

Strain distribution in zinc-blende and wurtzite GaAs nanowires bent by a one-sided (In,Al)As stressor shell: Consequences for torsion, chirality, and piezoelectricity

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We present a finite-strain model that is capable of describing the large deformations in bent nanowire heterostructures. The model incorporates a nonlinear strain formulation derived from the first Piola-Kirchhoff stress tensor, coupled with an energy functional that effectively captures the lattice-mismatch-induced strain field. We use the finite element method to solve the resulting partial differential equations and extract cross-sectional maps of the full strain tensor for both zinc-blende and wurtzite nanowires with lattice-mismatched core and one-sided stressor shell. In either case, we show that the bending is essentially exclusively determined by ε_{zz} . However, the distinct difference in shear strain has important consequences with regard to both the mechanical deformation and the existence of transverse piezoelectric fields in the nanowires.

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I. INTRODUCTION

Strain engineering is a powerful means for manipulating and tuning of the electronic band structure of semiconductors [1]. In planar heterostructures, combining layers with different lattice constants generates a spatially uniform biaxial strain that strongly modifies the energy and dispersion of the electronic bands in the strained layer, and which is routinely used for various electronic and optoelectronic applications of semiconductors [2–6].

However, strain *gradient* engineering, i.e., the use of the effects of spatially nonuniform strain, has thus far remained largely unexplored, and has only recently emerged as one of the key topics for future solid-state research. In fact, sufficiently large strain gradients in inorganic materials unlock new physical properties such as, most prominently, flexoelectricity [7–10], but may also induce ferroelectricity, superconductivity, and flexomagnetism [11]. Continuously tunable strain gradients can furthermore be utilized to realize spectrally indistinguishable quantum emitters [12]. While the magnitude of such gradients in inorganic bulk crystals is limited by their low fracture strength, freestanding nanostructures such as nanomembranes or nanowires are tolerant to loads

close to the elastic limit of the respective material [13,14] and can thus sustain strain gradients in excess of $2 \times 10^{-3}/\text{nm}$.

The flexibility and quasi-one-dimensional nature of nanowires offer new degrees of freedom for novel heterostructure design and strain engineering [15]. Bent nanowires have therefore attracted attention in both the semiconductor and the piezotronics fields. For example, dispersed ZnO microwires have been bent mechanically by micromanipulation to induce charge-carrier drift in the strain (and thus bandgap) gradient across the wire's cross section [16–19]. The bending of freestanding ZnO nanowires by an external load such as the tip of an atomic force microscope was theoretically investigated by several groups to compute the resulting piezo- and flexoelectric fields [20–25].

A novel method to uniformly bend all nanowires in an ordered array has been developed by researchers from the Paul-Drude-Institute [26,27] and McMaster University [28,29]. By exploiting the directional nature of the impinging atom fluxes in molecular-beam epitaxy, they fabricated nanowires that were bent in a controlled fashion by highly lattice-mismatched stressor shells deposited on a single side of the nanowires. This approach allows precise control over the degree of bending and the resulting strain gradients, eliminates the need for external mechanical micromanipulation, and produces arrays of freestanding nanowires with deterministic positioning and uniform bending. However, the current understanding of the strain distribution in these nanowires is rudimentary in the sense that it neglects all strain components except ε_{zz} [16–19,26].

In this paper, we use a three-dimensional finite-strain model based on the Green-Lagrange total strain tensor, including geometric nonlinearity, to describe the large deformations

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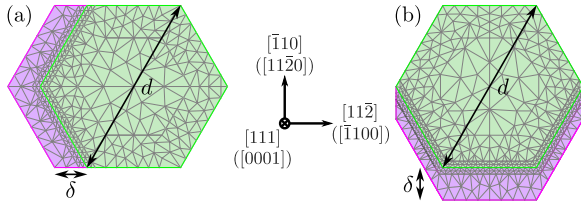


FIG. 1. Cross-sectional view showing the material composition, and the triangular mesh and refinement along the core/shell interface. The regular hexagonal with core diameter d (green color) consists of GaAs and the one-sided shell of thickness δ (purple color) contains the (In,Al)As alloy. The shell is deposited either along (a) the $[11\bar{2}]$ direction for ZB-[111] nanowires ($[\bar{1}100]$ direction for WZ-[0001]) and (b) along the $[\bar{1}10]$ direction for ZB-[111] nanowires ($[11\bar{2}0]$ direction for WZ-[0001]).

induced by the lattice mismatch between the nanowire core and a one-sided lattice-mismatched stressor shell [30,31]. We explicitly consider GaAs/(In,Al)As core/shell nanowire heterostructures as realized in Ref. [26]. These nanowires consist of a GaAs core with a regular hexagonal cross section and a one-sided (In,Al)As stressor shell.

Figure 1 shows two possible configurations of such nanowires and the mesh used, where the shell is deposited either along the $[11\bar{2}]$ (or $[\bar{1}100]$) crystallographic direction or along the $[\bar{1}10]$ (or $[11\bar{2}0]$) direction. The computational grid provides sufficient resolution to accurately capture the displacement and strain fields across the nanowire's interface. The coherent interface between the core and the shell leads to strain that bends the nanowire. Bending angles up to 180° with an associated strain gradient greater than $0.1\%/nm$ have been experimentally demonstrated [26]. Beyond this achievement, the GaAs-AlAs-InAs materials system constitutes the most mature compound semiconductor class with numerous important applications in microwave electronics, photonics, and photovoltaics. Furthermore, GaAs stands out as one of the very few materials that allows the synthesis of phase-pure nanowires with either zinc-blende (ZB) or wurtzite (WZ) crystal structures. Consequently, we derive the full strain tensor for both ZB and WZ nanowires, each for shells deposited in the two perpendicular crystallographic directions, and compare the numerical results to approximate analytical results. Furthermore, we point out important differences between the two polytypes and their implications for the existence of transverse piezoelectric fields in the nanowires.

II. FINITE-STRAIN MODEL

Our model is numerically solved in the reference (Lagrangian) configuration and is based on a predeformation tensor $\mathbf{M}$ which takes into account the influence of the lattice mismatch between the two materials (see the Julia package ELECTROMECHANICSFEM.JL [32]). Hence, $\mathbf{M}$ differs in each region of the composite structure. Let $\mathbf{u} \in \mathbb{R}^3$ denote the displacement, $\mathbf{F} := \nabla \phi = \mathbf{I} + \nabla \mathbf{u}$ the deformation gradient tensor, and $\mathbf{C} \in \mathbb{R}^{3 \times 3 \times 3 \times 3}$ the fourth-rank stiffness tensor. In our model, we use a linear stress-strain relation (Hooke's law) and consider the Green-Lagrange total strain tensor with a geometric nonlinearity, i.e., $\epsilon(\mathbf{F}) := \frac{1}{2}(\mathbf{F}^T \mathbf{F} - \mathbf{I}) = \frac{1}{2}(\nabla \mathbf{u} +$

$\nabla \mathbf{u}^T + \nabla \mathbf{u}^T \nabla \mathbf{u})$. Then, our model can be expressed by the partial differential equation [31]:

$$-\text{div}(\det(\mathbf{M})\mathbf{F}(\mathbf{u})\mathbf{M}^{-1}(\mathbf{C} : \epsilon(\mathbf{u}))\mathbf{M}^{-T}) = 0, \quad (1)$$

which is solved using the finite element method (FEM) for the displacement $\mathbf{u}$. In this equation, $\epsilon = \mathbf{M}^{-T}\epsilon(\mathbf{F})\mathbf{M}^{-1} - \frac{1}{2}(\mathbf{I} - \mathbf{M}^{-T}\mathbf{M}^{-1})$ is the elastic strain. The model is supplied with homogeneous Neumann boundary conditions at all facets except at the interface between the nanowire and the substrate, where we apply Dirichlet boundary conditions.

III. STRAIN PROFILES IN BENT ZB/WZ NANOWIRES

Since none of the strain components changes along the length of the nanowire (except in close vicinity to the nanowire ends), the problem can be reduced to two dimensions spanned by the cross-sectional coordinates perpendicular to the bending direction. Figure 2 shows the six elastic strain components in the center cross section (taken at $1 \mu\text{m}$) of a $2\text{-}\mu\text{m}$ -long GaAs/In_{0.5}Al_{0.5}As core/shell nanowire with a core diameter $d = 2s = 100/\sqrt{3} \text{ nm}$, where s denotes the circumradius, i.e., the side length of the regular hexagon forming the nanowire core, and a shell thickness $\delta = 10 \text{ nm}$ [33]. We consider two different polytypes [ZB in Figs. 2(a) and 2(c), WZ in Figs. 2(b) and 2(d)] and two different core/shell geometries (the two top and bottom rows) as shown in Fig. 1. The curvature κ of these four different bent nanowires is only slightly different and corresponds roughly to $0.52 \mu\text{m}^{-1}$. As an illustration, Fig. S1 in the Supplemental Material [34] provides a three-dimensional view of the ZB-[111] nanowire from Fig. 2(c).

In all four cases, the normal strain components ϵ_{xx} , ϵ_{yy} , and ϵ_{zz} are large and very similar in magnitude for both polytypes and crystallographic bending directions. The same applies to the in-plane shear strain component ϵ_{xy} . However, the values of the two out-of-plane shear strain components ϵ_{xz} and ϵ_{yz} differ drastically between the two crystal structures. These components have the same order of magnitude as the normal components for ZB-[111] nanowires [see Figs. 2(a) and 2(c)], but are actually zero for WZ-[0001] nanowires [see Figs. 2(b) and 2(d)]. The origin of this difference in magnitude of ϵ_{xz} and ϵ_{yz} lies in the structure of the stiffness tensors for the two different polytypes. For both direct comparison and numerical efficiency [35] we transform the stiffness matrix for the ZB structure (defined with the unit vectors along the $\langle 001 \rangle$ axes) into the nanowire coordinate system spanned by the $[111]$, $[\bar{1}10]$, and $[11\bar{2}]$ directions. No such transformation is necessary for the WZ structure, whose unit vectors naturally align with the nanowire coordinates.

In Voigt notation, the stiffness matrices $\mathbf{C}$ for WZ-[0001]- and ZB-[111]-oriented nanowires are given by [35]

$$\mathbf{C}^{0001} := \begin{pmatrix} C_{11}^{\text{WZ}} & C_{12}^{\text{WZ}} & C_{13}^{\text{WZ}} & 0 & 0 & 0 \\ C_{12}^{\text{WZ}} & C_{11}^{\text{WZ}} & C_{13}^{\text{WZ}} & 0 & 0 & 0 \\ C_{13}^{\text{WZ}} & C_{13}^{\text{WZ}} & C_{33}^{\text{WZ}} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{44}^{\text{WZ}} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{44}^{\text{WZ}} & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{66}^{\text{WZ}} \end{pmatrix},$$

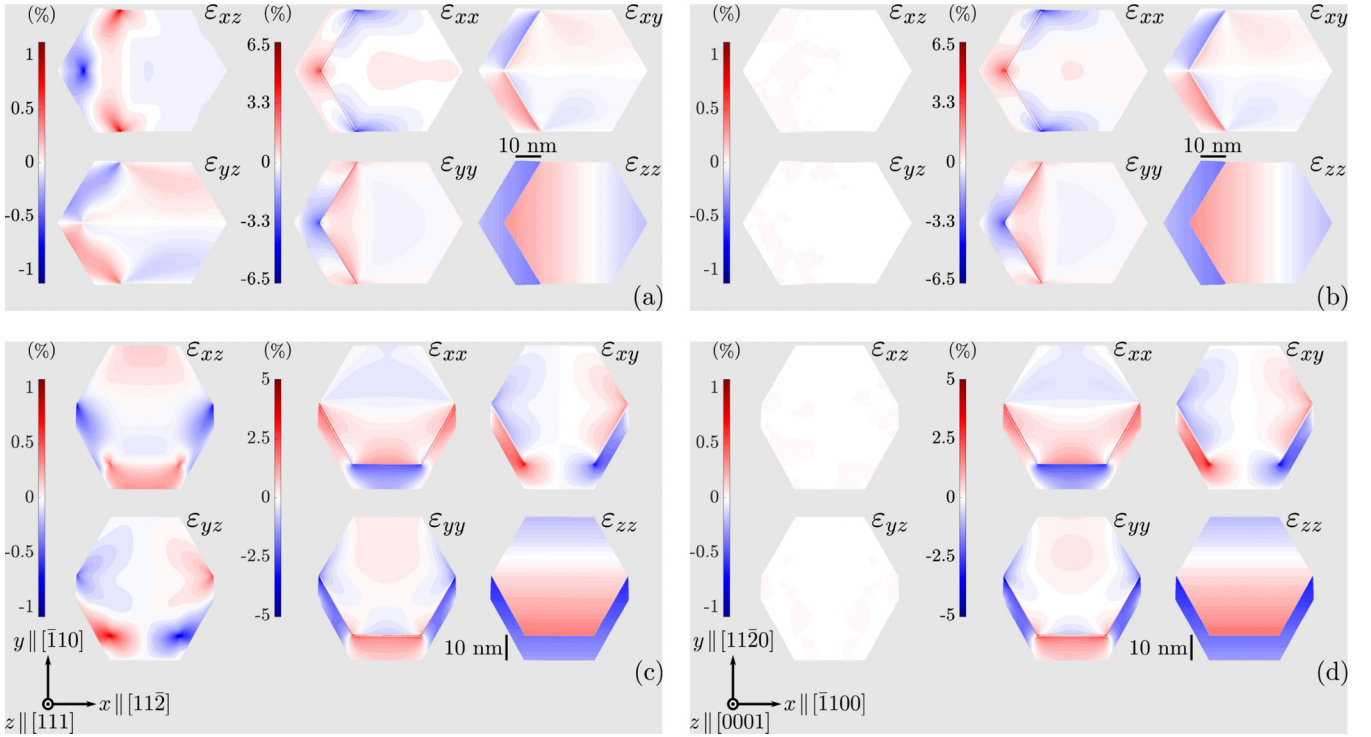


FIG. 2. Elastic strain components computed on the central cross section of a 2- μm -long GaAs/In_{0.5}Al_{0.5}As core/shell nanowire, using two different cross-sectional geometries. In the top panel, the shell is applied on a vertex of the hexagonal core [see Fig. 1(a)]: (a) along the $[11\bar{2}]$ direction for ZB-[111] nanowires, and (b) along the $[\bar{1}100]$ direction for WZ-[0001] nanowires. In the bottom panel, the shell is applied on the edge of the hexagonal core [see Fig. 1(b)], i.e., in (c) along the $[\bar{1}10]$ direction for ZB-[111] nanowires, and in (d) along the $[11\bar{2}0]$ direction for WZ-[0001] nanowires. In each case, we separate the ε_{xz} and ε_{yz} shear strain components since their values are smaller than the normal components. In the ZB-111 case [see (a) and (c)], the ε_{xz} and ε_{yz} components are approximately five to six times smaller than those of the normal strain, but in the WZ-[0001] case [see (b) and (d)], they are zero. The finite values on the order of 10^{-5} are a numerical artifact resulting from the comparatively coarse grid used for these computations. With increasing spatial refinement, these components asymptotically approach zero.

and

$$C^{111} := \begin{pmatrix} C_{11}^{\text{ZB}} & C_{12}^{\text{ZB}} & C_{13}^{\text{ZB}} & 0 & C_{15}^{\text{ZB}} & 0 \\ C_{12}^{\text{ZB}} & C_{11}^{\text{ZB}} & C_{13}^{\text{ZB}} & 0 & -C_{15}^{\text{ZB}} & 0 \\ C_{13}^{\text{ZB}} & C_{13}^{\text{ZB}} & C_{33}^{\text{ZB}} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{44}^{\text{ZB}} & 0 & -C_{15}^{\text{ZB}} \\ C_{15}^{\text{ZB}} & -C_{15}^{\text{ZB}} & 0 & 0 & C_{44}^{\text{ZB}} & 0 \\ 0 & 0 & 0 & -C_{15}^{\text{ZB}} & 0 & C_{66}^{\text{ZB}} \end{pmatrix}.$$

Since there is no complete set of parameters available for the WZ materials, particularly for InAs and AlAs, we use a linear transformation (quasicubic approximation) to obtain C_{ij}^{WZ} from the stiffness constants of the corresponding ZB materials in their natural ($\langle 001 \rangle$) basis [36]. Likewise, the relations between the C_{ij}^{ZB} in the rotated basis ($\langle 111 \rangle$) and those in the natural coordinate system ($\langle 001 \rangle$) of the ZB crystal are given in Ref. [35]. For this particular orientation the components of the stiffness matrices are identical ($C_{ij}^{\text{WZ}} = C_{ij}^{\text{ZB}}$), except for the additional component C_{15} in C^{111} . The values for the lattice, stiffness, and piezoelectric constants used in the present work for both ZB and WZ GaAs and (In,Al)As are given in Table S1 in the Supplemental Material [34].

The key difference between C^{111} and C^{0001} is the element C_{15} , which is zero for the WZ but nonzero for the ZB case. For

ZB-GaAs, for example, we obtain a value of 12.85 GPa. The structure of these matrices properly reflects the trigonal (C_{3v}) and hexagonal (C_{6v}) symmetry of ZB-[111] and WZ-[0001] nanowires. Note that different but equivalent representations of C^{111} can be obtained depending on the exact choice of the coordinate transformation [15,37].

IV. TORSION

An as unexpected as interesting consequence of this distinct difference in the strain distribution in ZB-[111]- and WZ-[0001]-oriented nanowires is displayed in Fig. 3, which views the nanowires along the normal of their top facet for our four different bent nanowire configurations. To maximize the displacements, we here consider GaAs nanowires with a pure InAs stressor shell, representing the maximum lattice mismatch available in this material's system. For the WZ-[0001] nanowires shown in Fig. 3(b), the nanowire bends strictly in the bending plane indicated by the red dashed lines. The same is true for the ZB-[111] nanowire shown in the left panel of Fig. 3(a), with the stressor shell applied along the $[11\bar{2}]$ direction. However, for the ZB-[111] nanowire shown in the right panel of Fig. 3(a), with the stressor shell applied along the $[\bar{1}10]$ direction, we observe a displacement of the nanowire

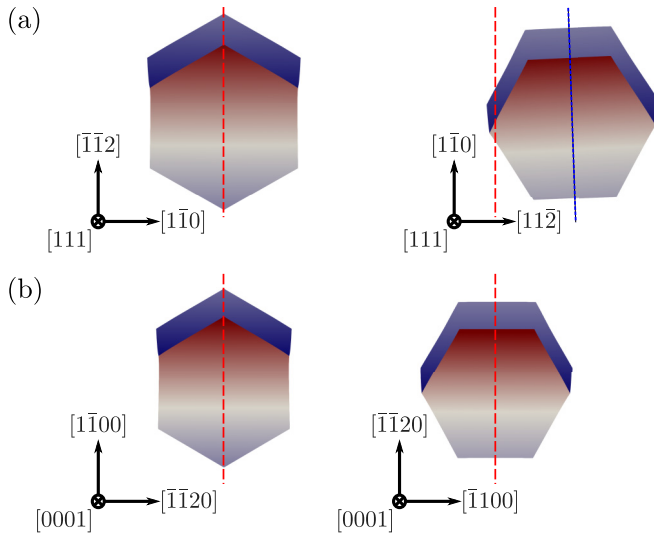


FIG. 3. Bent GaAs/InAs nanowires viewed along the normal of their top facet from the same viewpoint (inside the nanowire). Due to the different curvature and thus distance from the viewpoint, the nanowires seem to be of different size, but they all have an identical core diameter of $100/\sqrt{3}$ nm. The color gradient depicts the variation of ε_{zz} analogously to Fig. 2. In (a), we show ZB-[111] nanowires with the stressor shell deposited along the (left) $[11\bar{2}]$ and (right) $[1\bar{1}0]$ directions corresponding to Figs. 1(a) and 1(b). In (b), the corresponding WZ-[0001] nanowires are displayed, with the stressor shell deposited along the (left) $[1\bar{1}00]$ and (right) $[11\bar{2}0]$ directions, corresponding to Figs. 1(a) and 1(b). The red dashed line represents the bending plane for each of the four different cases. In three of these cases, the nanowire stays exactly in the bending plane. However, for ZB-[111] nanowires with the shell applied in the $[1\bar{1}0]$ direction, the nanowire is laterally displaced and exhibits a torsion visualized by the blue dotted line.

out of the bending plane, and an anticlockwise rotation about the nanowire's $[111]$ axis.

This torsion of the nanowire induces a left-handed helical chirality. At the first glance, this result may appear surprising, since the zinc-blende structure is cubic, and materials of cubic elastic symmetry are not chiral. However, as mentioned above, the rotated stiffness matrix of the ZB-[111]-oriented nanowires exhibits a trigonal elastic symmetry, which is in fact the highest elastic symmetry that permits chirality [38]. In contrast, the stiffness matrix of the WZ-[0001]-oriented nanowires belongs to the class of transverse isotropic materials, which are not chiral [39].

The torsion of the ZB-[111]-oriented nanowire is induced by the large out-of-plane shear strain components, which in turn originate from the finite value of the symmetry-breaking or chiral stiffness constant C_{15} [37,38]. The degree and handedness of the rotation are determined by the magnitude and the sign of C_{15} , respectively. Torsion only occurs when the nanowire bends along the $[1\bar{1}0]$ direction independent of the shell geometry, confirming that it is the material symmetry which is responsible for this effect (see Fig. S3 in the Supplemental Material [34]).

The effects of pure torsion in beams with a noncircular cross section have been traditionally modeled with Prandtl's stress equation [40]. In Ref. [41], this well-established

approach was used to compare the consequences of torsion in ZB and WZ nanowires on the respective strain distribution and the resulting piezoelectric fields. We note that the complex strain distributions arising in bent or twisted nanobeams are an area of very active research in the field of mechanical engineering, and are believed to require higher-order theories beyond classical linear elasticity, such as Cosserat elasticity [42,43] and strain- or stress gradient elasticity [44]. The various models developed in this field aim to describe primarily the size dependence of deformations, and thus include length-scale parameters to explicitly consider the actual size of the system under consideration [45,46]. Such a size dependence may arise due to the microscopic heterogeneity of the material [47]. Still, in the extreme nanoscopic limit, an intrinsic size dependence is also expected for homogeneous materials (such as for single-crystalline GaAs nanowires), since the magnitude of the strain gradients linearly increases with decreasing system size [48,49]. However, there are two major issues with the existing higher-order elasticity theories: They offer conflicting predictions with no consensus in the field for the underlying reasons [50] and, for any practical application, they rely on a large number of additional and in general unknown parameters [45,51]. Our model may be conceptually less advanced, but in the end more practical since all parameters involved are known with a fair degree of accuracy.

V. AXIAL ELASTIC STRAIN AND CURVATURE

The full strain distribution in the bent nanowires as depicted in Fig. 2 can only be obtained by numerical means. It is possible, however, to derive an analytical expression for the strain component ε_{zz} for a given shell thickness δ and core diameter d . In Ref. [31] we have taken the same approach to minimize the strain energy density in the nanowire, but modified the prestrain condition to ensure that the resulting expression coincides with the one obtained with the classical bending theory developed by Timoshenko [52]. This logical consistency is achieved only if we consider that the entire predeformation occurs in the shell, i.e., when $\mathbf{M}$ is the identity tensor in the core, and a diagonal matrix with elements corresponding to the full lattice mismatch in the shell [31]. In Fig. 4, we compare the analytically derived variation of ε_{zz} with the results obtained from the numerical simulations. Figures 4(a) and 4(b) depict the variation of ε_{zz} along the center horizontal and vertical line across the nanowire cross sections shown in Figs. 1(a) and 1(b), respectively. In both cases, the analytically derived ε_{zz} strain components are in excellent agreement with the numerical simulations.

Based on the analytical expression for ε_{zz} , we have derived a corresponding one for the curvature of the nanowire [31]. Figure 5 compares the curvature thus obtained as a function of δ and for different values of d with the one predicted by the numerical solution of (1) for both the ZB and the WZ structures. Evidently, the agreement between the analytical model based on ε_{zz} alone and the numerical model explicitly involving the full strain tensor is excellent, demonstrating that the bending of the nanowires is essentially exclusively determined by ε_{zz} . The slightly larger values of ε_{zz} for the WZ-[0001] nanowires [cf. Figs. 2(b) and 2(d), as well as Figs. 2(a)

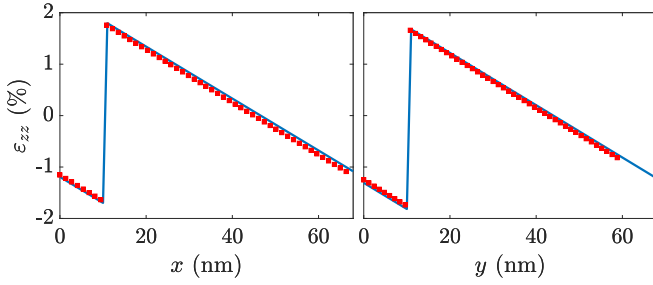


FIG. 4. Variation of ε_{zz} along the x and y directions of the ZB-[111] GaAs/In_{0.5}Al_{0.5}As nanowire with $d = 100/\sqrt{3}$ nm and $\delta = 10$ nm as depicted in (left) Fig. 1(a) and (right) Fig. 1(b). The lines represent the analytical expression for ε_{zz} [31] whereas the solid circles show the results of the FEM simulation. Similar results are obtained for the WZ-[0001] case.

and 2(c)] thus manifest themselves in a systematically larger curvature. For each core diameter, the curvature peaks at a certain shell thickness, the value of which is monotonically decreasing with decreasing core diameter. This behavior is easily understood: the smaller the core diameter, the easier it is for a mismatched shell of given thickness to bend the nanowire. With increasing shell thickness, the curvature initially increases until the shell becomes so thick that it switches roles with the core. From this point on, which is inversely proportional to the core diameter, it is the shell which is decreasingly bent by a core of constant diameter.

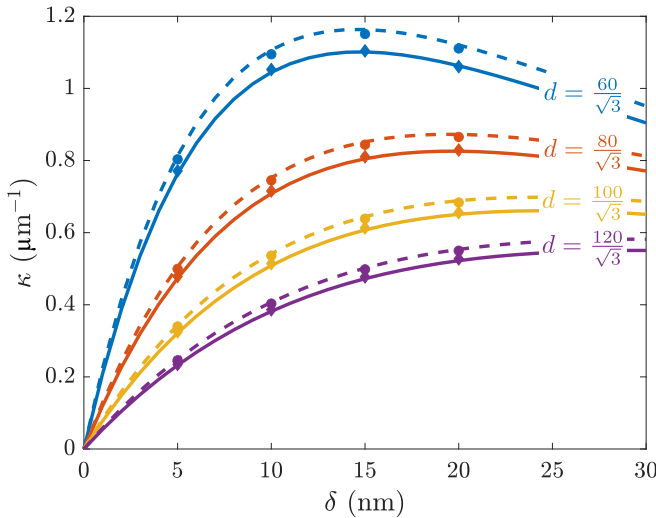


FIG. 5. Curvature of a bent GaAs/In_{0.5}Al_{0.5}As nanowire with varying shell thickness δ for hexagonal core diameters $d = \frac{1}{\sqrt{3}}\{60, 80, 100, 120\}$ nm (blue, red, gold, and magenta curves, respectively). The solid and dashed lines are obtained with the analytical curvature formula for a ZB-[111] and WZ-[0001] nanowire, respectively. The solid circles and diamonds indicate the respective values obtained by the FEM simulations. In both cases, the cross section of Fig. 1(b) has been used. Similar results are observed for ZB/WZ nanowires with cross sections as in Fig. 1(a).

VI. OUTLOOK: CONSEQUENCES FOR PIEZOELECTRICITY

Since GaAs is a piezoelectric material, it is important to consider the consequences of the distinct strain fields of the two polytypes for piezoelectric polarization and piezoelectric fields. The piezoelectric polarization $\mathbf{P} = (P_x, P_y, P_z)^T$ for the WZ polytype in [0001] orientation has the form [35]

$$\mathbf{P}^{0001} = \begin{pmatrix} 2e_{15}^{\text{WZ}}\varepsilon_{xz} \\ 2e_{15}^{\text{WZ}}\varepsilon_{yz} \\ 2e_{31}^{\text{WZ}}(\varepsilon_{xx} + \varepsilon_{yy}) + e_{33}^{\text{WZ}}\varepsilon_{zz} \end{pmatrix},$$

where the e_{ij}^{WZ} are the piezoelectric constants for the WZ structure (see Table S1 in the Supplemental Material [34]). Since $\varepsilon_{xz} = \varepsilon_{yz} = 0$, it follows that $P_x = P_y = 0$, i.e., there is neither an in-plane piezoelectric polarization nor a transverse piezoelectric field. Only the polarization component P_z does not vanish for the WZ-[0001] nanowires. However, since P_z does not change along z (except in direct vicinity of the bottom interface with the substrate and the free top surface of the nanowire), this polarization does not induce any longitudinal piezoelectric field.

For the ZB polytype in [111] orientation, the polarization vector in the rotated basis reads [35]

$$\mathbf{P}^{111} = \begin{pmatrix} 2e_{15}^{\text{ZB}}\varepsilon_{xz} \\ 2e_{15}^{\text{ZB}}\varepsilon_{yz} \\ 2e_{31}^{\text{ZB}}(\varepsilon_{xx} + \varepsilon_{yy}) + e_{33}^{\text{ZB}}\varepsilon_{zz} \end{pmatrix} + \begin{pmatrix} e_{11}^{\text{ZB}}(\varepsilon_{xx} - \varepsilon_{yy}) \\ 2e_{12}^{\text{ZB}}\varepsilon_{xy} \\ 0 \end{pmatrix},$$

where the e_{ij}^{ZB} are the piezoelectric constants for the ZB-[111] case (for their relation to the single piezoelectric constant e_{14} of the ZB crystal in its natural $\langle 001 \rangle$ basis; see Ref. [35] and Table S1 in the Supplemental Material [34]). In contrast to the case of WZ-[0001] nanowires discussed above, the polarization components P_x and P_y are not zero, and neither are $\partial P_x / \partial x$ and $\partial P_y / \partial y$ (see Fig. S4 in the Supplemental Material [34] for the corresponding polarization maps). Hence, in bent ZB-[111] nanowires, we encounter transverse electric fields of substantial magnitude.

VII. FINAL REMARKS

In summary and conclusion, our analysis of the strain distribution in GaAs nanowires bent by a one-sided stressor shell has revealed several important differences between the ZB and WZ polytypes. First, for the ZB-[111] case, all shear strain components are large, whereas the out-of-plane ones are zero for otherwise equivalent WZ-[0001] structures. The origin of this difference lies in the fact that the stiffness matrix for the ZB structure, rotated such as to align with the nanowire coordinates, contains a nonzero symmetry-breaking (chiral) stiffness constant C_{15} . The resulting large out-of-plane shear strain components lead to a torsion for a certain bending direction, and thus make these nanowires chiral.

Moreover, these shear strain components for the ZB case directly translate into large piezoelectric polarization compo-

nents P_x and P_y , which, due to their variation along x and y , will cause non-negligible transverse electrostatic fields. These fields may be strong enough to field ionize excitons and spatially separate charge carriers, and thus to profoundly modify the charge-carrier dynamics in these nanowires. To understand this dynamics, we are required to solve the drift-diffusion equations for electrons and holes in the potential landscape created by strain as well as by the resulting piezo- and flexoelectric potentials. As a first step, we are currently extending our model to include full electromechanical coupling for being able to compute the total electrostatic potential in nanowires bent by one-sided stressor shells.

Our methodology can be easily applied to other nanowire geometries, for example with different cross-sectional shape of the core and/or the shell. Additionally, the nanowire can be composed of arbitrary materials as long as the relevant material parameters are known with sufficient accuracy.

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DATA AVAILABILITY

The data that support the findings of this article are openly available [53], embargo periods may apply.

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