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Evidence for strain in and around InAs quantum dots in GaAs from ion-channeling experiments

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Strain in and around pyramidal InAs/GaAs quantum dots (QD’s) fabricated by molecular-beam-epitaxy influences the density of states of the confined charge carriers. The presence of strain in QD’s is required to explain their optical properties. In this paper MeV ion-channeling experiments are presented which provide evidence for the presence of strain in and around InAs QD’s in GaAs. The small dimensions of the QD’s (typical height 4 nm) and the presence of a wetting layer complicate the interpretation of channeling measurements, but our experiments show that extended strain fields around the QD’s induce ion steering which accounts for the observed channeling behavior.

I. INTRODUCTION

One of the hot topics in semiconductor physics is the production and study of low-dimensional structures, i.e., structures in which the charge carriers are confined to less than three dimensions. This confinement of the charge carriers changes the density of states, which leads to sharper optical transitions. The threshold current density and its temperature dependence are reduced, and furthermore, the energy of the transition can be controlled by the well thickness. These effects are more pronounced for higher levels of confinement, and can be achieved in either quantum wire lasers, where charge carriers are free to move in only one direction; or quantum box or quantum dot (QD) lasers, where there is total confinement with no direction of freedom.

It is very interesting that QD’s can be grown without using lithography via so-called self-assembly. Such QD’s are manufactured by the deposition of about 2 ML of InAs on GaAs, which results in the formation of InAs islands during growth. Since the critical layer thickness for the growth of a single coherent strained InAs film on GaAs is only 1.4 ML, island formation becomes favorable as a mechanism to relieve strain. Photoluminescence spectra, however, point to (partially) strained QD’s.

MeV ion channeling is a well-known technique to investigate strain of thin films. Usually it is restricted to an analysis of films with a thickness larger than approximately 20 nm. The typical height of QD’s, which is only 4 nm, and the low areal density of In in the investigated QD samples (10^10 QD cm^-2, 11×10^14 In atom cm^-2), complicate an experimental verification of the presence of strain. The goal of this paper is to investigate whether strain in QD’s can be measured with MeV ion-channeling.

II. EXPERIMENT

The QD samples were grown in a Varian GenII molecular-beam-epitaxy system. A buffer layer consisting of 675 nm GaAs was grown on a [001]-oriented GaAs wafer. Subsequently, a layer of 0.66 nm InAs (corresponding to 2 ML) was grown at a temperature of 555 °C. Due to the 7% lattice mismatch of InAs (lattice constant of 0.605 nm) with respect to GaAs (lattice constant of 0.565 nm), three-dimensional islands are formed when more than 1.4 ML of InAs are grown. This self-assembly of three-dimensional islands is known as the Straniski-Krastanov growth mode. In between the islands a 1-ML-thick wetting layer of InAs containing about 50% of the total In is present. The InAs is capped with 98 nm GaAs, 30 nm Al_{0.33}Ga_{0.67}As, and 17 nm GaAs. The fluctuation in the size of these self-organized quantum dots can be as small as 10%, and the InAs QD’s are typically 10 nm in diameter and about 4 nm high depending on the growth conditions.

For ion-beam analysis experiments, the QD sample was placed in a three-axes goniometer with an angular resolution <0.005°. Channeling experiments have been performed using 4-MeV He^+ ions from the 2-30-MeV AVF Cyclotron at the Eindhoven University of Technology. The beam divergence was 0.09° full width at half maximum (FWHM). Backscattered ions were detected with a 1200 mm² Canberra passivated implanted planar silicon (PIPS) detector positioned at a scattering angle of 160°. A 11.4-μm-thick mylar stopper foil (C_{10}H_{10}O_4) was placed in front of the detector to decrease the count rate of the GaAs substrate and to limit the pileup. The energy straggling of the ions in the foil was approximately 28 keV. The energy resolution of the system is also determined by the kinematic spread over the detector (26 keV) and its intrinsic energy resolution (~40 keV). The resulting FWHM of the In peak was 55 keV, which is still significantly less than the energy separation of the In peak and the GaAs edge in the backscattering spectrum (168 keV). Consequently, angular scans of In can be recorded by plotting the integrated In yield as a function of angle. A second 10 mm² Canberra PIPS detector was positioned at a scattering angle of 130°. This detector was used to obtain angular scans of GaAs from Rutherford backscattering spectrometry (RBS) spectra with a better energy resolution: the kinematic
spread over the detector is smaller and energy straggling in a foil is absent. The angular scans through the [011] axes are performed with an angle of 45° between the surface normal of the sample and the incoming beam.

III. RESULTS

Ion-channeling is usually applied in combination with RBS. This leads to energy (or depth) yield spectra as presented in Fig. 1. Figure 1 shows the random and [011] channeled RBS spectra of a QD sample measured with the 1200-mm² detector. The random spectrum was obtained during spinning the sample 90° around its surface normal after the beam was tilted away from the [011] axis by 2°. The minimum yield is the ratio between the channeling and random yields. For GaAs these are the integrated yields from the 10-mm² detector from a depth of 6 to 16 nm in the channeled and random spectra respectively, while for In the channeling and random yields are the integrated yields of the entire In peak in the channeling and random spectra respectively. The minimum yields found in this way are $\chi_{\text{min}} = 3.5\%$ for GaAs and 18.0% for In. The FWHM of the In peak is 54 keV. The energy difference between the ions scattered on Ga and As is too small to identify these contributions separately.

To determine the exact direction of a crystal axis, the yield in a certain depth interval is measured as a function of the angle $\psi$ between the incoming beam and the crystal axis. These so-called angular scans have been measured through the [011] and [001] axes of a QD sample, both in the (100) plane. They are shown in Figs. 2(a) and 2(b) respectively. In the same way as mentioned above, the GaAs yield has been determined in a depth interval of 6–16 nm and the In yield has been determined from the entire In peak. Table I summarizes the measured half-widths $\psi_{1/2}$'s and minimum yields $\chi_{\text{min}}$'s of GaAs and In for both angular scans.

The interpretation of the angular scans is complicated by the limited height of the QD’s, no more than approximately 4 nm, and the presence of an InAs wetting layer. For a buried ultrathin homogeneous layer (4 nm), the length of the atomic strings along which the ion steering occurs is far below the typical lengths ($\geq 10$ nm for ion energies $\geq 4$ MeV) required to obtain channeling characteristics representative of the crystal structure of the ultrathin layer. Consequently, the shape and position of an angular scan is not only representative of the ultrathin layer (or QD’s), but is also determined by the flux pattern (channeled or nonchanneled) emerging from the overlying (GaAs) crystal reaching the ultrathin layer (or QD’s).

Furthermore, in the samples containing the QD’s, about 50% of the In is in the tetragonally deformed homogeneous wetting layer. Because this wetting layer is only 1 ML thick, the channeling behavior of the In signal from this wetting layer will be determined by the position of the In atoms in the flux pattern emerging from the GaAs capping layer.

A. Strain

Using Poisson’s ratio $\nu = 0.35$ for InAs, the tetragonal distortion of a fully strained homogeneous InAs film on a GaAs crystal without relaxation (like the wetting layer in the QD samples) is $\varepsilon_T = 0.10$. Consequently, for a fully strained

<table>
<thead>
<tr>
<th></th>
<th>$\psi_{1/2}$</th>
<th>$\chi_{\text{min}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>GaAs[011]</td>
<td>(0.69 ± 0.02)°</td>
<td>(3.3 ± 0.1)%</td>
</tr>
<tr>
<td>GaAs[001]</td>
<td>(0.60 ± 0.02)°</td>
<td>(3.5 ± 0.1)%</td>
</tr>
<tr>
<td>In[011]</td>
<td>(0.44 ± 0.02)°</td>
<td>(18.0 ± 2.0)%</td>
</tr>
<tr>
<td>In[001]</td>
<td>(0.50 ± 0.02)°</td>
<td>(8.6 ± 1.4)%</td>
</tr>
</tbody>
</table>

FIG. 1. The random and [011]-channeled RBS spectra of a QD sample.

FIG. 2. The measured scans through the [011] (a) and [001] (b) axes of a QD sample.
InAs layer on GaAs the position of the [011] axis with respect to the [011] axis of the cubic GaAs substrate is shifted by 4.0° toward the [001] axis.

To relieve the strain in the InAs layer during growth, QD’s are formed, because strain energy can be relieved via surface tension, which in turn can be lowered by enlarging the surface. The surface tension can be minimized by creating crystal planes with the lowest surface energy. Crystal growth will also be lowest perpendicular to these planes, and they will become the boundaries of the crystal. For zinc-blende-type lattices, the planes with the lowest surface energy are the {111} planes, and although the shape of the QD’s is a controversial point in the literature, a truncated pyramid shape with {111} planes as sides is generally accepted. When free-standing QD’s are capped with GaAs, the strain energy again increases, and the presence of significant tetragonal distortion within the QD cannot be excluded. The strain present in the InAs wetting layer induces a shift of the [011] axis of 4.0°, which is the upper limit for the distortion in the QD’s.

Figure 2(a) shows that the minimum of the angular scan through the [011] axis in the (100) plane of the In signal coincides with the minimum of the angular scan through the [011] axis in the (100) plane of the GaAs signal. When the channeling behavior is assumed to be determined by the InAs strings, this would imply the absence of tetragonal distortion in the InAs QD’s. However, under this assumption, Fig. 2 reveals an anomaly in the width of both angular scans. For a bulk InAs crystal the half-width \( \psi_{1/2} \), is proportional to the characteristic angle \( \psi_1 \) as defined in the Lindhard model,

\[
\psi_1 = \left( \frac{2Z_1Z_2e^2}{4\pi\varepsilon_0Ed} \right)^{1/2},
\]

in which the atomic number of the incoming particle and the target atom are represented by \( Z_1 \) and \( Z_2 \), respectively, \( E \) is the energy of the incoming particle, and \( d \) is the lattice spacing along the channeling direction. The half-width \( \psi_{1/2} \) is related to the characteristic angle \( \psi_1 \) by a constant \( C_\psi \) (≈1), which depends predominantly on the vibrational amplitude of the atoms: \( \psi_{1/2} = C_\psi \psi_1 \). An In angular scan in bulk InAs is thus expected to be broader than a GaAs angular scan in bulk GaAs, because of the larger \( Z_2 \). With a 4-MeV He\(^+\) beam and an average \( Z_2 = 32 \) for GaAs, the characteristic angles are \( \psi_1(\{001\}) = 0.52°(d = 0.565 \text{ nm}) \) and \( \psi_1(\{011\}) = 0.62°(d = 0.400 \text{ nm}) \). For the In strings in InAs \( (Z_2 = 52) \) these characteristic angles are \( \psi_1(\{001\}) = 0.62°(d = 0.606 \text{ nm}) \) and \( \psi_1(\{011\}) = 0.74°(d = 0.429 \text{ nm}) \) respectively.

The characteristic angles for InAs have also been obtained by measurements on a [001]-oriented bulk InAs wafer. The measured half-widths are \( \psi_{1/2} = (0.65 ± 0.02)°(C_\psi = 1.05) \) and \( \psi_{1/2} = (0.77 ± 0.02)°(C_\psi = 1.04) \) for the [001] and [011] axes, respectively. Undoubtedly, the half-widths for both the [001] and [011] axial directions of the InAs QD’s in GaAs are anomalously small compared to both the calculated and measured characteristic angle.

From Table I the ratio of the half-widths of the [001] and [011] angular scans of the GaAs is consistent with the predicted dependence, but the ratio of the \( \psi_{1/2} \) values for the [001] and [011] angular scans of the InAs QD’s is opposite to that expected for a bulk InAs crystal. One possible explanation could be that the QD’s have a crystal orientation with the [011] axis of the InAs lined up with the [001] axis of the GaAs substrate. Such an orientation can easily be verified by measuring, for example, the orientation of the [001] and [011] planes and the [111] planes relative to the surface normal, because they will be different for [001]- and [011]-oriented crystals. The [001] axis is intersected by two [011] planes and two [001] planes, symmetrically placed at 45° rotations. The [011] axis has one [011] plane and one [001] plane perpendicular to each other, and also two [111] planes at 35.3° on either side of the [011] plane. Figure 3 shows the results of measurements on the orientation of the planes in the QD. It can be seen that the orientation of these planes coincides with those of the [001]-grown GaAs; thus the InAs seems to be [001] oriented in spite of the peculiar ratio of the \( \psi_{1/2} \) values from the In angular scans.

Calculations show that small displacements from substitutional sites (which is the case for the position of the In atoms in the wetting layer compared to the strings of the GaAs capping layer) result in a significant narrowing of the angular yield curve. It is, however, important to realize that for displacements caused by tetragonal distortion this narrowing would only apply for angular scans for off-normal axes, because the In atoms in the wetting layer have a displacement perpendicular to the channeling direction only for off-normal axes. Thus the geometry of the wetting layer influences only the measured half-width of the In angular scan for the [011] axis in the QD sample, being smaller than in a perfect bulk InAs crystal. But, from Fig. 2(b), it can be seen that the In angular scan is also smaller than the GaAs angular scan for the [001] axis. This implies that the narrowing is also a result of the specific crystal structure of the InAs in the QD’s.

**B. Minimum yield**

In channeling experiments the formation of a shadow cone reduces the nuclear encounter probability for atoms in a string, i.e., the first few atoms in a string shield the underlying atoms from the incoming particles. The first few atoms which make a substantial contribution to the formation of this shadow cone give rise to a surface peak. This is the peak in the yield of a channeled RBS spectrum that usually can be seen, because the nuclear encounter probability is much higher for the first few atoms in the strings in case of chan-
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FIG. 4. The nuclear encounter probability of the atoms in (011) and (001) axes of a cubic InAs lattice as calculated with the FLUX6 simulation package.

nelling. The number of atoms making a substantial contribution to this surface peak can be estimated from the number of atoms in a string (in terms of an areal density) contributing to the surface peak, which can be determined according to Feldman et al. 12 using the Coulomb shadow cone radius \( R_C \) and the two-dimensional, root-mean-square vibrational amplitude normal to the beam, \( \rho \), which depends on the temperature. Computer calculations allowed them to generate a universal curve, making it possible to calculate the surface peak intensity (atoms/row) from the ratio of \( \rho \) to the Molière radius \( R_M \), which in turn can be calculated from \( R_C \).

In our experiments the energy of the incoming particle is \( E = 4 \) MeV, the atomic number of the incoming particle is \( Z_1 = 2 \), and that of the target particle is \( Z_2 = 49 \) (In). \( \rho \) is taken to be 15 pm for InAs, 13 and the lattice spacing \( d \) depends on the channeling direction. Under these conditions 5 (whole) atoms per string contribute to the surface peak for In strings along the (001) axes and 6 atoms per string do so for In strings along the (011) axes of a perfect InAs crystal. 12 These sums contain substantial contributions (contribution to the total surface peak > 1%) from approximately 9 and 11 atoms in a string, respectively. If a uniform flux impinges on a layer that consists of all the atoms that make a substantial contribution to the surface peak, the minimum yield of this layer will be approximately 50%.

Figure 4 shows the results of nuclear encounter probability calculations for In atoms in a string along the [011] and [001] axes of a bulk cubic InAs crystal with 4-MeV \( \text{He}^+ \) ions as incoming particles. These calculations were done with the FLUX6 simulation package, 14 which calculates the two-dimensional, root-mean-square vibrational amplitude normal to the beam using a Debye temperature of 249 K. 15 The sum of the nuclear encounter probabilities as a function of the number of atoms in a string is plotted in Fig. 5. In this graph it can be seen that the contribution of the next atom to the surface peak is smaller than 1% from 8 atoms on for the (001) axes, and from 10 atoms on for (011) axes. This is in good agreement with the estimation made above.

For zinc-blende-type lattices, the 60° perfect dislocation is the most probable type of misfit dislocation to relieve compressive tetragonal strain (epitaxial growth of InAs on GaAs), when the layer is grown thicker than the critical layer thickness. 6 The perfect dislocations glide through the \{111\} planes, and are called perfect because the stacking sequence of the \{111\} planes remains intact. At the substrate interface, however, dislocation lines are formed. Only 1 ML is involved in the relaxation of compressive tetragonal strain via perfect dislocations in the \{111\} planes, while the rest of the crystal on both sides of the perfect dislocation is not deformed. If the QD’s have an equilibrium cubic InAs lattice structure, the misfit with the GaAs crystal is most likely to occur in the \{111\} planes, which form the boundaries of the pyramidal QD’s. Then, due to the 7% lattice mismatch of InAs with the GaAs, the flux pattern emerging from the GaAs averages out and appears as a uniform flux to the buried relaxed InAs QD’s. Just as a surface peak occurs for a nonburied InAs surface, an interface peak will occur in this case.

Scanning tunneling microscopy (STM) and TEM measurements show that the QD’s have a height of \( \sim 4 \) nm. 16 For the [001] direction this corresponds to a maximum string length of 6.6 atoms. Considering the truncated pyramid shape of the QD’s, an estimated maximum average string length of about 4.1 atoms InAs is seen by the channeled \( \text{He}^+ \) ions, which is far less than the 8 atoms calculated to make a substantial contribution to the interface peak. For the [011] direction the maximum string length is 13.2 atoms, and the estimated maximum average string length is about 9 atoms in the QD’s, while the first 10 atoms in a string would contribute to the interface peak. Thus, if the InAs in the QD’s is fully relaxed via 60° perfect dislocations, the minimum yield from the In in the QD’s is expected to be at least 50% of the random yield for the [011] axis.

The minimum yield from the In atoms in the wetting layer is fully determined by their position in the flux pattern emerging from the GaAs channels in the capping layer. Because the InAs wetting layer is fully strained, for the [011] axis the In atoms will be shifted 28% toward the center of the GaAs channels. Feldman et al. gave a model that roughly describes the depth-independent spatial flux distribution within the channels as a function of angle of incidence relative to the channel axis assuming cylindrical symmetry and the small \( r \) approximation to the standard potential. 17 From
this model for incidence parallel to the channels the flux at 28% of the distance to the center of the channel is about 10% of the flux for random incidence. Then, the minimum yield of the In atoms in the wetting layer will also be about 10% for the [011] axis. For the [001] axis the In atoms are not shifted, and the minimum yield will be a little lower than for the surrounding GaAs, because of the higher atomic number.

Remembering that half of the In atoms are in the QD’s and half of them are in the wetting layer, the separate contributions to the minimum yield can be combined. If the QD’s relieve their strain completely via 60° perfect dislocations, the total In minimum yield has to be at least 30% for the [011] axis and 25% for the [001] axis. However, from Table I it is clear that the measured minimum yield values are significantly less for both axes.

C. Strain fields

From the discussion presented above it can be concluded that the interface between the InAs QD’s and the GaAs capping layer does not behave like the interface between a cubic InAs film and a cubic GaAs capping layer. The minimum yield values must be the result of deformation in and around the QD’s: apparently, the crystal lattices of the capping layer and the QD’s are distorted near the interface in such a way that the channeled particles are steered from the GaAs channels into the InAs channels, i.e., the strings in the GaAs capping layer continue in the strings in the InAs QD’s. These channelling experiments thus provide evidence of the presence of extended strain fields in the GaAs required to induce steering into the InAs, which typically occurs at a length scale of >10 nm for 4-MeV He ions in GaAs and InAs. In literature, strain fields in and around the InAs QD’s have been suggested.1,8,18–20 It is interesting to note that the experimentally found width of the base of the pyramids (~10 nm) is able to accommodate one unit cell more of GaAs than InAs. If the strain is relieved via misfit dislocations, this would result in two GaAs half-planes per QD. Although these misfit dislocations cannot be excluded from our ion-channeling experiments, the optical performance of the QD’s and STM measurements point to the absence of these misfit dislocations.16,21 Thus the QD and the surrounding GaAs crystal structure are pseudomorphic, and it must be concluded that the difference in lattice constants of InAs and GaAs induces strain fields which induce a steering of the ions in a similar fashion as known to occur in the presence of misfit dislocations.

Furthermore, in the areas of a crystal which induce ion steering, the half-widths will be smaller than measured in a perfect crystal: the ions in the flux distribution in the channels which come closest to the strings will have a greater probability of being dechanneled in a curved crystal than in a perfect crystal, depending on the curvature. In combination with the channeling behavior in the wetting layer, this qualitatively explains the measured half-widths in the In angular scans for both the [001] and [011] directions.

IV. CONCLUSIONS

The present measurements confirm previous speculations about possible strain in and around QD’s, and exclude the presence of 60° perfect dislocations. The lattice mismatch between the InAs islands and the GaAs substrate causes strain fields, which extend from the QD’s into the surrounding GaAs matrix over a typical length scale of >10 nm. These extended strain fields induce a steering of the channeled particles from the GaAs channels into the InAs channels. This explains the observed channeling behavior, i.e., the measured minimum yields are low, despite the fact that the QD’s are too thin for shadow cone formation, and the half-widths of the angular scans are anomalously small.

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17 L. C. Feldman, J. W. Mayer, and S. T. Picraux, Materials Analysis by Ion Channeling (Ref. 11), Chap. 3, pp. 73–79.


