Size Effects and Scaling in Misfit Dislocation Formation in Self-Assembled Quantum Dots

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ABSTRACT

Growth islands due to large mismatch strain arising in Stranski-Krastanow (SK) and Volmer-Weber (VW) film growth can be used to produce large arrays of quantum dots. This same mismatch strain may also cause misfit dislocations to form, presenting a quality control problem. Johnson and Freund (J. Appl. Phys. 81(9), 1997, p6081) developed a two-dimensional model of misfit dislocation nucleation in SK and VW growth islands whereby they predict a power-law relation between misfit strain, ϵ_m, and the minimum island size to nucleate a misfit dislocation, R_c: $R_c \propto \epsilon_m^{1/(\lambda-1)}$, where $\lambda < 1$ is a function of the island-substrate contact angle. This problem is treated here in three dimensions as an application of a numerical dislocation simulation using the finite element method to take proper boundary conditions into account. The predictions are analyzed in the context of the Johnson–Freund model, and modification of the power-law is shown to be necessary.

Keywords: dislocations, modelling, stress-concentration, quantum dots, self-assembly

1 Introduction

Stranski-Krastanow (SK) and Volmer-Webber (VW) epitaxial growth modes are being used as a tool to produce self-assembled quantum dots. Typical systems for this method of dot production include Ge/Si, GeSi/Si, InAs/GaAs and InGaAs/GaAs [1], [2]. The self-assembled dots form due to the lattice mismatch between the deposited material and the substrate. As a mismatch strain relief mechanism, the deposited material grows in the SK or VW mode (Fig. 1) where islands form, rather than in the F. van der Merwe mode, monolayer by monolayer. The same mismatch strain that drives three dimensional growth also drives the formation of defects such as misfit dislocations. Motivated by the two-dimensional model of Johnson and Freund [2], a three-dimensional model of misfit dislocation nucleation at the island corners is presented here as an application of a three-dimensional dislocation dynamics simulation with treatment of arbitrary boundary conditions using the finite element method [3], [4]. A key result of the two-dimensional model was a power-law relating the transition island radius at which a coherent growth island will form a misfit dislocation, R_c, to the island's mismatch strain, ϵ_m,

$$R_c = K\epsilon_m^{\frac{1}{\lambda-1}}, \tag{1}$$

where the coefficient and the exponent are obtained analytically. A major goal of the three-dimensional modelling is to verify that the power-law holds in three dimensions,

$$R_c = K_{2D}\epsilon_m^{\frac{1}{\lambda-1}} \Longleftrightarrow R_c = K_{3D}\epsilon_m^{\frac{1}{\lambda-1}}. \tag{2}$$

In addition to the technological interest in self-assembled quantum dots, there is a more general interest in developing models of dislocations with full treatment of boundary conditions. In the development of such models, it is useful to have a simplified quantitatively treatable example that is also scientifically or technologically significant, and misfit dislocation formation in epitaxial islands is such an example. It is also of interest to improve micro-scale models or develop multi-scale models. The example presented here can be treated by both micro-level models such as dislocation dynamics and atomistic models, thus making an important connection between these two scales.

An additional point of interest is the use of computationally more efficient two-dimensional models [5] in place of three-dimensional models. Therefore, in addition to making a connection between scales, it is important to make a connection between dimensions. The three-dimensional model of misfit dislocation formation is designed to be easily compared with the two-dimensional Johnson and Freund model.

2 Two-Dimensional Model

2.1 Growth and Dislocation Formation

The formation of misfit dislocations in coherent epitaxial islands is a transition driven by changing the scale of the system, and it fits inside the larger context of island growth which is also characterized by changing

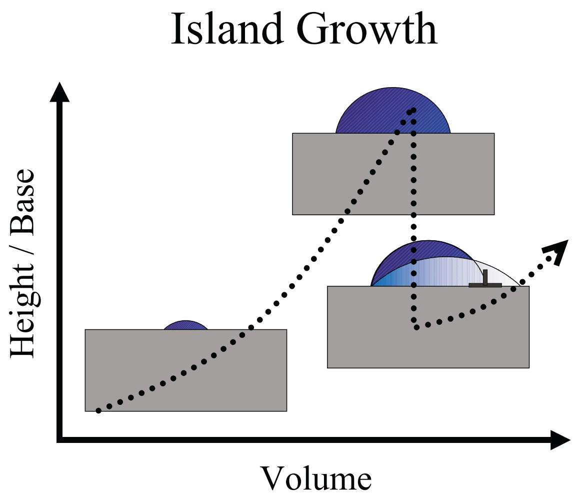

Figure 1: *Island Growth* Schematic of how epitaxial strained shape evolves with increasing volume. Initially, islands are flat in shape due to the effect of the surface energy. Later, as the island grows, mismatch strain causes the island to assume a taller shape. At a critical size, mismatch strain is relieved by misfit dislocation formation and a flatter shape is once again assumed. The process can continue with more growth and further misfit dislocations forming.

scales. At the simplest level of analysis, there are three important contributions to the energy of growth islands, each with a different scaling law. First, there is the mismatch strain energy that scales as volume $[L^3]$ and drives three-dimensional growth and misfit dislocation formation. Second, there are the surface and island–substrate interface energies that compete with the strain energy to drive two-dimensional growth and that scale as area $[L^2]$. Finally, there is the dislocation line energy that scales approximately linearly but more accurately as $[L \ln L]$. The progress of island growth is depicted in Fig. 1, but the part of interest here is only the misfit dislocation formation where at a large enough island radius, R, the island relieves its volume strain energy in exchange for dislocation line energy. This transition defines the critical island radius, R_c.

2.2 "Virtual" Dislocation Model

The energy scaling aids in understanding the mechanisms behind the transition from coherent to dislocated islands, but in the Johnson-Freund model, dislocation nucleation is modelled as kinetically controlled, and the same approach is adopted here. The Johnson–Freund model is equivalent to a "virtual" dislocation model, where a virtual test dislocation is placed an atomically small distance, d, from the island edge. The response of the test dislocation is used to determine whether a real dislocation would nucleate in a similar context. Approximations used by Johnson and Freund include assuming

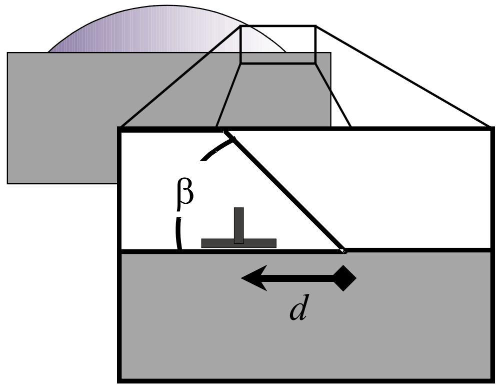

Figure 2: According to [2], dislocations nucleate at island corners where mismatch stress is concentrated. Singular mismatch and image fields are cut off by placing the dislocation the cutoff distance, d, inside the island. β is the contact angle between the island surface and substrate and determines the scaling exponent, $(\lambda - 1)$.

homogeneous isotropic linear continuum elasticity and restricting the island shapes to sections of circles.

The key result of the two-dimensional model was a power-law relating the maximum coherent (dislocation-free) island size to the mismatch strain. It is, however, more convenient to solve the inverse problem: what is the maximum mismatch strain a coherent island of a given shape and size can sustain before it nucleates a misfit dislocation? Johnson and Freund theorized that dislocations nucleate due to concentration of mismatch stress at the island corners (Fig. 2). Nucleation occurs when the singular mismatch stress term which scales with island size and mismatch strain as $\sigma_m \propto \epsilon_m R^{\lambda-1}$ is equal to the dislocation image stress, σ_I, which is due to interaction with the nearby free surface and which remains constant with island size. The result is a power-law

$$\epsilon_m^c = K R^{\lambda-1}, \tag{3}$$

where λ and K are functions of the island–substrate contact angle; λ is obtained from the theory of elastic wedges [6], and K is obtained from the analytic solution of the stress field throughout the island–substrate system [7]. It should be noted that this scaling cannot actually be observed since island shapes are not similar; they are a function of the size, surface energies and mismatch strains. However, the power-law is a useful analytic form to summarize the model predictions.

3 Three-dimensional model

In three dimensions, the islands are modelled as spherical sections corresponding to the two-dimensional circular sections. Unfortunately, the analytic methods used in two-dimensions are not available, and a numerical

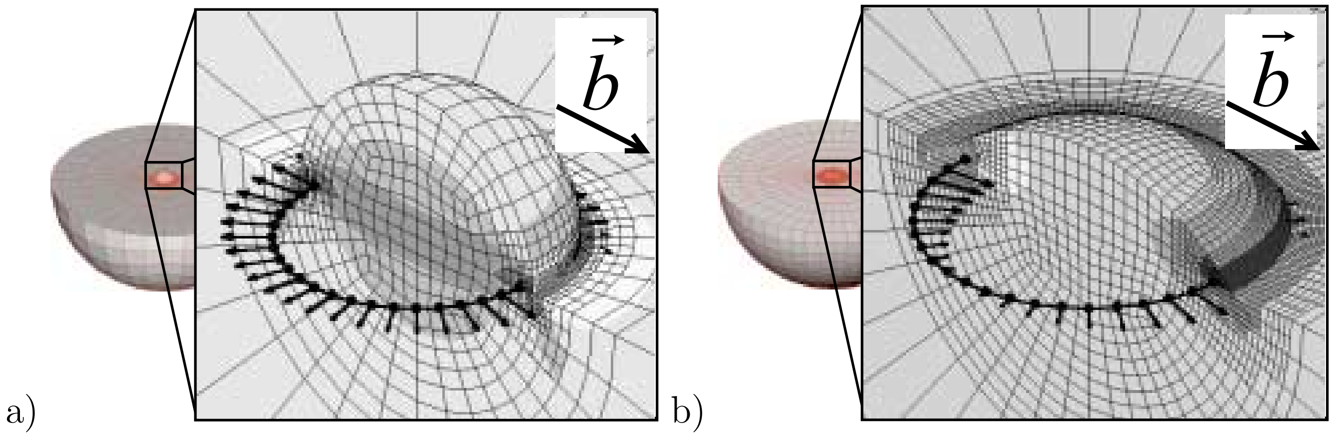

Figure 3: 90° (a) and 45° (b) island–substrate systems. Misfit dislocation Burgers vector is as shown. The image stress and resulting Peach-Koehler force is depicted in the 90° island (a), and the mismatch stress and resulting Peach-Koehler force is depicted in the 45° island (b). The shear stress component projected onto the misfit dislocation glide system is plotted. Dark/light shading indicates negative/positive stress values. The discretized virtual dislocation is also shown. The arrows indicate the local Peach-Koehler force due to the plotted stress field.

approach is required. To calculate the mismatch stress concentration and the dislocation image stresses, it is necessary to discretize both the dislocation and the space containing the island and substrate. This is done using one-dimensional first order finite elements for the dislocation and three-dimensional second order elements to discretize space [3], [4]. This discretization is done for two island configurations, one with 90° contact angle, and one with 45° contact angle (Fig. 3). The finite element method is used to calculate the mismatch stress and the image stress which compete to respectively cause and hinder dislocation formation. In Fig. 3a, one can see that the image stress field pulls the entire virtual dislocation towards the surface, thus hindering dislocation nucleation. In Fig. 3b, it is demonstrated that the mismatch stress pulls the part of the dislocation that relieves mismatch strain into the island.

The dislocation configuration shown is chosen to correlate closely with the two-dimensional model. As in two dimensions, the dislocation is everywhere parallel to the the island surface. In the future, the predictions using the chosen configuration will be compared with predictions using configurations similar to that used by Schwarz and Chidambarrao [8] where the virtual dislocation forms a small semi-loop intersecting the surface. Other than the initial configuration, the essential difference between [8] and the model presented here is the inclusion of the image stress field. With the chosen configuration, it can be seen in Fig. 3b that one part of the dislocation that has edge character most effectively relieves mismatch strain and is most strongly pulled into the island by the mismatch stress. This point on the virtual dislocation is tested as the nucleation criterion.

4 Results

By taking the ratio of the image stress to the stress per unit mismatch strain, the critical mismatch strain, ϵ_m^c can be found for an island of a given shape and radius, R. For an island with 90° contact angle, a power-law of the type predicted by Johnson and Freund is found, along with the predicted exponent, $(\lambda - 1) = -0.456$ (Fig. 4a). For the 45° dot, the power-law form with $(\lambda - 1) = -0.326$ is not justified at all (Fig. 4b). However, by including higher order terms, a much better fit is obtained. This fit has the form

$$\epsilon_m^c = \frac{\sigma_{M1}(R)}{\sigma_I(R)} = \frac{a_0 R^{\lambda-1} + a_1 R^{\lambda'-1}}{\sigma_I(\infty) + c_0 R^{-\lambda} + c_1 R^{-\lambda'}}. \quad (4)$$

a_0, a_1, c_0, c_1 are fit parameters, and the form and exponents, λ and λ', are justified by elastic wedge theory. σ_I and σ_{M1} are fit separately so that there are only two fitting parameters for each the numerator and denominator. The added terms are finite-size corrections. They are due to the finite dislocation cutoff, d. Setting a_1, c_0 and c_1 to zero, the power-law is recovered.

5 Discussion/Conclusions

A numerical model of misfit dislocation nucleation in epitaxial growth islands arising during Stranski-Krastanow and Volmer-Webber growth was implemented as an application of a numerical three-dimensional dislocation dynamics simulation where boundary conditions are enforced by means of the finite element method. This model predicts the maximum mismatch strain that can be sustained by a coherent growth island before a misfit dislocation nucleates as a function of the island radius,

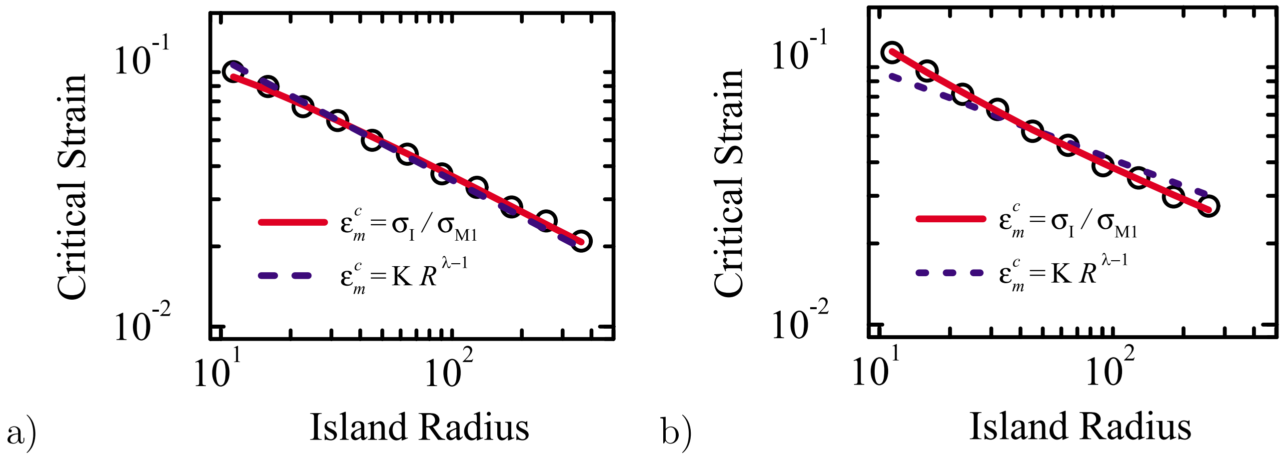

Figure 4: Log-log plots of predicted critical mismatch strain, ϵ_m^c, as a function of island radius, R. (a) and (b) shows data and fits for 90° and 45° contact angle islands respectively. Data is fit to power-law form, Eq. 3, and to extended form, Eq. 4. Strain is in dimensionless units of b/d (Burgers vector/cutoff), and radius is in units of d. A poisson ration of 0.3 was used.

R. It was constructed to be closely compared with a previous two-dimensional model [2]. The two-dimensional model was formulated analytically, assuming the asymptotic limit, that the dislocation core cutoff parameter, d, is much smaller than the island radius, R. This assumption was facilitated by the theory of elastic wedges [6], and leads to a power-law predicting the maximum mismatch strain for a given island radius or the maximum island radius for a given mismatch strain. The present three-dimensional model did not agree with this power-law, but still yielded predictions that were consistent with elastic wedge theory. However, higher order terms must be included that account for the finite size of the growth island, *i.e.* that the asymptotic limit had not been reached for the modelled islands.

The interpretation of the model results is somewhat difficult. How literally should the model be taken? Are the finite-size corrections discussed here an artifact of the model? These questions can be answered from a purely scientific and a practical point of view. One can argue that the observed finite-size effects is an artifact of the contrived "virtual" dislocation configuration. Dislocations nucleate at the island edge, not d inside. Therefore, the distance d should only be used to cutoff the most singular term, and only the most singular term should be kept, thus reproducing the power-law of Johnson and Freund. The problem with such an interpretation is that any corrections to linear elasticity will be similar in size to the finite-size correction observed here and may couple to the higher order stress fields in a similar manner. Thus, the deviation from the power-law can be seen as an estimate of the importance of the higher order effects and a reasonable formalism by which such effects can be included into a continuum level picture of an essentially atomic scale process. Furthermore, if one is interested in the further evolution of the dislocation, continuum level simulations can be very advantageous. For these purposes, it will be necessary to have on hand a dislocation nucleation criterion which will be consistent with the further evolution. For such an application, it will be necessary to interpret the predictions literally.

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