The features of moiré pattern on electron-microscope images of free-standing quantum dots containing dislocations

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Abstract. Simulation of moiré pattern arising on plan-view transmission electron-microscope image of nanoisland (quantum dot) containing dislocations was performed on the base of finite-element method. The presence of dislocations with a screw component of Burgers vector in the nanoisland is shown to be energetically unfavourable. On the contrary, edge dislocations allow relieving mismatch stress most effectively. The simulation results provide a means to determine the type of dislocation inside quantum dot by the specific features of the moiré pattern on transmission electron microscope image.

1. Introduction
Transmission electron microscopy (TEM) is one of the most common methods for studying microstructure of materials. The TEM image is known to be a projection of electron transparent volume of TEM specimen on registration plane along the incidence beam, therefore the image of an object within the area under study may overlaps with the image of another one. When two overlapping objects are crystalline and rotated relative to each other or lattice mismatched rotational or translational moiré pattern may appear on the TEM image. The translational moiré pattern is often observed on plan-view TEM images of free-standing quantum dots which, from standpoint of microstructure, are crystalline nanoislands (NI) on the surface of crystalline substrate with different lattice constant. If NI is coherent to the substrate the translational moiré pattern consists of periodic parallel fringes which appear due to elastic relaxation in the upper part of NI [1, 2]. However, when NI contains a defect it causes crystal lattice distortions which result in the significant modification of moiré pattern that is demonstrated in Figure 1.

Figure 1 (a, b). Plan-view TEM images of InSb/InAs nanoislands representing (a) moiré fringes and (b) complicated moiré pattern obtained under two-beam conditions with diffraction vector g=220 and 2-20, accordingly.
Contrast from dislocations on the plan-view TEM image appears to be overlaid with moiré pattern that hinders visualization and analysis of the dislocation type [3].

The purpose of this work is to study the impact of different dislocation types in NI on the appearance of the moiré pattern.

2. Experimental method

In order to determine the type of defect contained in the sample from plan-view TEM image, we carried out a simulation of moiré patterns. Moiré patterns received from simulation were used then for comparison with experimental ones. The modeling of images consisted of two stages:

1) Calculation of the displacement field according to the elasticity theory (isotropic case);
2) Calculation of TEM images using the Howie-Whelan equations on the base of calculated displacement field.

The nanoisland-substrate model was based on the results of TEM studies of InSb/InAs quantum dots (Figure 2, a) [3]. The faces of the island are formed by \{111\} planes. Experimental images have shown the presence of misfit dislocations at NI/substrate interface (Figure 2, a). Also NI contained a stacking fault.

To simplify the calculations, the shape of the nanoisland in NI-substrate model was taken as a truncated cone with an angle of 55° at the base (Figure 2, b). The simulated NI had a height of 7 nm and base diameter of 40 nm.

![Figure 2](image)

**Figure 2 (a, b).** (a) Cross-section HREM image of an InSb/InAs nanoisland containing dislocations and stacking fault; (b) the geometry of the nanoisland-substrate model.

The displacement field was calculated for a NI containing various configurations of dislocations:

- without dislocations;
- one Shockley dislocation (screw, Burgers vector \(b=a/6*[121]\));
- one Frank dislocation (edge, Burgers vector \(b=a/3*[111]\));
- two Frank dislocations (configurations with parallel and perpendicular Burgers vectors);
- one perfect 60°-dislocation (mixed, \(b=a/2*[101]\));
- two perfect 60°-dislocations (configurations with parallel and perpendicular Burgers vectors);
- one perfect 90°-dislocation (edge, \(b=a/2*[101]\));
- two perfect 90°-dislocations (configuration with parallel and perpendicular Burgers vectors).

Using the finite-element method we calculated general displacements and elastic stress fields in NI, which arise due to the NI and substrate lattice mismatch and the presence of structural defects. For the calculation, conventional equations of the elasticity theory for a homogeneous isotropic material were solved, namely differential equilibrium equations (1), Hooke’s law (2), and the Cauchy equation (3):

\[
\frac{\partial \sigma_{ij}}{\partial x_j} = 0
\]

(1)
\[ \sigma = E\varepsilon \]  
\[ \varepsilon_{ij} = \frac{1}{2} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \]  

where \( \sigma_{ij} \) – are the components of the stress tensor \( (i, j = x, y, z) \); \( \varepsilon_{ij} \) – are the components of the elastic strain tensor; \( u_i \) – are the components of the elastic displacements vector; \( E \) – is the elastic modulus (or Young's modulus, for InAs – 5.09 Pa, for InSb – 4.28 Pa).

The initial strain \( \varepsilon_0 \) in the NI was expressed as the compression of the NI lattice \( (a_{OD}) \) with respect to the lattice of the substrate \( (a_{sub}) \):

\[ \varepsilon_0 = \frac{a_{OD} - a_{sub}}{a_{sub}} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \]  

For the InSb/InAs system lattice mismatch is 6 %.

To take into account the contribution of the displacement field caused by dislocations, a thin material layer was introduced into the NI model with an initial strain determined by the direction and magnitude of the Burgers vector.

By solving equations of the elasticity theory the total elastic energy of the system was calculated for each configuration by:

\[ W_s = \sum_{i,j} \frac{1}{2} c_{ij} (\varepsilon_i - \varepsilon_{i0})(\varepsilon_j - \varepsilon_{j0}) \]  

where \( c_{ij} \) – are the components of the elastic modulus tensor.

The elastic energy depended on the type of defects introduced and their position in the NI. For each configuration, the dislocation position in the NI corresponding to the elastic energy minimum was determined (for example, for the perfect 90°-dislocation in Figure 3). These dislocation positions were used later to simulate the TEM images.

\[ \text{Figure 3 (a, b). Total elastic energy of a nanoisland-substrate system with one (a) and two (b) complete 90°-dislocations. The axes are the distance from the dislocation to the island center (x, nm) and the elastic energy of the system (*10^{-26} J).} \]  

Based on the calculated displacement field, a simulation of the TEM images of a coherent NI and NI containing various type dislocations was carried out. To describe electron diffraction in a crystal, we used the dynamic Howie-Whelan approximation, which contains two differential equations for the wave functions of the transmitted \( (\Phi_t) \) and diffracted \( (\Phi_d) \) beams [2]:
\[
\frac{d\Phi_s(z)}{dz} = \frac{\pi i}{\xi_g} \Phi_s(z) \exp(2\pi i \tilde{g} \tilde{u})
\]
\[
\frac{d\Phi_u(z)}{dz} = \frac{\pi i}{\xi_g} \Phi_u(z) \exp(-2\pi i \tilde{g} \tilde{u}) + 2\pi i \tilde{s} \Phi_s(z)
\]

where \( \tilde{g} \) is the diffraction vector, the diffraction vector \( g \) is perpendicular to the direction of incidence electron beam \( z \), \( \xi_g \) is the extinction length, \( \tilde{s} \) is the parameter of deviation (in our model \( s = 0 \)), \( \tilde{u} \) is the displacement vector obtained from the solution of the elasticity theory equations.

3. Experimental results

The calculation showed that after the elastic stress relaxation, the total elastic energy of the system decreases by 10 times, and after the dislocations introduction, by another 6-27%, depending on their type and quantity (Figure 4). Of the considered models, NI with two 90°-dislocations had the lowest energy. The minimum energy was obtained for symmetrically located dislocations relative to the island center and a distance between them was 8.5 nm. It correlates well with the experimental data – the distance between dislocations founded from cross-section HREM image of an InSb/InAs nanoisland was 8.2-8.8 nm (Figure 2, a).

It was also found that the introduction of the edge dislocation makes it possible to relieve the stresses in the system most effectively, and the introduction of the screw dislocation, on the contrary, leads to increase in the system energy for any arrangement in the island.

As a result of TEM image simulation, it was found that the introduction of dislocations in the NI leads to different distortions in the moiré pattern (Figure 4). It can be seen that moiré pattern of NI with dislocations undergoes considerable changes when rotating the diffraction vector \( g \). TEM image loses symmetry under the conditions \( g = 400 \) and \( g = 0-40 \). It is also seen that the introduction of dislocations in NI leads to appearance of additional moiré fringes in the image with the diffraction vector \( g = 220 \). At \( g = 2-20 \) moiré pattern for NI with edge dislocations does not differ from the images of coherent nanoisland, unlike the dislocations with screw component of the Burgers vector.

The introduction of dislocations in NI leads to bending of the moiré fringes at \( g = 400 \) and \( g = 0-40 \) for edge dislocations and at \( g = 2-20 \) for screw dislocations. The number of bend fringes is determined by the number of dislocation.

The obtained results showed that moiré patterns obtained under various diffraction conditions allow to identify the dislocation type in NI. For example, the perfect 60°-dislocation presence can be determined from the moiré fringes at \( g = 2-20 \). But to distinguish the perfect 90°-dislocation from the Frank partial dislocation occur very difficult from the moiré pattern.

The simulated images of NI with dislocations correlate well with experimental ones and explain the observed features of the moiré pattern (Figure 5).
| Nanoisland                                                                 | System energy, \(10^{-26}\) J | g = 220                                      | g = 400                                      | g = 2-20                                    | g = 0-40                                    |
|----------------------------------------------------------------------------|---------------------------------|---------------------------------------------|---------------------------------------------|---------------------------------------------|---------------------------------------------|
| Coherent NI                                                               | 8,30                            | ![Image](image1)                             | ![Image](image2)                             | ![Image](image3)                             | ![Image](image4)                             |
| NI with Frank particle dislocation                                        | 7,24                            | ![Image](image5)                             | ![Image](image6)                             | ![Image](image7)                             | ![Image](image8)                             |
| NI with two Frank particle dislocations with parallel Burgers vectors     | 6,53                            | ![Image](image9)                             | ![Image](image10)                            | ![Image](image11)                            | ![Image](image12)                            |
| NI with two Frank particle dislocations with perpendicular Burgers vectors | 6,51                            | ![Image](image13)                             | ![Image](image14)                            | ![Image](image15)                            | ![Image](image16)                            |
| NI with perfect 60°-dislocation                                           | 7,83                            | ![Image](image17)                             | ![Image](image18)                            | ![Image](image19)                            | ![Image](image20)                            |
| NI with two perfect 60°-dislocation with parallel Burgers vectors          | 7,66                            | ![Image](image21)                             | ![Image](image22)                            | ![Image](image23)                            | ![Image](image24)                            |
| NI with two perfect 60°-dislocation with perpendicular Burgers vectors     | 7,46                            | ![Image](image25)                             | ![Image](image26)                            | ![Image](image27)                            | ![Image](image28)                            |
| NI with perfect 90°-dislocation                                           | 6,89                            | ![Image](image29)                             | ![Image](image30)                            | ![Image](image31)                            | ![Image](image32)                            |
| NI with two perfect 90°-dislocation                                        | 6,05                            | ![Image](image33)                             | ![Image](image34)                            | ![Image](image35)                            | ![Image](image36)                            |

**Figure 4.** Simulated electron microscope images of coherent nanoisland and a nanoisland containing partial Frank dislocations, perfect 60°- and 90°-dislocations. The images are calculated for different directions of the diffraction vector g.
Figure 5 (a–h). Comparison of experimental (a – d) and simulated (e – h) TEM images from InSb nanoislands in the presence of a different type dislocations: with two Frank particle dislocations (a, e), with one Frank particle dislocation (b – c, f – g) and with perfect 90°-dislocation (d, h).

4. Conclusion
A model of NI with dislocations at the nanoisland/substrate interface is constructed. From the calculation of the total elastic energy minimum is obtained that the distance between dislocations in the NI is in good agreement with found experimentally. It confirms the consistency of the constructed model and the calculations performed.

It is shown that the presence of dislocations with a screw component of the Burgers vector in the NI is unlikely, since this is energetically unfavourable. Edge dislocations, on the contrary, allow relieving the system stresses most effectively and, therefore, happen in real objects more often.

The simulation results allow determining the type of dislocation inside quantum dot by moiré pattern on TEM image of NI in plan-view geometry. For example, the experimentally observed features of the moiré pattern from the InSb quantum dot are possible to explain by the presence of Frank particle dislocations and perfect 90°-dislocations in it.

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