Shape-mediated anisotropic strain in self-assembled InP/In_{0.48}Ga_{0.52}P quantum dots

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InP quantum dots grown on (001) InGaP/GaAs exhibit a pronounced size anisotropy with respect to the [110] and $[1\bar{1}0]$ directions. This asymmetry leads to a remarkable polarization dependence of photoluminescence spectra and to different elastic relaxation in these directions. The strain distribution is investigated by x-ray diffuse scattering along with respective kinematical simulations using linear elasticity theory. The geometric aspect ratios of island height and island base widths are evaluated with high accuracy and the influence of these ratios on the strain field inside the quantum dots is discussed.

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Structural properties such as size, shape, elastic strain, and its spatial distribution strongly influence the optical properties of semiconductor quantum dots (QD's).¹ In principle, the electronic energy levels and respective optical matrix elements are determined by the explicit (e.g., asymmetric) shape and its associated anisotropic strain field inside the QD and the surrounding barrier layers. For reasons of feasibility, however, a fixed QD shape is often used in theoretical calculations of strain and electronic structure, and the dependence of the optical properties on simple geometric parameters is discussed. Among them are the vertical aspect ratio $Q = w/2h$ of island base width w and height h ,^{2,3} and the lateral aspect ratio w_1/w_2 reflecting different QD base widths w_1 and w_2 in different lateral directions.⁴

The characterization, understanding, and control of the QD size and shape are important not only for a fundamental understanding of the optical properties, but also for future applications in optical devices. In III-V materials systems such as InAs/GaAs or InP/InGaP, the most popular way of generating QD's is through the use of the Stranski-Krastanow growth mode. It is generally accepted that the equilibrium shape of such self-assembled strained islands is determined by the balance of surface free energy and elastic strain energy. Since real surfaces are often strongly anisotropic, remarkable deviations from highly symmetrical islands (e.g., hemispherical QD's or lens shaped rotationally symmetric QD's⁵) may appear. This anisotropy in surface free energy may cause a faceting of the island surface, resulting in a complicated QD shape.⁶ The situation can be further complicated by kinetic limitations during growth; e.g., anisotropic surface diffusion lengths may also have a large influence on the QD shape.⁷ Consequently, a large variety of QD shapes has been reported experimentally.^{4,8-13} These observations were accompanied by various theoretical studies calculating the equilibrium shape of a QD and its dependence on growth kinetics.¹⁴⁻¹⁷ In the present paper we report on InP QD's grown on (001)In_{0.48}Ga_{0.52}P/GaAs which exhibit a pronounced shape asymmetry with respect to the [110] and $[1\bar{1}0]$ directions.¹⁸

Samples were grown by gas source molecular beam epitaxy (GSMBE) on GaAs (001) substrates. First, a 100-nm-

thick GaAs buffer was grown at 500 °C at a rate of 0.9 $\mu\text{m/h}$, followed by the growth of In_{0.48}Ga_{0.52}P at 415 °C. The surface of In_{0.48}Ga_{0.52}P shows a (2×1) reconstruction. During the growth process reflection high-energy electron diffraction (RHEED) patterns were monitored *in situ*. At the beginning of InP growth ($T = 410$ °C), the RHEED pattern appears streaky and becomes gradually spotty after the deposition of about 3 monolayers (ML) InP. In this study we focus on a sample with free-standing InP QD's resulting from a deposition of 5 ML of InP on the surface of 500 nm In_{0.48}Ga_{0.52}P. A high QD density of about $5 \times 10^{10} \text{ cm}^{-2}$ was achieved. A similar sample with buried InP QD's (6 ML InP), but capped with 15 nm In_{0.48}Ga_{0.52}P was prepared for photoluminescence (PL) investigations.

An atomic force micrograph (AFM) as displayed in Fig. 1 clearly shows the elongated shape of the free-standing InP quantum dots. A statistical analysis from these and other AFM pictures yields average island base widths along [110] and $[1\bar{1}0]$ of about $w_1 := w_{110} = 45 \text{ nm} \pm 10 \text{ nm}$ and $w_2 := w_{1\bar{1}0} = 30 \text{ nm} \pm 10 \text{ nm}$, respectively, with an average height of about $h = 8 \text{ nm}$. Cross-sectional transmission electron microscopy (TEM) reveals flat lens-shaped objects or

FIG. 1. Atomic force micrograph of free-standing InP quantum dots grown on (001) In_{0.48}Ga_{0.52}P/GaAs.

flat faceted objects rather than steep domelike features.¹⁹ Also scanning electron microscopy (SEM) at free-standing QD's gives some hints into a weak shape anisotropy, although the contrast is only poor. Surprisingly, on-zone bright field images in plan view TEM seem to show InP QD's with their edges aligned to the $\langle 100 \rangle$ directions.¹⁹ However, as demonstrated by Liao *et al.*²⁰ the interpretation of these images is not straightforward but requires multiple-beam dynamical image simulations.

The InP QD's as reported here are elongated along the $[110]$ direction. By contrast Jin-Phillipp and Phillipp have observed InP QD's that extend along the $[1\bar{1}0]$ direction with a higher lateral aspect ratio of $w_2/w_1 = 60 \text{ nm}:20 \text{ nm}$.²¹ Also Sugisaki *et al.*²² found InP islands which are elongated along $[1\bar{1}0]$ with a, however, rather small lateral aspect ratio. It is maybe interesting to note that, also, InAs QD's grown on (001)GaAs tend to elongate along the $[1\bar{1}0]$ direction.^{4,23,24} In order to avoid misinterpretation by a possibly wrong assignment of the crystallographic orientation of the GaAs substrate the $[110]$ and $[1\bar{1}0]$ directions have been checked by evaluating the orientation of oval defects²⁵ of the GaAs substrate. Our results agree with the data sheet as given by the producer.

The reasons for the elongation of the InP QD's along $[110]$ are not yet clarified and need theoretical modeling. The equilibrium island shape can be determined by density functional theory (DFT). Calculations that combine elasticity theory with microscopic parameters and surface free energies as determined by DFT are available for, e.g., InAs quantum dots¹⁷ but—to our knowledge—have not been carried out yet for InP quantum dots. They would clarify as to what extent the asymmetric shape can be explained in terms of total energy minimization. Another important parameter that can modify growth is the surface miscut which has been shown to be important in determining the shape anisotropy. At sufficiently large values of typically 2° the size, shape, and positional correlation of quantum dots can be manipulated by the terrace width of the substrate (see, e.g., Ref. 26). The terrace width, on the other hand, depends on the state of step bunching at the sample surface which can be changed by employing different growth conditions and different buffer layer thicknesses. The GaAs substrates that are used in the present paper do not exhibit any remarkable surface miscut. It is smaller than 0.05° as determined by x-ray diffraction. This small value of 0.05° corresponds to a terrace width of at least 300 nm which is far too high in order to influence the three-dimensional (3D) growth of the InP islands. We do not, therefore, expect the small miscut of $\approx 0.05^\circ$ to play a role. A possible reason for the elongated shape could be kinetic limitations during growth. It is well known from kinetic Monte Carlo simulations that anisotropic diffusion lengths lead to elongated islands.⁷ It is possible that different diffusion lengths can be induced by the (2×1) surface-reconstruction. A detailed analysis on how surface reconstruction is influencing growth has, however, not been carried out yet.

In order to get a statistically relevant measure of the size asymmetry, grazing-incidence small-angle x-ray

FIG. 2. In-plane grazing incidence small angle x-ray scattering (GISAXS) of the sample as shown in Fig. 1. The elliptically shaped intensity distribution with the main axis along $[1\bar{1}0]$ is a consequence of the elongated QD shape along $[110]$. The aspect ratio of the ellipse, $\Delta q_{1\bar{1}0}/\Delta q_{110}$, in reciprocal space inversely scales with the corresponding lateral aspect ratio $w_{1\bar{1}0}/w_{110}$, in real space. Four peaks are superimposed on the ellipse which are due to positional correlation along the $\langle 100 \rangle$ directions.

scattering^{27,28} (GISAXS) has been performed. The elliptically shaped intensity distribution as shown in Fig. 2 reflects the asymmetric quantum dot shape. In good approximation the horizontal aspect ratio β of the ellipse is connected to the island base widths along $[110]$ and $[1\bar{1}0]$ via $\beta := \Delta q_{1\bar{1}0}/\Delta q_{110} = w_{110}/w_{1\bar{1}0} \approx 1.5$ which is in good agreement with the aspect ratio as estimated by AFM. Superimposed on the ellipse in Fig. 2 are four strong peaks that are connected to positional correlation along the lateral $\langle 100 \rangle$ directions. The evolution of positional correlation as a function of InP deposition has been already described in a previous paper¹⁹ and will not be further discussed here.

The optical matrix elements and thus the PL spectrum of QD's often show a pronounced polarization anisotropy. In order to study the effect of the asymmetric dot shape and the anisotropic strain field, we investigated the lateral linear polarization of the PL from capped InP QD's. The PL was excited using the 413.1 nm line of an Ar⁺ laser. The PL signal was dispersed in a DILOR spectrograph XY800 and detected by a charged coupled device (CCD) camera. Since the dots are elongated along the $[110]$ direction, we expect polarization anisotropy between the $[110]$ and $[1\bar{1}0]$ directions.^{4,23,24} Indeed, the photoluminescence (Fig. 3) reveals a remarkable polarization anisotropy of $\rho = (I_{[110]} - I_{[1\bar{1}0]})/(I_{[110]} + I_{[1\bar{1}0]}) \approx 36\%$, where $I_{[110]}$ and $I_{[1\bar{1}0]}$ denote the integrated PL intensities along the $[110]$ and $[1\bar{1}0]$ directions, respectively. No PL polarization anisotropy was observed with respect to the $[100]$ and $[010]$ directions, and also the polarization anisotropy of the In_{0.48}Ga_{0.52}P buffer and GaAs substrate vanished.

Interpretation of the PL data requires detailed theoretical investigations. It is known from these that the optical polarization anisotropy is caused by the mixing of heavy-hole and light-hole states.²⁹ This coupling can be induced by asymmetric lateral confinement and anisotropic lateral strain.²⁴ The asymmetric lateral confinement due to an asymmetric QD shape yields an increased lateral polarization in the direction of the QD elongation,⁴ i.e., in our case the $[110]$

FIG. 3. PL spectra (10 K) of buried InP QD's polarized linearly along $[110]$ and $[1\bar{1}0]$. The orientation and the different island base widths along $[110]$ and $[1\bar{1}0]$ have been sketched schematically.

direction. On the other hand, as will be discussed below in more detail, lateral strain relaxation is most efficient along the shorter axis of the QD, leading to a reduced lateral polarization along the $[1\bar{1}0]$ direction. Consequently, both different lateral confinement and strain anisotropy enhances the degree of polarization along $[110]$.

Anisotropic lateral strain inside the QD's is, however, not necessarily connected to an asymmetric QD shape. This has been recently shown by Sugisaki *et al.*²² who observed a strong optical polarization dependence of InP quantum dots that exhibit nearly identical island base widths along $[110]$ and $[1\bar{1}0]$. Moreover, strong anisotropy was found also for the PL signal from the InGaP matrix. The authors claim that the polarization anisotropy is induced by anisotropic strain in the InGaP barrier layers which is due to the formation of horizontal composition changes along the $[110]$ and $[1\bar{1}0]$ directions.³⁰ Since we do not observe any polarization dependence of the InGaP buffer, we can exclude this interpretation for the samples investigated here. Instead, the measured optical polarization anisotropy is induced by the size elongation along $[110]$. This result, therefore, also proves that the QD's are still asymmetric with respect to $[110]$ and $[1\bar{1}0]$ even after they have been overgrown by $\text{In}_{0.48}\text{Ga}_{0.52}\text{P}$.

We will now discuss how the shape influences the strain relaxation inside the QD. From elasticity theory it is known that the strain distribution inside a QD is—at a given fixed shape—independent of the QD size.³¹ However, as will be addressed in this paper, it is critically sensitive to the shape. The strain distribution may, therefore, serve as a sensitive probe of the QD shape. In this work, an indirect method is used, whereby the strain distribution inside and around QD's is measured by x-ray diffuse scattering. The experimental x-ray scattering pattern is then compared with respective kinematical simulations using the finite element method (FEM) which is based on elasticity theory. Since structural properties such as shape, size, and composition sensitively enter these simulations, the calculations can be refined until satisfactory agreement with experiment is achieved. A detailed description of this method is given in Refs. 32 and 33.

The rather moderate lattice mismatch—as compared to InAs/GaAs—of 3.8% between InP ($a = 5.87 \text{ \AA}$) and

FIG. 4. X-ray diffuse scattering of free-standing InP QD's in the vicinity of the $1\bar{1}3$ and 113 reciprocal lattice points: (a),(b) experimental and (c),(d) respective simulations. The intensity scale logarithmically varies from black to white as indicated at the right side. The InGaP buffer layer and GaAs substrate Bragg peaks are not shown here since they do not reveal information about the InP quantum dots. They are located at $q_{001} = 3.335 \text{ \AA}^{-1}$ and $q_{110} = q_{1\bar{1}0} = 1.572 \text{ \AA}^{-1}$ as marked by vertical white lines. These correspond to the crystal truncation rods (CTR's) of the sample surface, whereas the thin white line at the right side of the CTR's is an experimental artifact.

$\text{In}_{0.48}\text{Ga}_{0.52}\text{P}$ ($a = 5.65 \text{ \AA}$) ensures that linear elasticity theory can be used in very good approximation. The continuum elastic properties of III-V materials exhibit fourfold symmetry, and, in particular, the $[110]$ and $[1\bar{1}0]$ directions are treated equivalently. Nevertheless, different strain relaxations may occur due to an asymmetric QD shape with respect to these two directions. This shape-induced anisotropic strain relaxation is much stronger than effects that are caused by the implementation of the exact atomistic twofold symmetry as discussed by Pryor *et al.*³⁴

Intense synchrotron radiation as provided by the BW2 wiggler station at HASYLAB/DESY has been used in the x-ray scattering experiments. Details of the experimental setup are given in Ref. 32. In order to obtain complete information, a variety of reflections was investigated with consistent results. In Figs. 4(a) and 4(b) the experimental x-ray diffuse intensity in the vicinity of the $1\bar{1}3$ and 113 reciprocal lattice points is displayed for the free-standing InP QD's, respectively. The diffuse intensity is widely spread out in reciprocal space and the peak position is shifted by $\delta q_{1\bar{1}0}$ and δq_{110} with respect to the corresponding values $q_{1\bar{1}0}$ and q_{110} of the InGaP buffer reflection (as marked by vertical

FIG. 5. Measured x-ray diffuse scattering of free-standing InP QD's in the vicinity of the (a) 404 and (b) 044 reciprocal lattice points, (c) simulation. The close similarity of (a) and (b) proves that there is no strain anisotropy with respect to the $[100]$ and $[010]$ directions. The intensity scale logarithmically varies from black to white. The InGaP buffer layer and GaAs substrate Bragg peaks (not shown here) are located at $q_{001} = 4.445 \text{ \AA}^{-1}$ and $q_{100} = q_{010} = 4.445 \text{ \AA}^{-1}$ as marked by vertical white lines. These correspond to the crystal truncation rods (CTR's) of the sample surface, whereas the thin white line at the right of the CTR's is an experimental artifact.

white lines in Fig. 4). These shifts are in good approximation related to the respective mean values of total elastic strain components³⁵ through

$$\langle \varepsilon_{110} \rangle = -\frac{\delta q_{110}}{q_{110}}, \quad (1a)$$

$$\langle \varepsilon_{1\bar{1}0} \rangle = -\frac{\delta q_{1\bar{1}0}}{q_{1\bar{1}0}}. \quad (1b)$$

Evaluation of Figs. 4(a) and 4(b) yields values of $\langle \varepsilon_{1\bar{1}0} \rangle = (9.2 \pm 0.5) \times 10^{-3}$ and $\langle \varepsilon_{110} \rangle = (5.0 \pm 0.5) \times 10^{-3}$. It is striking that the elastic relaxation is different for the $[110]$ and $[1\bar{1}0]$ directions. This is related to the elongated shape of the QD's along the $[110]$ direction. Since the influence of the underlying GaAs substrate and InGaP buffer is larger in the elongated direction than along the shorter direction, the lattice can relax more efficiently along $[1\bar{1}0]$ than along $[110]$. On the other hand, as depicted in Figs. 5(a) and 5(b), the diffuse intensities in the vicinity of the 404 and 044 reciprocal lattice points are identical proving that the strain field is identical along the $[100]$ and $[010]$ directions.

A detailed understanding of the experimental data requires careful theoretical modeling. First, a certain island model, i.e., shape, size, and lattice mismatch, is created. Second, the elastic strain field inside and around the islands is calculated numerically by using the FEM. Finally, this strain field is used to calculate the diffuse x-ray scattering within the kinematical scattering approach.³² In subsequent steps, the shape and size are refined until satisfactory agreement with experiment is achieved.

The simulations can be only fitted to the experimental data by using a somewhat reduced lattice mismatch of

FIG. 6. (a) Mean total strain—as evaluated from calculated x-ray diffuse scattering maps similar to Figs. 4(c) and 4(d)—inside free-standing InP QD's $[\varepsilon_{110}]$ ($\bullet$) and $[\varepsilon_{1\bar{1}0}]$ ($\circ$) as a function of the QD height h . QD base widths of $w_1 = 50 \text{ nm}$ and $w_2 = 30 \text{ nm}$ have been used. (b) Calculated mean asymmetry ratio $\langle \alpha \rangle = \langle \varepsilon_{1\bar{1}0} \rangle / \langle \varepsilon_{110} \rangle$ ($\bullet$) plotted against the lateral aspect ratio Q_1/Q_2 of the QD. The horizontal dashed lines represent respective experimental values as taken from Figs. 4(a) and 4(b). Solid lines are guides for the eyes.

$\Delta a/a = 2.58\%$ between the QD's and the underlying $\text{In}_{0.48}\text{Ga}_{0.52}\text{P}$ buffer. It is thus very likely that intermixing of In and Ga takes place during growth. The reduced mismatch corresponds to $\text{In}_{0.83}\text{Ga}_{0.17}\text{P}$ QD's. The influence of a possible composition gradient of In inside the QD's has not been considered in this study and the QD's as used for the simulations are modeled as having a homogeneous composition.

For islands exhibiting steep side faces (e.g., truncated pyramid with steep facets) simulations and experiment are at clear variance. By contrast, the use of QD's with shallow faces leads to remarkably better results. Therefore, simulations as further discussed in this paper use flat faceted pyramids with rectangular base. The remaining free parameters of the simulations are the respective QD base widths w_1 and w_2 along $[110]$ and $[1\bar{1}0]$ and the QD height h . The simulations turn out to be very sensitive to these parameters and very good agreement with experiment is achieved for $w_1 = w_{110} = 50 \text{ nm} \pm 5 \text{ nm}$, $w_2 = w_{1\bar{1}0} = 30 \text{ nm} \pm 5 \text{ nm}$, and $h = 7 \text{ nm} \pm 1 \text{ nm}$ which is in good agreement with AFM.

The corresponding calculated x-ray diffuse scattering around the $1\bar{1}3$, 113 , and 044 reciprocal lattice points is displayed in Figs. 4(c), 4(d), and 5(c), respectively. In particular, we would like to emphasize the following points: (i) the simulations reproduce the overall shape of experimental diffuse intensity [Figs. 4(a), 4(b), 5(a), and 5(b)], proving that the calculated elastic strain field matches the real one; (ii) the absolute positions of the maximum of the diffuse

FIG. 7. Calculated strain tensor components (a) ε_{110} and (b) $\varepsilon_{1\bar{1}0}$ in $(1\bar{1}0)$ and (110) planes, respectively, through the symmetry axis of a strained pyramid ($w_1=50$ nm, $w_2=30$ nm, $h=7$ nm, lattice mismatch 2.58%) attached on a $\text{In}_{0.48}\text{Ga}_{0.52}\text{P}$ buffer layer.

intensity distribution in reciprocal space are—within the given error bars—identical for both experiment and simulations; and (iii) the experimentally determined and simulated values of the mean strength of asymmetry $\langle\alpha\rangle$ given by

$$\langle\alpha\rangle = \frac{\langle\varepsilon_{1\bar{1}0}\rangle}{\langle\varepsilon_{110}\rangle} \quad (2)$$

agree within the estimated uncertainties: experimentally we find $\langle\alpha\rangle = 1.84 \pm 0.10$ and the simulated value is $\langle\alpha\rangle = 1.71 \pm 0.10$.

Since the QD size (at fixed shape) does not influence the strain distribution, only two of the parameters w_1 , w_2 and h are independent. The two remaining relevant quantities which determine the strain distribution are the geometric aspect ratios defined as

$$Q_1 = \frac{w_1}{2h}, \quad (3a)$$

$$Q_2 = \frac{w_2}{2h}. \quad (3b)$$

When increasing the QD height h at fixed base widths w_1 and w_2 the strain inside the QD may relax more efficiently. This is demonstrated in Fig. 6(a). Here the mean total strains $\langle\varepsilon_{1\bar{1}0}\rangle$ and $\langle\varepsilon_{110}\rangle$ —which have been evaluated from the peak positions in simulated x-ray diffuse scattering maps—are plotted as a function of the island height h . As a result of our simulations the mean lateral strain tensor components $\langle\varepsilon_{1\bar{1}0}\rangle$ and $\langle\varepsilon_{110}\rangle$ linearly increase as a function of the island

FIG. 8. Calculated strain tensor components: (a) selected line scans through symmetry axis of the pyramid shown in Fig. 7 for $\varepsilon_{110}(z)$ (■), $\varepsilon_{1\bar{1}0}(z)$ (●), and $\alpha = \varepsilon_{1\bar{1}0}/\varepsilon_{110}$ (△). (b) Respective line scans through a pyramid with $w_1=50$ nm, $w_2=30$ nm, and $h=15$ nm.

height. On the other hand, at fixed QD height h the mean total strain components $\langle\varepsilon_{110}\rangle$ and $\langle\varepsilon_{1\bar{1}0}\rangle$ inversely scale with the QD base widths w_1 and w_2 , respectively. As a consequence, $\langle\alpha\rangle$ varies linearly with the lateral aspect ratio Q_1/Q_2 [Fig. 6(b)]. This useful scaling behavior facilitates a systematic refinement of the simulation.

Although appearing quite reasonable, the linear scaling laws for the *mean* total strains (i.e., averaged over the entire island) as plotted in Fig. 6 are not obvious. This can be demonstrated by finite element calculations. We first focus on a pyramid with $w_1=50$ nm, $w_2=30$ nm, and $h=7$ nm. In Figs. 7(a) and 7(b) calculated values of ε_{110} and $\varepsilon_{1\bar{1}0}$ are shown in respective $(1\bar{1}0)$ and (110) planes through the symmetry axis of the pyramid. Please note that Fig. 7 displays only a part of the sample that has been calculated by the FEM. The calculations prove that ε_{110} and $\varepsilon_{1\bar{1}0}$ are different inside the pyramid and underlying InGaP buffer, and—inside the pyramid—they monotonically increase with larger values of z . This means that areas inside the island close to $z=0$ are strongly stressed and not able to relax horizontally. Only with increasing position z above the wetting layer may elastic relaxation take place to some extent. This behavior is also illustrated in selected line scans for $\varepsilon_{110}(z)$, $\varepsilon_{1\bar{1}0}(z)$ and $\alpha(z) = \varepsilon_{1\bar{1}0}(z)/\varepsilon_{110}(z)$ along the symmetry axis of the pyramid [Fig. 8(a)]. Note that the island is totally relaxed nowhere; i.e., ε_{110} and $\varepsilon_{1\bar{1}0}$ are always smaller than the lattice mismatch of $\Delta a/a = 2.58\%$ between

the pyramid and the buffer. As a consequence the ratio $\alpha(z)$ is nearly constant for $z \geq 0$. This behavior—which can be observed for island heights h up to about 10 nm—is the main reason for the linear scaling law as plotted in Fig. 6(a) for the *mean* total strains. At sufficiently large island height h the situation will, however, change. This is illustrated in Fig. 8(b) where respective line scans for a pyramid with $w_1 = 50$ nm, $w_2 = 30$ nm, and $h = 15$ nm are shown. Here, both $\varepsilon_{1\bar{1}0}(z)$ and $\varepsilon_{1\bar{1}0}(z)$ merge at the top of the pyramid, and, consequently, $\alpha(z)$ is locally varying inside the island. This is also reflected in Fig. 6(a) for the mean total strains which show remarkable deviations from the linear scaling at $h = 15$ nm.

The calculated diffuse scattering exhibits pronounced shape-induced diffuse scattering that gives rise to intensity oscillations (“fringes”). One expects, however, that these fringes may not be observable in the experimental data due to size fluctuations of the QD’s and, in fact, no fringes are experimentally observed. As pointed out before, the strain field scales solely with the geometric aspect ratios Q_1 and Q_2 . Therefore, a possible QD size distribution does not change the distribution of strain-induced x-ray diffuse scattering in reciprocal space as long as the shape is not changed. The good agreement between experiment and simulation is, therefore, indicative of a rather uniform shape of the QD’s although the size fluctuations (15% rms) as estimated by AFM are remarkable.

For a faceted pyramid with rectangular base the evaluated values of $Q_1 = 3.57$ and $Q_2 = 2.14$ correspond to QD side faces which are tilted by 15.6° and 25.0° with respect to the (001) surface and are thus close to (115) (15.8°) and (113) (25.2°) facets, respectively.

In summary, we have determined the shape of free-standing InP quantum dots with a pronounced shape anisotropy with respect to the [110] and $[1\bar{1}0]$ directions. The elongation of the QD’s along the [110] direction leads to a polarization dependence of photoluminescence spectra both because of the directional difference in spatial confinement as well as because of the resulting strain anisotropy. X-ray diffuse scattering along with respective calculations makes it possible to evaluate the geometric aspect ratios Q_1 and Q_2 with rather high accuracy. The asymmetry ratio $\langle \alpha \rangle$ of mean horizontal elastic relaxation of free-standing QD’s is (at fixed lateral aspect ratio Q_1/Q_2) constant for island heights below 15 nm and it solely scales linearly with Q_1/Q_2 . At larger island heights deviations from that simple scaling are expected.

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- ³⁵ ε_{110} and $\varepsilon_{1\bar{1}0}$ are the diagonal elements of the strain tensor ε_{ij} with respect to the $[110]$ and $[1\bar{1}0]$ directions, respectively. Please note that the total strain is used in the presentations; i.e., the $\text{In}_{0.48}\text{Ga}_{0.52}\text{P}$ buffer (which is lattice matched to GaAs) is used as a reference everywhere.