InAs/GaAs (7.2 %). However, because the conditions of InSb/InAs QD formation are not optimized yet the big islands appear among small ones during the epitaxial growth of InSb on InAs substrate [2–3]. Such big dots are incoherent and contain misfit defects.

The subject under study was determination of misfit defect nature in big incoherent InSb/InAs QDs. For this purpose the microstructure of InSb/InAs QDs was studied by TEM. Based on TEM results the model of the structure of such QDs was developed, and calculations of displacement fields and modeling of diffraction contrast TEM images were done.

2. Experimental

The samples were grown using the LPE or MOCVD technique. The LPE growth was carried out in a horizontal set-up equipped with a conventional graphite slider boat under purified H₂ flow on InAs(001) substrate in the temperature range of 420–445°C during 2 seconds, the temperature was lowered from the saturation point down to the growth temperature at a ramp rate of 0.3–0.6°C/min. The MOCVD growth of InSb/InAs QDs was performed in a standard horizontal reactor under atmospheric pressure at temperatures of 420–440°C and at the rate of TMIn supply to the reactor of 5.6–8 μmol/min. The details of the QD growth were reported elsewhere [1–5].
The samples with arrays of InSb QDs on the InAs surface were prepared for the study by TEM using the conventional procedure of preliminary mechanical thinning followed by final ion beam milling (4 keV Ar⁺ ions). The TEM study was carried out in a JEOL JEM 2100F microscope at an accelerating voltage of 200 kV in the diffraction and high-resolution modes. Both cross-section and plan-view TEM specimen configurations were used.

3. TEM results

TEM observation showed the QD ensemble to have bimodal size distribution [2]. There were small QDs of the typical size of 5 nm in height and 18–22 nm in diameter as well as big QDs of 9–10 nm in height and 38–50 nm in diameter. The majority of QDs looked lens-like in the cross-section TEM image. Also there were some QDs having a truncated spherical shape.

Under two-beam diffraction conditions the regular moiré fringes appeared in plan-view TEM images of small InSb QDs. Such fringes were shown to occur [6-7] due to fine difference in atomic plane distance in the InAs matrix and elastically relaxed free-standing QD. An example of the fringed image obtained from small InSb QD under two-beam diffraction conditions is shown in figure 1 (a). The fringes always run perpendicular to the diffraction vector, and when the diffraction vector rotates to orthogonal direction the fringes lay-out also becomes orthogonal.

As distinct from small QDs the big ones were discovered to exhibit whether the complicated moiré pattern (figure 1 (b)) or the specific "tick"-like contrast features. Additionally, the fringe pattern from big QD did not rotate accordingly to the rotation of the diffraction vector \(\mathbf{g}\) but showed a significant change as can be seen in figure 2.

![Figure 1. Plan-view TEM images with the moiré pattern of small (a) and big (b) InSb/InAs QD](image1.png)

![Figure 2. TEM images of big InSb/InAs QDs taken under various diffraction conditions](image2.png)
The study of big QDs in high-resolution mode using the cross-section specimen revealed the presence of dislocations near the QD-substrate interface. Such a dislocation is seen in the cross-sectional image of big QD presented in figure 3.

4. Modeling
In order to understand the observed features of TEM/HREM image a theoretical structure modeling and subsequent simulation of image contrast is usually required. To interpret the complicated moiré pattern we have calculated diffraction contrast from QD containing a misfit defect.

A partial Frank dislocation (FD) often occurring in incoherent QDs in the well studied InAs/GaAs system [8] was selected to represent a misfit defect in our model. The dislocation with the Burgers vector $b=\frac{1}{3}[111]$ was placed at the QD-InAs substrate interface along [110] direction and displacement fields inside and outside QD were calculated relative to unstrained part of InAs substrate using the finite element method.

We examined QD of a cylindrical, a lens-like and a truncated spherical shape. The last two cases – a lens-like shape and a truncated sphere – were observed in TEM.

The results of the displacement field calculation for the developed model have demonstrated that the QD shape has insignificant influence on the magnitude and distribution of the displacement field.

The insertion of FD into QD of each shape essentially changes the distribution of the local displacement field and reduces strain at the edges of QD almost by 30%. As an example, the calculated displacement field for cylindrical QD is exhibited in figure 4. One can compare the position of equal displacement lines for QD without FD in figure 4 (a) and for QD with FD in figure 4 (b).

Calculated displacements were then used in simulation of diffraction contrast TEM images. The Howie-Whelan dynamic approach [9–10] was applied to simulate the plan-view image of QD containing FD. The approach is commonly used for the solution of electron diffraction problem in the
crystals containing defects and is based on two differential equations for the amplitudes of incident ($\Phi_0$) and diffracted ($\Phi_g$) electron waves:

\[
\frac{d\Phi_0(z)}{dz} = \frac{\bar{m}}{\xi_g} \Phi_g(z) \exp(2\pi ig \cdot \bar{u}) \\
\frac{d\Phi_g(z)}{dz} = \frac{\bar{m}}{\xi_g} \Phi_g(z) \exp(-2\pi ig \cdot \bar{u}) + 2\bar{m}\bar{s} \Phi_g(z)
\]

where $\bar{g}$ is the diffraction vector, $\xi_g$ is the extinction distance, $\bar{s}$ is the parameter of deviation (in our calculations $\bar{s} = 0$).

5. Results and discussion
The results of TEM image simulation showed that the shape of QD had insignificant influence on the final diffraction contrast.

Behavior of diffraction contrast in the simulated TEM image depending on the operating diffraction vector and a lattice mismatch value is presented in figure 5.

As can be seen, the insertion of FD into QD leads to various changes in the moiré pattern. It causes the appearance of additional moiré fringes in the diffraction contrast image with the diffraction vector of $g = 220$. The introduction of FD also breaks the symmetry of the image with the diffraction vector of $g = 400$ or $0–40$.

The increase in a lattice mismatch results in reduction of the moiré fringes period and, therefore, leads to the increase in the number of observable fringes.

| $g$ | QD without FD | QD with FD |
|-----|----------------|-------------|
| $3\%$ | $6\%$ | $3\%$ | $6\%$ |
| 220 | ![Figure 5](a) | ![Figure 5](b) |
| 400 |  |  |
| 220 |  |  |
| 0-10 |  |  |

Figure 5. Simulated contrast from QD without FD and with FD for 3% and 6% lattices mismatch (a) and the position of stacking fault (it is shown by the counter) associated with FD in QD (b).

Comparison of simulated and experimental images exemplified in figure 6 shows that the observed period of the moiré pattern from small QD under 220 reflection (figure 6 (e–f)) is very close to that in the simulated image of QD with a 6% lattices mismatch (figure 6 (l–m)). It means that QD consists of pure InSb and does not contain arsenic (or a quite low As concentration).
The characteristic “tick”-like contrast observed in the experimental TEM image taken from big QD under the operating diffraction vector 400 occurs in simulated images of QD containing FD at the interface (figure 6 (a–d) and figure 6 (g–k)).

| Calculated contrast images | Experimental images |
|----------------------------|---------------------|
| QD with FD and 3% mismatch at $g=400$ and 0-40 | ![Image](a) ![Image](b) ![Image](g) ![Image](h) |
| QD with FD and 6% mismatch at $g=400$ and 0-40 | ![Image](c) ![Image](d) ![Image](j) ![Image](k) |
| QD with FD and without FD 6% mismatch at $g=220$ and 2-20 | ![Image](e) ![Image](f) ![Image](l) ![Image](m) |

Figure 6. Comparison of experimental and simulated InSb QD image contrast.

6. Conclusion
Some structural features of InSb QDs free-standing on InAs substrate were investigated by TEM supplemented with image simulation. The specific contrast features were observed in the plan-view diffraction images of big QDs (9–10 nm in height and 38–50 nm in diameter). To understand the origin of such distortions in the TEM image the model of InSb QD on InAs substrate was developed and used for calculations of the displacement field and the subsequent diffraction image simulation of InSb QD for the first time.

The shape of QD was established to influence insignificantly the magnitude of radial displacements. The insertion of a misfit defect (a partial Frank dislocation) into QD reduces the strain at the edges of QD almost by 30%.

The simulated images of QD correlate well with the specific “tick”-like contrast in the experimental electron micrographs in the case of a Frank dislocation inserted into the QD-substrate interface.

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