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Full characterization and modeling of graded interfaces in a high lattice-mismatch axial nanowire heterostructure

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I. INTRODUCTION

Semiconductor nanowires offer the unique opportunity to realize coherent axial heterostructures which associate materials having vastly different lattice parameters [1–3] or crystalline structures [4,5]. In addition, the nanowire geometry can be adjusted to finely engineer its photonic and electronic properties [6–10]. Brought together, these appealing features promise a wealth of applications in optoelectronics [6,10].

Prototypes of laser diodes [10,11] and quantum light sources [12], white light emitting diodes [13,14], solar cells [7–9], and high efficiency photodetectors [15,16] were recently developed in nanowire heterostructures.

Today, numerous material combinations have been explored to realize axial nanowire heterostructures [4,17–19]. In all cases, the control of the strain level around the interface is critical, because above a certain threshold, elastic energy is plastically released via the formation of dislocations [20,21]. Dislocations act as recombination centers for photons and electrons and degrade the materials properties by reducing the light emission or detection efficiency, and the carrier density. One solution to realize defect-free interfaces is to reduce the nanowire lateral dimensions. Indeed, for a given couple of materials A and B, and thus a given lattice mismatch, there exists a critical nanowire radius below which coherent growth of B on top of A is possible regardless of the height of B.

The mismatch strain is then partially and elastically relaxed at the nanowire sidewalls. This critical radius, which separates the domains of elastic and plastic strain relaxation, is well understood in the case of a sharp interface [20,22].

However, sharp interfaces still present a large residual strain, which may be detrimental for applications. For example, the electron-hole wave-function overlap decreases in InAs/GaAs quantum dot nanowires, resulting in longer exciton lifetimes and nonradiative recombination [23]. High interface strains also lead to potential barriers for charge carriers, which limits their transport in quantum dot nanowire devices [24]. Moreover, a high interfacial strain can enhance piezoelectric effects which degrade performances of nanowire based solar cells [25]. Finally, in the case of large lattice mismatch, coherent growth is only possible for a very limited range of radii, severely limiting the accessible geometries. As an example, for a lattice mismatch of 7%, the critical radius is as low as 10 nm. Implementing graded interfaces, with a smooth chemical profile, offers a solution to overcome these limitations. Despite a few works [25–27], this strategy remains to be thoroughly explored.

In this work we investigate both theoretically and experimentally graded interfaces in axial nanowire heterostructures. A theoretical model specifies the wire radii compatible with coherent growth for various interface lengths and lattice mismatches. While we specifically consider the representative case of interfaces whose chemical profile is described by an error function, these calculations could be easily extended to...
other profiles. We compare these predictions to experiments realized with the highly mismatched InAs/GaAs material system. The nanowire heterostructures are grown by molecular beam epitaxy (MBE), using a gold droplet as a catalyst. We perform a complete characterization of the interface: the chemical profile is obtained by energy dispersive x-ray spectroscopy (EDX) analysis, while the structural characterization is conducted through high-resolution transmission electron microscopy (TEM). In the case of coherent growth, the maps of the mismatch strain obtained by geometrical phase analysis (GPA) are in excellent agreement with finite element simulations. This analysis confirms in particular that mechanical strain is largely reduced by interface grading. More generally, interface grading constitutes a novel tuning knob to adjust the physical properties of nanowire heterostructures.

II. RESULTS AND DISCUSSION

As schematized in Fig. 1(a), we consider an infinitely long nanowire oriented along the \( z \) direction, with a circular section of radius \( R \). The nanowire features a graded interface between two materials A and B. They have different lattice parameters \( a_a \) and \( a_b \), which leads to the lattice mismatch \( \varepsilon_m = (a_b - a_a)/a_a \). The interface is centered at \( z = 0 \), and the fractions \( n_A = 1 - n_B \) of the two species follow a smooth profile. For small-scale compositional gradients (on the order of the nanowire diameter), the interface chemical profile is usually well represented by an error function [28–30]. Specifically, we assume:

\[
n_B = \frac{1}{2} \left[ 1 + \text{erf} \left( \frac{z}{L} \right) \right] \quad \text{with} \quad \text{erf} \left( \frac{z}{L} \right) = \frac{2}{\sqrt{\pi}} \int_0^z e^{-u^2} du,
\]

where \( L \) measures the interface length [Fig. 1(b)]. For a given couple of materials, and in the framework of linear elasticity, the amplitude of the strain generated around the interface is controlled by the normalized interface length \( \alpha = L/R \). Intuitively, one thus expects that the critical radius \( R_c \) below which coherent growth is possible increases with \( \alpha \). To determine \( R_c \) for a given lattice mismatch and interface profile, we compare the energies of the system in two states, namely state (1) with a purely elastic relaxation of the mechanical strain, and state (2) with a single dislocation segment lying perpendicular to the nanowire axis. The critical radius is then defined as the radius above which state (2) has an energy lower than state (1). In state (1), the system energy reduces to elastic energy. This quantity is evaluated with finite element software, assuming mechanical isotropy for the materials. The energy in state (2) is obtained with the method of Spencer and Tersoff considering an edge dislocation [31,32]. More details on these calculations are given in Sec. S1 of the Supplemental Material [33]. Figure 1(c) gives the variation of the critical radius \( R_c \) as a function of mismatch \( \varepsilon_m \), each curve corresponding to a given normalized interface length \( \alpha \). Alternatively, the curves can be read as giving the critical mismatch (below which the system should remain coherent) as a function of nanowire radius. They thus separate, in the \( R-\varepsilon_m \) plane, the domains of elastic/plastic (below/above) growth. The case \( \alpha = 0 \) corresponds to a sharp interface. Strikingly, increasing \( \alpha \) leads to a dramatic increase in \( R_c \). Composition-graded interfaces thus considerably extend the domain where coherent growth is possible: an interface length over tens of nanometers is sufficient to completely suppress the constraint on the nanowire dimensions. This is in contrast to thin film epitaxy [34] where composition-graded buffer layers need to be larger than hundreds of nanometers and to selective area growth of planar nanowires where composition-graded interfaces of tens of nanometers are not sufficient to release the mechanical strain and suppress misfit dislocations at the interface [35]. These results, obtained with the parameters of the InAs/GaAs material system, capture the general benefits of interface grading. Furthermore, they can be used to estimate \( R_c \) for graded interfaces involving other material systems. When precise values are required, one can employ the same method to determine \( R_c \) using the specific
In this work we have grown several nanowire heterostructures to form either sharp or controlled graded interfaces [38–40]. Interface grading occurs in particle-seeded nanowire systems and is attributed to the solubility of the growth species [36]. The nanowire radius is determined by the catalyst dimensions, while the interface length can be controlled by adjusting the growth conditions. The evolution of microscopic and mechanical properties of the materials as well as the actual composition profile of the interface is very well reproduced by an error function. The fit of the data to Eq. (1) leads to an interface length \( L = 5.9 \) nm.

FIG. 2. InGaAs/GaAs axial nanowire heterostructure: chemical characterization. (a) Dark-field TEM image of NW\(_1\) taken along the [2-1-10] zone axis. The position of the interface is indicated by the white arrow. Moiré fringes are visible in the nanowire and are due to the coincidence periods between the scanning step of the electron beam and the interatomic potential. (b) EDX composition profile measured along the nanowire axis [blue arrow in (a)]. (c) Zoom on the interface profile. The fit to an error function yields \( L = 5.9 \) nm.

To investigate the crystalline quality of the nanowire heterostructure, we image different areas of NW\(_1\) by high resolution HAADF STEM followed by fast Fourier transform. Both GaAs and InGaAs segments have the wurtzite (WZ) crystal structure except for a small zinc blende (ZB) insertion in the interface region (Supplemental Material S3). Figures 3(a) and 3(b) are additional HR STEM images in two different orientations and do not reveal any misfit dislocation in the crystal at the InGaAs/GaAs interface. As predicted by our calculations, the crystalline integrity of our nanowire is preserved and the mismatch strain at the interface is relaxed elastically.

Across the interface, the lattice parameters \( a \) and \( c \) are modified both by compositional changes and by mechanical strain. We employ geometric phase analysis (GPA) to image the \( c- \) and \( a- \) lattice strain, i.e., the \( c- \) and \( a- \) lattice deformations with respect to a reference chosen here as unstrained \( c- \) GaAs and \( a- \) GaAs: \( \Delta c / c = \epsilon_{m,c} / \epsilon_{m,c}^{\text{GaAs}} \) and \( \Delta a / a = \epsilon_{m,a} / \epsilon_{m,a}^{\text{GaAs}} \), respectively [41]. To map the \( c- \) lattice (a-lattice) strain around the interface, we use the high resolution [2110] [0110] HAADF-STEM image shown in Fig. 3(a) [Fig. 3(b)]. GPA is then performed to the image by applying a mask around the (000\( \bar{2} \)) \( \bar{2} \) Bragg peak in the Fourier transform visible in the inset of Fig. 3(a) [Fig. 3(b)] (Supplemental Material S3). We choose a medium-size mask of \( \sim 0.15 \) \( \bar{g} \) (with \( \bar{g} \) the reciprocal lattice vector) in order to preserve a balance between a good spatial resolution and a high signal-to-noise ratio [42,43].

Figure 3(c) [Fig. 3(d)] shows the resulting color-coded map of \( \Delta c / c \) (\( \Delta a / a \)) in the \( a- \) plane. The bottom part of the wire corresponds to unstrained GaAs (\( \Delta c / c = \Delta a / a = 0\% \)). The top part of the nanowire features a maximum deformation of the \( c \) and \( a \) planes with respect to GaAs which is consistent with unstrained wurtzite In\(_{0.5}\)Ga\(_{0.5}\)As (composition found by EDX), which indicates full relaxation far from the interface. We observe a transition region around the InGaAs/GaAs interface indicating that the lattice is gradually stretched. Importantly, there is no discontinuity (or defects) in the transition regions for \( \Delta c / c \) and \( \Delta a / a \), confirming the absence of misfit dislocations at the interface [44,45]. The transition region is thicker in the center than on the nanowire edges, showing that the \( a- \) and \( c- \) lattice parameters recover faster their unstrained characteristic value near the nanowire sidewalls than at the nanowire center. It is indeed more difficult to release strain in the core of the nanowire than on the free sidewalls.
To get a complementary insight on strain relaxation, we visualize the arrangement of the crystal planes with a numerical moiré technique [46] [Figs. 3(e) and 3(f)]. We obtain a moiré pattern from the geometric phase images of Figs. 3(a) and 3(b) using Fourier filtering of the (000 2) and (2 110) Bragg peaks, respectively. We observe that the distance between planes is larger in the upper segment than in the bottom segment. Far from the interface, the planes are parallel to each other and are strain-free. Near the InGaAs/GaAs interface, at the sidewalls, the planes bend dramatically. This large deformation is due to elastic relaxation of the mismatch strain at the nanowire free surfaces. Note that plane bending is also evidenced in lattice rotations maps obtained by GPA (not shown).

We now quantitatively compare the experimental GPA data to numerical simulations. We first calculate the mechanical strain tensor \( \bar{\varepsilon} \) around the nanowire interface using finite element software (COMSOL Multiphysics), the values of lattice constants [47,48] and stiffness coefficients [49] for WZ InAs and WZ GaAs, and all the measured characteristics of NW1. We consider a cylindrical wire of radius \( R = 10.5 \, \text{nm} \). The lengths of the GaAs and InGaAs sections (200 and 60 nm, respectively) correspond to the dimensions of NW1. Since these lengths are already both much larger than \( R \), the results will also apply to nanowires featuring longer segments. We also include the interface chemical profile as determined from the fit to the EDX measurement [Fig. 2(b)]. Finally, we take into account the mechanical anisotropy associated with the wurzite nanowire crystal (see the Supplemental Material S4 Methods). The \( a \)-lattice strain is then deduced using the relation \( \Delta a/a = [c_{\text{loc}}(\varepsilon_{xx} + 1) - a_{\text{GaAs}}]/a_{\text{GaAs}} \). Here \( a_{\text{loc}} \) is the local unstrained lattice parameter, determined from the measured chemical profile in Fig. 2(c) and using a linear interpolation between GaAs and InAs. \( a_{\text{GaAs}} \) is the unstrained lattice parameter of GaAs and \( \varepsilon_{xx} = \frac{a - a_{\text{GaAs}}}{a_{\text{loc}}} \) is the mechanical strain along the \( x \) axis. Similarly, we have \( \Delta c/c = [c_{\text{loc}}(\varepsilon_{zz} + 1) - c_{\text{GaAs}}]/c_{\text{GaAs}} \). In addition, in order to account for the depth of focus of STEM imaging (around 10 nm), the theoretical data are averaged along the nanowire depth (details in the Supplemental Material S4).

Figure 4(a) and 4(b) compare the experimental and simulated \( a \)- and \( c \)-lattice strain along the nanowire axis. Without any free parameter, we obtain for \( \Delta c/c \) an excellent agreement between the simulated and experimental profiles (the discrepancy is lower than 0.5%). For \( \Delta a/a \), the agreement is good, but the theory predicts a slightly lower In composition in the In\(_{0.8}\)Ga\(_{0.2}\)As segment than observed in the experimental data. We attribute this to the noise in the experimental GPA data [Fig. 3(d)], which increases the uncertainty on the unstrained reference region. Both \( \Delta c/c \) and \( \Delta a/a \) increase gradually from 0% (GaAs reference) to about 5.9% and 5.7% (In\(_{0.8}\)Ga\(_{0.2}\)As segment) respectively, which is consistent with
The maximum hydrostatic strain to 6. We note here that interface grading has a stronger
to decrease
L
of the interface length
and plot the maximal values of
ε
nanowire with the same dimensions and composition as NW1
grading on the strain fields. We consider an InGaAs/GaAs
nanowire devices.
[23,24] which should be taken into account in the design of
will introduce a spatial modulation of the band structure
formation. Importantly, these marked strain inhomogeneities
longitudinal oscillations between tensile and compressive de-
spatial inhomogeneities. In particular,
ε
0.5%, indicating that the mismatch strain is largely decreased
roughly set by the nanowire diameter, in agreement with the
structural properties of the interface.

We build on this understanding to discuss the distribution
of mechanical strain around the InGaAs/GaAs interface. Fig-
ures 4(c) and 4(d) show the calculated strain components εzz
and εxx along the nanowire axis (z). Both components are
zero far from the interface, and feature significant amplitude
over a domain which is 30–40 nm long. Its size significantly
exceeds the interface length (L = 5.9 nm), and is in fact
roughly set by the nanowire diameter, in agreement with the
Saint Venant’s principle. εzz and εxx show a maximum around
0.5%, indicating that the mismatch strain is largely decreased
but not fully released. Finally, both εzz and εxx feature large
spatial inhomogeneities. In particular, εxx presents several
longitudinal oscillations between tensile and compressive de-
formation. Importantly, these marked strain inhomogeneities
will introduce a spatial modulation of the band structure
[23,24] which should be taken into account in the design of
nanowire devices.

Figure 5 illustrates the dramatic influence of interface
grading on the strain fields. We consider an InGaAs/GaAs
nanowire with the same dimensions and composition as NW1
and plot the maximal values of εxx, εyy, and εzz as a function
of the interface length L. In the case of a sharp interface
(L = 0) εzz and εxx reach 1.7% and 2.6%, respectively. A
graded interface with L = 5.9 nm (NW1) is already sufficient
decrease εzz by a factor of 3, and εxx by a factor close
to 6. We note here that interface grading has a stronger
influence on the transverse strain components. Of course,
increasing L leads to a further decrease of the strain but for
the investigated interface lengths, the spatial extension of the
strained region is roughly the same (Supplemental Material
S4). We next consider the hydrostatic strain ∆Ω/Ω = εxx +
εyy + εzz, which has an important impact on the band gap and
the conduction band offsets [23]. Its maximum value is also
plotted in Fig. 5: it is reduced from 4.2% down to 0.8% as the
interface length increases from 0 to 8.4 nm. Moderate interface
grading thus already results in a strong reduction of the strain
level.

Next, we consider additional nanowire samples to further
support the theoretical predictions of the coherent growth
domains. The results are summarized in Fig. 6, which confronts
the theory to experimental results obtained with two families
of samples. The first set of nanowires (NW2 to NW4) features
εm of 5.7%, R around 10 nm, and α ranging from 0.25 to
0.56. For all these nanowires, the mismatch strain is always
elastically released by the sidewalls, as shown on HRTEM
images by the absence of dislocations at the interface and on
GPA color-coded maps by the curvature of the a and c planes
(Supplemental Material S5). As shown in Fig. 6, this nanowire
family falls in the predicted coherent domain. The second set
of InAs/GaAs nanowire samples with α being 0.48 and 0.67
for a unique εm of 7.1% (NW5 and NW6). We observe by
HRTEM that the nanowires present defects at the InAs/GaAs
interface. GPA color-coded maps confirm the presence of
misfit dislocations and reveal plane bending (Supplemental
Material S6). In those nanowires the mismatch strain is re-
leased both via plastic and elastic relaxation. We finally plot
the experimental data in Fig. 6: these thick nanowires fall in
the plastic relaxation region, confirming here as well the
predictions.

Our study is of particular significance when it comes to
realize optoelectronic devices using semiconductor het-
erstructures. Material combinations such as, for example,
InP/InSb (εm = 10%) and GaN/InN (εm = 11%) are
important for photovoltaic and optoelectronic applications but suffer from an extremely high lattice mismatch. As seen in previous works, reducing the diameter is not always possible or sufficient to prevent plastic relaxation \cite{44,50}. Thus, the design of nanowire devices with compositionally graded interfaces has the potential to reduce materials constraint on the device dimensions. Importantly, a compositional grading over few nanometers at nanowire interfaces is sufficient to reduce most of the strain without altering the required physical properties.

### III. CONCLUSION

In conclusion, we fully characterized high lattice-mismatch axial In(Ga)As/GaAs heterostructure nanowires featuring graded interfaces. The heterostructure shows a preserved crystalline quality with a mismatch strain released elastically, via plane bending. Full elastic relaxation occurs at the nanowire sideways while the remaining strain is localized in the central area of the nanowire, larger than the interface length. Theoretical predictions confirmed by our experimental data show that the domains for coherent growth can be extended using compositional gradients of few nanometers. Beyond the realization of coherent heterointerfaces, interface grading offers an additional tuning knob to control residual strain in the nanowire, and thus to fine-tune its optoelectronic properties.

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The authors declare no conflict of interest.

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