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Collective formation of misfit dislocations at the critical thickness for equilibrium nanowire heterostructures

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ABSTRACT

In this work we model the evolution of strain energy during different growth stages of heterostructure nanowires. We find that the minimum energy configuration changes abruptly from fully elastically strained to partially relaxed at the critical thickness. The transition at the critical thickness, when the crystal growth is close to equilibrium, is associated with a collective formation event of misfit dislocations. These insights are based on a technique developed to simulate misfit dislocations in a finite element framework, incorporating both elastic and plastic relaxation in a stationary heterostructure. We argue that these results have general relevance for mismatched heterostructures.

1. Introduction

The presence of misfit dislocations (MDs) in epitaxial heterostructures alters the structural, mechanical, optical and electronic properties. The stress induced from elastic strain, originating from the mismatch between the lattice parameters of a growing thin film and the substrate, acts as a driving force for the formation of structural defects when the critical thickness is exceeded. Understanding the mechanisms that lead to formation of MDs at the critical thickness is therefore an important step towards finding the limits of coherence for engineered epitaxial devices. The transition from elastic strain to plastic relaxation at the critical thickness in thin films has for these reasons been studied intensively in the past decades, and several general models for the formation of MDs have been proposed and tested [1–13]. Most of these models examine the limit for nucleation of a singular MD in an otherwise elastically strained and pseudo-infinite planar thin film, implicitly assuming a singular MD nucleation event.

A challenge in simulating the general case of MD formation for a simple interface (pseudo-infinite system) is finding boundary conditions which reduce the model to a finite size, while not affecting the physics. Using for instance symmetric or periodic boundary conditions will hinder modeling MDs as ‘additional’ or ‘missing’ crystal planes in a pseudo-infinite film, since the outer boundaries need the ability to move freely. For this reason, we choose Selective Area Growth (SAG) as a model system, given that a full SAG nanowire (NW) geometry can be modelled to avoid challenges associated with boundary conditions for pseudo-infinite systems. Additionally, SAG offers the opportunity to design complex networks in the plane of the substrate, which makes it a promising platform for production of scale-able devices. For this reason, SAG methods for synthesis of NW heterostructure networks have received increasing interest in the field [14–21].

Meanwhile, the initial growth stages of SAG NWs closely resemble the trends observed from planar films, and studies of SAG allow us to probe the mechanisms for MD formation in general. We note the important difference between a SAG structure grown on top of a mesa-like buffer which will have dilatational and rotational degrees of freedom, and a bulk section of a planar structure which is constrained due to the surrounding bulk. These degrees of freedom give rise to overhangs with rotation of crystal planes, further discussed in section 2.

The non-trivial morphologies found in SAG NWs may be difficult to handle in a purely analytical framework, but they are easier to define with the finite element method (FEM) software employed in our model. The morphologies add an interesting study of interplay between strain relaxation along different interfacial directions, and compared to large planar films, the previously mentioned additional degrees of freedom may alter the critical thickness.

From studies of the free-standing Vapor-Liquid-Solid (VLS) radial type NWs, we know that critical thickness can change dramatically

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[22–24] due to additional degrees of freedom from the change in morphology, with a limited NW radius in the VLS case. Theoretical models explain this phenomenon from comparison of a fully elastic model and a model exhibiting a single pair of perpendicular, interfacial MDs [25, 26]. The models predict how the critical thickness should scale with parameters such as NW radius and mismatch, and these are nicely summarized in a review by Kavanagh [27]. Unfortunately, the VLS method lacks reliable ways of forming more complex NW networks in an experimental setting, and so our choice of SAG lets us work with a promising method somewhere between the planar thin film and the VLS NWs.

Starting with the simplest case in section 2, we study purely elastic strain relaxation in SAG NWs, to characterize the strain energy evolution for different growth stages. The shapes studied are those observed in experiments [14–16], appearing to be approximately equilibrium shapes given lowest surface energy configuration for the NW cross section. Building on these examinations, in section 3 we subsequently study elastic and plastic relaxation in SAG NWs with dislocations as ‘additional’ crystal planes. The FEM simulations are carried out for a wide range of mismatches and MD densities, finding the equilibrium configurations at the critical thicknesses from comparison between the elastic and plastic configurations. We study elastic strain relaxation of a (110) orientated NW on a (001) substrate and buffer, finding a first order-like transition as a function of the extensive parameter film thickness, from a fully elastic configuration to one with a network of MDs formed collectively - a conclusion expected to carry over to other hetero-structures subject to in-plane strain caused by a lattice mismatch. In later sections it will be discussed how dislocation formation observed experimentally in literature, for instance in islands, does not represent a SAG system of these conditions, and we propose an experiment to investigate our simulated predictions empirically. Lastly, we analyze the stationary MD densities and show critical thicknesses and MD densities as functions of mismatch, finding a weak dependence on mismatch, suggestive of a stronger dependence on other parameters, e.g. morphology. This further allows for study of different fractions of plastic relaxation as opposed to elastic.

2. Purely elastic strain relaxation

Fig. 1a presents a stereographic projection of the typical NW types available on (001) substrates. The purely elastic simulation features a translationally invariant segment, using three symmetry planes as illustrated in Fig. 1b along with an example of a preliminary mesh. We assume for simplicity that the buffer (mesa-like structure) is relaxed to the underlying substrate. See Supplementary Material for information on strain implementation and calculation of strain energy density (SED) in the FEM software COMSOL [28].

Varying geometric parameters allows for analysis of the dependence on dimensions, shape and size of the structure. In an actual growth environment these parameters can be controlled by lithographic patterning and adjusting growth time, flux compositions and temperature. See Supplementary Material for example results of varying size effects.

These simulations are carried out for an InAs NW on an InGaAs buffer grown in the ⟨100⟩ direction with {110} side facets (see Fig. 1a). In Fig. 1c we show three different variations of this
morphology, where stage I represents a transport channel grown from a thin layer on the buffer to a full pyramid shape with fully formed facets. We regard this shape to be an approximation of the lowest-energy shape as dictated by the surface energy densities associated with different crystallographic orientations.

The other morphologies represent overgrowth, where stage II A) specifically represents a layer beginning to form on a fully grown stage I NW, and the transition is marked with an arrow in Fig. 1c. We conclude that for our model, overgrowth contributes to total strain at a lower rate than stage I growth. We also see that stage II B) can accommodate higher mismatch for lower transport channel volumes, but also that this becomes unfavorable at larger channel volumes. All three stages exhibit sublinear increase in total strain energy for very large transport channel volumes. We note that the simulated interface area is kept constant between these morphologies for comparison.

In Fig. 1d we investigate stage I and stage II B) and the strain energy dependence on the thickness of the InAs layer. For stage II B) we consider only half of the wire cut along the axial direction with suitable symmetry conditions, re-dimensionalized so the interface area is equal for both morphologies, considered a normalization to interface area. We further compare to a free-standing NW with identical interface area, which is not constrained by symmetry planes. We find this free-standing type NW to be favorable in comparison to SAG at all thicknesses, which is expected since the free-standing NW is less constrained. We note that the graphs for stage I and stage II B) cross each other at approximately 11 nm in panel 1d. This is due to stage I gaining less volume per unit layer thickness, as the triangular cross section becomes thinner towards the top. Hence, this crossing is absent in the panel 1c displaying the energy as a function of transport channel volume.

All cases compare favorably to the planar growth of thin film on a planar substrate, which is shown as the dashed line in panel 1d. The thin film is simulated as a rectangular structure with symmetry planes on all four sides to emulate a pseudo-infinite plane. For the thin film case, a mismatch of 1.8% (InAs/In0.75Ga0.25As) corresponds to a critical thickness of 4.8 nm according to Matthews model [6], depending on the exact Burgers’ vector in the strained top layer. This highlights the morphological advantages of a SAG buffer, where the NW can relax strain by a rotational degree of freedom which has also been shown by other authors [14].

3. Plastic strain relaxation

As the crystal volume of a lattice mismatched heterostructure increases during growth, the excess energy increases until a critical thickness is reached, at which point MDs are formed to lower the total energy, most often edge dislocations along the interfaces [14]. We are interested in understanding the limits of fully elastically strained heterostructures as a function of shape, volume and composition (which defines the lattice mismatch).

In a simple 1-dimensional case, the spacing between dislocations is generally given by \( d = |b|/(\delta - \epsilon) \), with \( |b| \) being the length of the Burger’s vector, \( \delta \) being the mismatch and \( \epsilon \) being the average remaining elastic strain. Therefore ‘full plastic relaxation’ corresponds to \( \epsilon = 0 \) with a corresponding density of dislocations. However, there will be a certain fraction of elastic vs. plastic relaxation that will display the minimum strain energy, and we can not in general expect full plastic relaxation. As such, we need to examine configurations with different MD densities in order to determine the critical thickness and the associated equilibrium configuration. As a first approach the dislocations are assumed to be equidistant, but as discussed in Supplementary Information the distribution of strain may not be spatially uniform. Should material concentrations of e.g. In and Ga also be spatially non-uniform, it may be expected that dislocations form a non-equidistant network. This can be further compounded by edge effects for finite size systems, where the relaxation behavior in bulk may differ from regions near free boundaries.

Fig. 2d shows a model of a (110) type NW with edge MDs of in-plane Burger’s vectors of type \( \langle \frac{1}{2} 110 \rangle \), where \( a \) is the lattice parameter. The dislocations are here modeled as planes in the buffer with thickness matching the length of the Burger’s vector and positive unity strain (tensile, normal to the planes) simulating ‘additional’ crystal planes due to misfit dislocations at the interface. This ensures the correct effect of MDs in the transport channel, while leaving artifacts in the simulations of the buffer and substrate where the ‘additional’ planes should not in general be strained relative to the surrounding material far from the interface (see Fig. 2d and 2f). We emphasize that this method works for finite-size structures such as the SAG morphologies chosen here, and conversely this method is incompatible with simulations of pseudo-infinite systems using fixed position symmetry planes, because they inhibit the strain-relaxing displacement generated by the additional crystal planes.

An alternate method simulates the same dislocations as ‘missing’ planes in the transport channel with negative unity strain (Fig. 2e). This creates the correct effect in the buffer and substrate, while the unwanted artifacts are now found in the transport channel. The dislocation planes end at the NW-buffer interface where the dislocations are situated [14]. In panels 2a-e we compare these two methods in two dimensions to the analytical solution of stress fields associated with dislocations at the interface of two semi-infinite solids in 2D as found by Head [29], which combined with mesh convergence studies give us confidence that we have reached a sufficient resolution. While we find a clear convergence in the elastic simulations at cell sizes of 10–20 nm, the characteristic cell size near the dislocation cores is on par with the length of the Burger’s vector (\( b \approx 0.4 \) nm).

The two methods can be combined graphically to yield the results shown in Fig. 2h, with a complete solution being to run both simulations and consider in each only the correctly affected domains. Since by far the biggest contribution to the strain energy (\( \approx 99\% \)) is found in the transport channel on top of the buffer, we continue only with the MD model first described (Fig. 2d).

As seen in figure 2a-c, a small region around the dislocation cores becomes highly strained. As a result, the elastic theory employed for evaluation of the SED is locally no longer valid, and an alternate method is needed if one wishes to evaluate the strain energy included in regions near the dislocations. We are concerned with the total strain energy in the transport channel (NW), which comprises by far the dominant energy contribution compared to the buffer and substrate. In order to evaluate the ‘invalid regions’ mentioned above, we modify the ‘Volterra method’ [1] or ‘empirical method’ [30], excluding slightly larger cylindrical cores of radius \( r_{\text{core}} = |b|/2 \), with \( b \) being the Burger’s vector, arguing that the dominant energy contribution inside this range is due to the rearrangement of chemical bonds. We account for these bonds by adding an energy per unit dislocation length from the melting approximation given as \( E_{\text{MD}} = GB^2/2a \) where \( G \) is the shear modulus of the transport channel, in this case InAs. This is likely an overestimate of the dislocation line energy density, which we will reflect upon below. Our simulations were carried out using models of the type in Fig. 3a (interface width 125 nm, channel length 4 \( \mu \)m, with ‘transverse’ dislocations as equidistantly spaced ‘additional’ planes in the substrate and then buffer. The orientation was chosen with \( (110) \) along the NW axis and \( (111) \) type side facets (see Fig. 1a). The material composition of the buffer was varied with corresponding changes in material parameters following Vegard’s Law, choosing to emulate mismatches from 1% to 4% corresponding to InAs on In\( _{0.75} \)Ga\( _{0.25} \). As with \( x \) between 0.86 and 0.44.

In all cases the composition within each region (substrate, buffer, NW) was chosen as spatially uniform for simplicity, and the distribution of dislocations as equidistant to simulate an equilibrium layer-by-layer growth as opposed to e.g. island growth. Note that the condition of layer-by-layer growth will likely be broken for the higher end of mismatches simulated here. The thickness of the thin film was varied (akin to the method employed for Fig. 1d) to emulate different stages of
approximate layer-by-layer growth throughout.

4. Results

Fig. 3b shows the strain energy of plastic configurations in units of the strain energy for the purely elastic configuration as a function of film thickness for a mismatch of $\delta = 2\%$. See Supplemental Material for similar results for other mismatches.

From closer examination we notice the first plastic configuration to become favorable is not the one with a singular dislocation. This is a general feature across the mismatches examined, but more notable for higher mismatches. This suggests that onset of misfit dislocations at the critical thickness is a first order-like transition in an extensive parameter, to a state which becomes stable when a certain equilibrium MD density is achieved. The transition from elastically strained to a partially plastically relaxed state is characterized by both a critical thickness and

Fig. 3. Model and strain energy as function of film thickness. a) Model along with a zoom section displaying a preliminary mesh with increased density near the dislocations. b) Total strain energy of different plastic configurations in units of the elastic configuration at the corresponding film thickness for a mismatch of $\delta = 2\%$. Note that the first plastic configuration to become favorable compared to the elastic case displays a network of MDs rather than one singular MD. The dimensions of the interface in the model are 125 nm by 4 $\mu$m.

Fig. 2. FEM simulations of dislocations. Top row: XY-components of stress fields caused by an edge dislocation at the markers. a) Analytical solution by Head. b) and c) Results from 2D FEM simulations with dislocations modeled as a planes indicated by markers, with strain (+1) and (-1) respectively. Panel c) additionally shows the region near the core excluded from energy calculations, size greatly exaggerated for clarity. d) and e) 3D FEM models of $(110)$ type NW (substrate not shown) with $\frac{1}{2}(110)$ dislocations modeled as vertical planes with strain (+1) and (-1), respectively. f) and g) Horizontal components of strain resulting from models d) and e) with 3% mismatch (InAs/In$_{0.58}$Ga$_{0.42}$As buffer). h) Composite image of results from the two models in panels f) and g). Colorbar applies to a-c) and f-h).
a characteristic density of MDs. We note that a lower value for the dislocation line energy density would lead to configurations with a higher MD density being more energetically favored. Thus, our results for the characteristic density of MDs at the critical thickness should be considered a lower bound, based on the melting approximation mentioned in section 3 above.

In this study, we have limited ourselves to a maximum of one axial dislocation running along the center of the NW, and note that a more complete examination would have to deal with a much larger parameter space of both number and positions of axial MDs.

We also note the general feature that higher mismatches tend to favor configurations with more MDs. For the 1% mismatch case the equilibrium configuration at the critical thickness has only transverse dislocations (MD), which could be interesting for engineering of MDs in heterostructures. However, for the mismatches of 2%, 3%, and 4% the equilibrium configurations at the critical thicknesses have both the axial and transverse dislocations present. This could prove useful for analysis, as the lack of an axial MD from cross-sectional TEM of a high mismatch structure could indicate that the entire structure is elastically relaxed.

The question of MD configuration at the critical thickness is examined further in Fig. 4a which shows the points where different configurations become favorable compared to the purely elastic case. For a given mismatch the lowest of the critical thicknesses is the predicted equilibrium critical thickness, and a specific MD density is associated with this.

The guidelines in Fig. 4a are fits to the form $h_c = a n_{\text{disl}} + b + c/(n_{\text{disl}} + d)$, where $n_{\text{disl}}$ is the number of dislocations. The minima from Fig. 4a (marked) are extracted from the fits and plotted in Fig. 4b along with the associated number of MDs and new fits of the simpler form $h_c = a/(\delta + \beta)$ where $\delta$ is again the mismatch.

The variables $a_{\perp} = 22.8 \text{ nm, } \alpha_{\perp} = -0.26\%, \alpha_{||} = 12.1 \text{ nm, and } \beta_{||} = -0.69\%$ are found from the fits for configurations without and with the axial dislocation, respectively. For mismatches below $\delta = 1.2\%$ (marked by an arrow in Fig. 4b), the configuration at the critical thickness shows no axial dislocation. Interestingly, the density of transverse MDs at the critical thickness only increases slightly while increasing the lattice mismatch from 1% to 4%. In the entire range, spacing between MDs is found to be around 200 nm, corresponding to a partial plastic relaxation of approximately 0.2% axial misfit strain (emphatically not 0.2% of the misfit strain). In the case of 2% mismatch we thus find the fraction of plastic relaxation to be $1/10$. The weak dependence on misfit strain and low value suggests the equilibrium configuration at the critical thickness is more dependent on e.g. morphology, and the melting approximation overestimating the dislocation line energy density. Further work for investigating this is discussed below.

The fit forms and variables found suggest a divergence of the critical thickness at a mismatch of a quarter of a percent. To ensure a fully elastic growth in stage 1 however, it is only necessary for the critical thickness to be larger than the thickness of the transport channel grown. Due to the geometry chosen for the model, the stage 1 transport channel can grow to a maximum thickness of $h_{\text{max}} = w/2$, where $w = 125 \text{ nm}$ is the width of the interface. In our model this can be accommodated elastically at a mismatch of $\delta = 0.52\%$, meaning a buffer of In$_{0.93}$Ga$_{0.07}$As. While a buffer this high in In concentration may cause issues in containing the wavefunction to an intended transport channel, we note the height of 125 nm is only an example, as are the chosen elements of In, Ga and As. We note that while all the critical thicknesses quoted are specific to the morphology, dimensions and materials, the method presented can be used for examination of other combinations and structures.

5. Discussion and conclusion

We find the mechanisms of strain relaxation in lattice-mismatched SAG NWs to be distinctly different from reports in literature on planar heterostructures and on free-standing NWs [25, 26]. Compared to planar thin films, the additional elastic relaxation for SAG stems from the rotational degree of freedom for relaxation transverse to the NW axis which in principle can overshoot the bulk relaxed values, giving additional room for elastic relaxation along the NW axis through the Poisson effect. We identify three different growth stages, all of which are energetically favorable compared to planar thin film growth, and all of which are sublinear but quickly become approximately linear with different dependencies on layer thickness, favoring stage II A).

Our findings establish a relationship between transport channel layer thickness and MD density for a SAG NW morphology, like that between NW radius and misfit percentage as found by Ertekin et al. [25] and Glas [26] for VLS NWs. This highlights the difference between SAG and free-standing NWs. For comparison we quote the experimentally found critical thickness of $h_{\text{film}} = 1.71 \text{ nm}$ for planar thin film growth of InP on GaAs at 3.8% lattice mismatch [31]. This further indicates the ability for elastic relaxation in SAG NWs as somewhere between the highly constrained planar thin films and the nearly unconstrained free-standing NWs of VLS.

We compare to previous efforts in using FEM to analyze misfit dislocations such as Ye et al. [32], which also use initial strain as a numeric technique, but fails to include both elastic and plastic relaxation simultaneously and naturally does not take the spatial freedoms and lattice directions of SAG NWs into account. Therefore, we believe our methods are novel and relevant for finite-size morphologies across materials, and the results can be compared to physical samples by analysis of e.g. atomic resolution TEM with GPA [33, 34]. It is appropriate to

![Fig. 4. Fitting critical thicknesses. Panel a) shows the predicted critical thicknesses, assuming a set number of dislocations for each of the four mismatches. Markers denote minima from fits. Panel b) shows the minima from a) for each mismatch ($\delta$) along with the corresponding number of dislocations found from fits. Fit types are described in the main text. The dimensions of the interface in the model are 125 nm by 4 nm.](image-url)
to observe singular MD formations in island growths, with accompanying changes in growth velocity immediately before and after nucleation events. They provide rudimentary theoretical considerations with equilibrium assumptions, but we consider their model incomplete as it does not include strain energy as a driving force and does not explain the preference for island growth over layer-by-layer. We understand that in our study we have specifically simulated an equilibrium environment and created a rigorous framework incorporating strain energy and additional references. We also emphasize the model employed in this work specifically applying to layer-by-layer growth.

A later study by Merdzhanova et al [36] uses a more time-efficient AFM method, noting higher growth temperatures consistently giving rise to more frequent and higher numbers of singular nucleation events, as well as a dramatic change in the size of islands. Particularly the balance between coalescence of neighbouring islands growing simultaneously, as opposed to islands growing smaller when located in the depletion zone of a larger island, is affected. They do not present a complete theory for this behavior but suggest a scenario qualitatively involving material intermixing.

We note these points to be different from the assumptions within our model, and that temperature dependencies agree well with a non-equilibrium nature of the process. As such we find the discrepancies to our model as expected, and they underline the potential in understanding the equilibrium and non-equilibrium divide in phenomena and behavior. In particular, the role of material intermixing could be introduced and studied within our framework, posing an immediate candidate for further work. Among other things it would affect the spatial distribution of strain, which may cause the optimal network of dislocation to be non-equidistant.

Additionally it would be possible to design an experiment using low growth rate, high temperatures and low mismatch, which would be a better representation of the simulation in reality. High thermal energy presumably allows for breaking of kinetic barriers and avoiding local minima, approaching our predicted global minimum of collective formation, and low mismatch with a low growth rate allows for true layer-by-layer growth, seeing as the island growth seen in literature is not well-represented in our current model. We propose using in-situ observation of strain in the layer-by-layer growth, for instance using a curvature tool as done by Gilardi et al [37], to investigate to which degree the stationary (non-time dependent) assumptions of the model are correct, when the other conditions as described above are fulfilled. We expect the results to be strictly different from the discussed literature, where conditions differ.

In summary we present a novel method for introducing plastic relaxation from MDs as localized FEM features in heterostructure simulations, allowing an examination covering different morphologies and MD densities. This leads to our prediction of collective rather than singular onset of MDs at the critical thickness, which is a novelty. For SAG NW growth in stage I, we find critical thicknesses of $h_t$,1% = 30.7 nm, $h_t$,2% = 9.6 nm, $h_t$,3% = 4.8 nm, and $h_t$,4% = 3.3 nm for 1%, 2%, 3%, and 4% mismatch, respectively, as summarized in Fig. 4. In all cases examined we find that collective formation, as a first order-like transition as a function of film thickness, is favorable compared to singular onset. For mismatches below $\delta_t$,1% = 1.2% we find that the equilibrium configuration shows only transverse dislocations, while for mismatches above the value both axial and transverse dislocations are expected. At the critical thickness, the density of MDs suggests initial plastic relaxation of approximately 0.2% misfit strain in the range of misfits examined. Further studies are needed in order to examine in more detail how this initial plastic relaxation changes with morphology, compositions and different values for the dislocation line energy density. We argue that our results are relevant for general heterostructures, predicting that a first order-like transition in our finite-size case carries over to e.g. a pseudo-infinite planar heterostructure.

CRediT authorship contribution statement

**Thue Christian Thann:** Conceptualization, Methodology, Validation, Formal analysis, Investigation, Visualization, Writing - original draft, Writing - review & editing. **Tobias Sørkjaer:** Conceptualization, Methodology, Validation, Formal analysis, Investigation, Visualization, Writing - original draft, Writing - review & editing. **Sergej Schuwalow:** Formal analysis. **Peter Krogerstrup:** Supervision, Funding acquisition, Conceptualization.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

Data will be made available on request.

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Appendix A. Supplementary data

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