Three-dimensional mapping of the strain anisotropy in self-assembled quantum-wires by grazing incidence x-ray diffraction

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Citation: Applied Physics Letters **85**, 3581 (2004); doi: 10.1063/1.1808493

View online: http://dx.doi.org/10.1063/1.1808493

View Table of Contents: http://scitation.aip.org/content/aip/journal/apl/85/16?ver=pdfcov

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Three-dimensional mapping of the strain anisotropy in self-assembled quantum-wires by grazing incidence x-ray diffraction

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(Received 12 January 2004; accepted 23 August 2004)

Three-dimensional strain mapping of InAs self-assembled nanowires on an InP substrate using grazing incidence x-ray diffraction is reported. A remarkable anisotropy was observed for the strain components, parallel [−220] and perpendicular [220] to the wire axis. The highest strain relaxation was measured along the [220] direction. The relationship between the interatomic distances along the [−220] and [220] directions, for each *z* position (height) in the nanostructure, was obtained by angular scans in the vicinity of the (040) reciprocal lattice point. © *2004 American Institute of Physics*. [DOI: 10.1063/1.1808493]

The strain distribution is one of the significant factors that determine the shape, size, and facet formation in self-assembled nanostructures obtained from strained heteroepitaxial growth. For coherently strained islands, the continuous variation of the lattice parameter inside the nanostructure (from bottom to top) makes it energetically stable against the formation of a uniform (flat) strained layer. The characterization of the strain distribution can be performed using grazing incidence x-ray diffraction (GIXRD), an accurate method sensitive to both local lattice parameter variation and nanostructure lateral size. Kegel *et al.*[1] demonstrated, assuming iso-strain disk scattering, that three-dimensional strain maps can be obtained in dots with full symmetry around the axis perpendicular to the substrate surface. Strain distribution and composition profiles of self-assembled nanostructures of InAs/GaAs[1–3] and Ge/Si[4] have been well characterized using GIXRD. Earlier x-ray studies of InAs/InP nanowires also revealed the presence of strain relaxation.[5] So far, however, there are no detailed studies of the anisotropic strain distribution in self-assembled nanowires. In particular, InAs self-assembled nanostructures on an InP substrate is a very attractive system for optoelectronic applications. In this case, both InAs quantum-wires and/or dots can be obtained by changing the buffer layer properties[6,7] or by tuning the growth conditions.[8,9] Recently, it has been shown that anisotropic strain relaxation could play an important role not only during the formation of InAs nanowires[10] but also in determining their optical behavior.[11]

In this letter, we report the study of strain distribution of InAs self-assembled nanowires on an InP substrate as shown schematically in Fig. 1. A remarkable anisotropy was observed for the strain components, parallel and perpendicular to the wires. The highest strain relaxation was measured along the [110] direction, perpendicular to the wires. Here, we describe a procedure to obtain the correlation between the strain components parallel to the substrate surface with their *z* position (height) in the nanostructures. In this way, one can construct a three-dimensional strain map of a self-assembled nanostructure system.

The InAs self-assembled nanowires were grown by chemical beam epitaxy.[9] Semi-insulating (001) InP substrates, misoriented by 2° toward [011], were used. After growth of the InP buffer layer, six monolayers of InAs were deposited at approximately 1.3 Å/s at 500 °C. The samples were then cooled in vacuum in order to avoid postgrowth surface redistribution.[9] Details of the growth process were published elsewhere.[9] Reflection high-energy electron diffraction (RHEED) was carried out *in situ* on the growing surfaces. After removal from the growth chamber, in-air AFM was used to analyze the surface morphology of the samples. Cross-section TEM images were obtained by using a JEM 3010 URP 300 kV TEM.

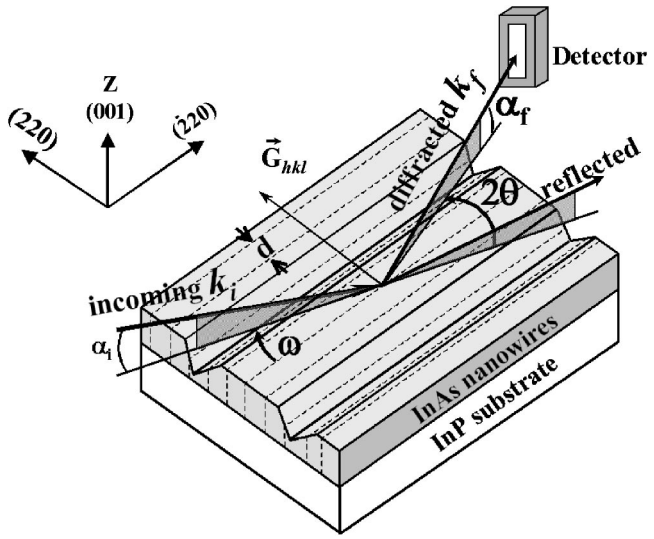

FIG. 1. Scheme of the GIXRD scattering geometry. Our InAs nanowires are oriented along the [−220] directions as previously reported (Refs. 8 and 9). For the case presented, the diffraction from (220) crystalline planes can be studied. Diffraction from (−220) planes can be obtained by rotating the sample 90° in the ω direction.

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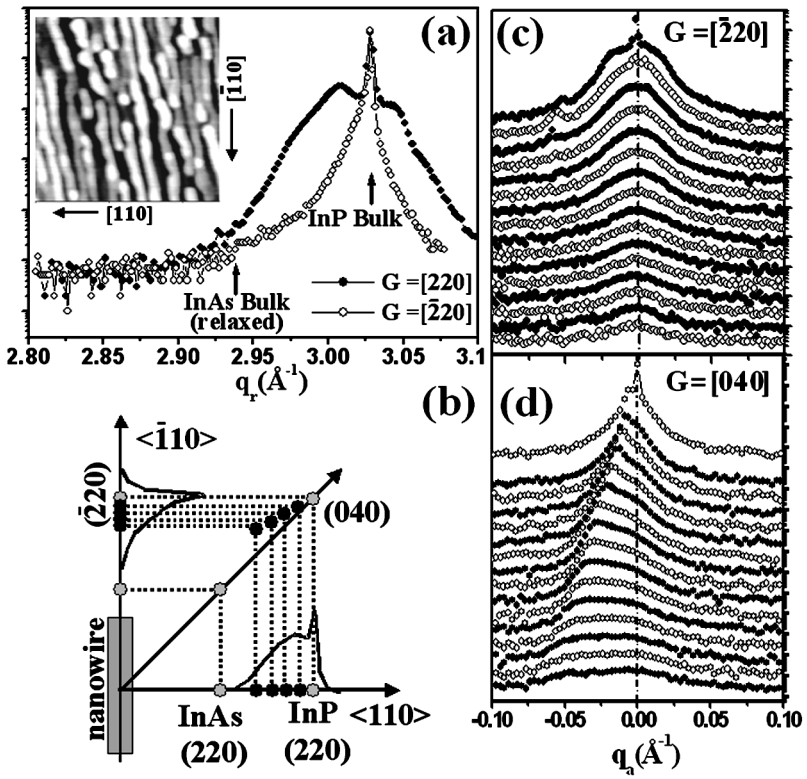

FIG. 2. (a) Radial scans along the [220] and [−220] directions. Inset shows an AFM image of the wires with the crystalline orientation. Scheme in (b) shows the shift of the intensity peak position, with respect to the [040] direction of the fcc structure, when anisotropic strain is present in the nanostructures. (c) and (d) Angular scans at different radial q_r positions in the vicinity of (−220) and (040) reciprocal lattice points, respectively, the curves were vertically shifted for clarity.

The x-ray experiments were performed at XRD2 beam line of the Brazilian National Synchrotron Laboratory.[12] The experimental setup was described in Ref. 4. All measurements were done in GIXRD geometry, as a function of the scattering angle (2θ, radial) and the sample rotation (ω, angular). The wavelength and the incidence angle of the x-ray beam were set to $\lambda = 1.192$ Å and $\alpha_i = 0.3°$, respectively.

In the GIXRD geometry, the measured x-ray intensities are due to diffraction from atomic planes perpendicular to the substrate surface. In Fig. 2(a), the x-ray scattered intensities measured as a function of $q_{\text{radial}} = q_r = (4\pi/\lambda)\sin(2\theta/2)$ are shown. The radial scan, which is sensitive to the strain in the sample, is performed by coupling ω to 2θ (Fig. 1). We mapped the vicinity of InP (220) and (−220) reciprocal lattice points that correspond to crystalline directions (G_{hkl}) perpendicular and parallel to the InAs nanowires, respectively [see the inset in Fig. 2(a)]. The spreading of the intensity distributions is associated to the strain relaxation; it can be understood qualitatively from Bragg's law [$\lambda = 2d\sin(2\theta/2)$]. Regions of the nanostructure with slightly different interplanar spacing (d_{hkl}) diffract the beam at slightly different angles (2θ). Thus, from Fig. 2(a), we can see that strain relaxation inside the InAs nanowires is highly anisotropic. The highest relaxation occurs in the [110] direction, perpendicular to the wires. Notice that at position (q_r) corresponding to (220) and (−220) points of bulk InAs, the intensity is very low, indicating that InAs nanowires are coherently strained.

In order to determine the interdependence of strain and shape we obtained angular scans for different values of q_r. In this case, the scattered intensities are measured as a function of $q_{\text{angular}} = q_a = q_r \sin[(2\theta/2) - \omega]$. The size L of the nanostructure region associated with a q_r value (and thus to a strain value) is determined from the full width at half maximum Δq_a in the angular scan, i.e., $L = 2\pi/\Delta q_a$. This size represents the nanostructure length along the direction perpendicular to the vector G_{hkl}. For instance, the sizes along the (220) direction are obtained from angular scans in the vicinity of the (−220) reciprocal lattice point and vice versa. For symmetric quantum dots both directions are equivalent and the island strain map can be obtained assuming iso-strain planes parallel to the substrate surface for each z (height) position.[1,5] However, our InAs nanowires are very asymmetric in shape and exhibit significant strain anisotropy. In this case, two problems are encountered: (i) we cannot determine the length of the wires since the lower measurable full width at half maximum (FWHM) of the angular scans is limited by experimental error and (ii) the assumption of iso-strain planes parallel to the substrate surface for each value of z cannot be made, and must be extended to the case in which the in-plane lattice constants are different due to anisotropic strain relaxation.

To solve these problems, we found a relationship between the interatomic distances along [220] and [−220] directions (d_{220} and d_{-220}, respectively) for each z position in the nanostructure. In this sense, angular scans in the vicinity of the (040) reciprocal lattice point were made. The scheme in Fig. 2(b) shows the deviation (with respect to the [040] crystalline direction for the fcc structure) of the angular scan maximum peak position when anisotropic strain relaxation is present in the nanostructures. This peak position shift was observed experimentally as shown in Fig. 2(d); using Gaussian fits we obtained the peak positions (q_a) for each value of (q_r). For small variations of the ω angle, the component q_a is perpendicular to q_r. Therefore, taking in account that [040] is 45° rotated with respect to [220] and [−220] [see Fig. 2(b)], we calculated the q_r components along these last directions using a coordinate rotation transformation. In this way, we obtained the relationship between d_{-220} and d_{220} for each "iso-strain plane" [$d_{-220} = F_2(d_{220})$] that is plotted in Fig. 3.

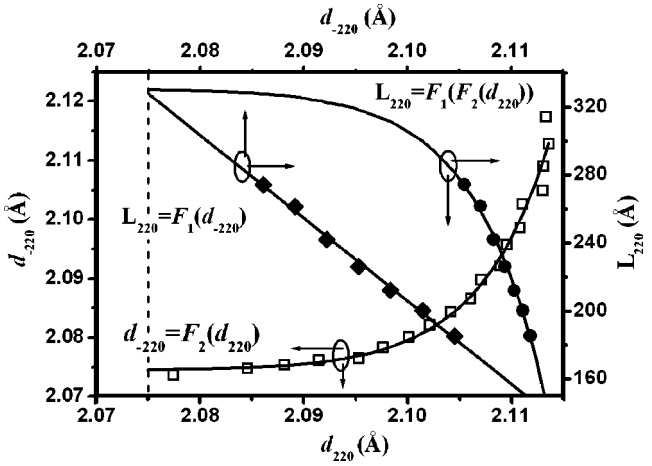

FIG. 3. The data (closed diamonds) for the relation $L_{220}=F_1(d_{-220})$ was obtained from the FWHM's of curves in Fig. 2(c). The data (white squares) for the relation $d_{-220}=F_2(d_{220})$ was obtained from the maximum peak position in curves of Fig. 2(d). Solid curves are linear and exponential fittings, respectively. The data points and the solid curve for the relation between L_{220} and d_{220} were obtained making the composed function of F_1 and F_2. The vertical dashed line indicates the bulk InP interplanar distance (substrate).

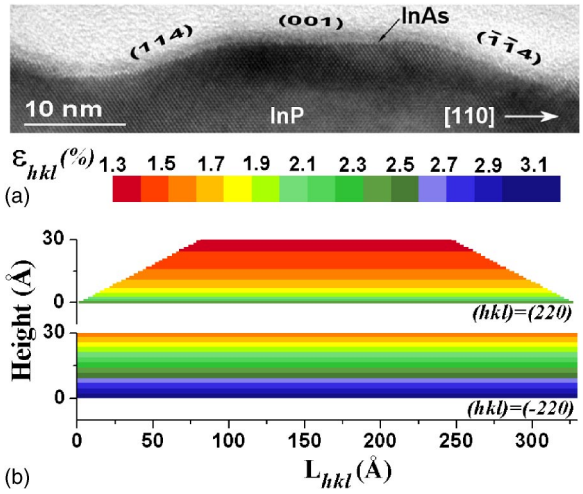

FIG. 4. (Color online). (a) Cross-section TEM image of an InAs nanowire. (b) Strain maps along the [220] and [−220] crystalline directions. The strain along each direction [*hkl*] was defined as: $\varepsilon_{hkl}=[(d_{\mathrm{InAs}}-d_{hkl})/d_{\mathrm{InAs}}]\times 100\%$. The *z* dependence was obtained correlating the RHEED and TEM results with curves in Fig. 3.

The F_2 function is an exponential growth-type fitting function with optimized parameters given by $d_{-220}=2.074+0.00026\,\mathrm{Exp}[(d_{220}-2.08)/0.0067]$.

On the other hand, the lateral size along the [220] direction as a function of d_{-220} [$L_{220}=F_1(d_{-220})$, shown in Fig. 3] was obtained from the FWHM of angular scans (Δq_a) in Fig. 2(c) for each q_r value. In this case, a linear fitting function ($L_{220}=10\,429-4868\,d_{-220}$) was used. If we consider the function $L_{220}=F_1(F_2(d_{220}))$, we can obtain the relationship between the lateral size and the interplanar distance both along the [220] direction, i.e., $L_{220}=333-1.27\exp[(d_{220}-2.08)/0.0067]$ (Fig. 3). From this equation, for $d_{220}=d_{\mathrm{InP}}=2.075$ Å the lateral size L_{220} is around 332 Å, in good agreement with the average wire base of 335 Å measured by AFM.

RHEED[8,9] and HRTEM results have shown that the InAs nanowires present (114) and (−1−14) facets parallel to the [−220] direction [see Fig. 4(a)]. Taking in account the shape of the wire cross section and the average base width measured by GIXRD, we obtain a direct relationship between the strain and the *z* position in the nanowire. Figure 4(b) shows the strain maps of the wires along directions [220] and [−220]. Clearly there is a much larger strain relaxation across the wires than along them, as expected from Fig. 2(a). The large relaxation of the elastic energy across the wires could justify the formation of these strained nanostructures instead of a flat and strained InAs layer. However, the high strain anisotropy could be at the origin of the shape transition (from wires to dots) previously reported.[8]

In summary, we have studied the strain relaxation of self assembled InAs/InP(001) nanowires using grazing incidence x-ray diffraction. A remarkable strain anisotropy was observed and quantified by mapping out the x-ray intensity near reciprocal lattice points of the substrate in two crystalline directions parallel to the substrate surface. These results can play a very important role in not only understanding the metastability of the InAs nanowires with respect to quantum dots, but also to study the influence of strain in the electronic properties of these asymmetric nanostructures.

H.R.G. and J.R.R.B. acknowledge financial support from FAPESP. This work was supported by FAPESP, CNPq, and FINEP. The HRTEM and GIXRD measurements were made at the National Laboratory of Synchrotron Light (LNLS-Brazil).[12]

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