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Configuration of the misfit dislocation networks in uncapped and capped InN quantum dots

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A transmission electron microscopy study of the misfit dislocation (MD) networks between InN quantum dots (QDs) and GaN substrate/capping layer is presented. Applying the geometric phase algorithm in planar-view orientation, a complete characterization of the first interface shows a set of three families of 60° MDs lying along the three $\langle 11\bar{2}0\rangle$ directions without node formation. The growth of a GaN capping layer decreases the plastic relaxation degree of the InN QDs by a rearrangement of the MDs. The full relaxation of the capping layer suggest that no changes will occur in the QD strain state during later growths. © *2007 American Institute of Physics*. [DOI: 10.1063/1.2770776]

Indium nitride (InN) has the best electronic and transport properties among the nitrides[1] and has become of increasing interest in recent years. Furthermore, the recent establishment of its band gap as ~0.7 eV (Refs. 2 and 3) makes it a very promising material for the fabrication of optoelectronic devices working in the infrared range or for high efficiency solar cells.[4] Moreover, the combination of the intrinsic properties of InN with quantum confinement phenomena,[5] resulting from the growth of self-assembled quantum dots (QDs), promises further applications. Finally, the optical properties of nitrides can be strongly modified by strain due to high intrinsic piezoelectric polarization field coefficients.[6] Thus, an understanding and control of the mechanisms involved in strain relief are of great importance for the development of future InN QD-based devices.

For highly mismatched heterosystems it is well known that, from the very beginning of epitaxial growth, a large part of the lattice misfit is plastically relieved by the introduction of a high density of geometrical misfit dislocations (MDs).[7] These MDs are seen as extra half-planes in the material with lower lattice parameter that separate coherent regions with pseudomorphic growth. As a result, these epilayers have a strain state with lattice parameter close to the unstrained crystal and a highly dislocated interface that can be a source of threading dislocations. To achieve the functionality of a device, these active layers need to be capped, generating new stress fields that influence the residual strain state of the buried layer. In the present work, a complete description of the strain state and MD network generated at the interface during the growth and capping of InN QDs on GaN pseudosubstrates is presented. It will be shown in both cases that most of the strain induced by the lattice mismatch is accommodated by the generation of 60° MDs lying along the three main $\langle 11\bar{2}0\rangle$ directions without interaction between them. The effect of the introduction of a 20 nm thick, low temperature GaN capping layer on the strain state and configuration of the MD dislocation network is also discussed.

Two InN QD samples were grown on GaN/Al_2O_3 by metal-organic vapor phase epitaxy,[8] with the second sample containing a low-temperature (LT)-GaN capping layer. First, a buffer layer of GaN was grown on (0001) sapphire using the usual two-step process at a temperature close to 1000 °C. The temperature was then lowered to 550 °C and InN QDs with an average height of 12 ± 2 nm were deposited using a V/III ratio of 15 000 and NH_3 as a nitrogen precursor. This concluded the growth for the first sample. For the second, we used a process where a capping layer of GaN is deposited at low temperature (550 °C) in order to cover the dots and to prevent their decomposition at higher temperature. Once protected in this way, the growth temperature was raised to 1050 °C to recrystallize the low temperature GaN capping layer, resulting in a 20 nm thick single crystal GaN encapsulating the InN QDs. Conventional and high resolution transmission electron microscopy (HRTEM) in cross section (XTEM) and plan-view (PVTEM) geometries were carried out using JEOL 2011 and JEOL JEM2500 microscopes, both working at 200 kV.

For both samples, the QDs have a truncated hexagonal pyramidal shape with a density of $\sim10^8$ cm^{-2}; a complete characterization of the morphology of these QDs can be found elsewhere.[9] The nucleation of these QDs occurs preferentially on top of pure edge threading dislocations from the GaN substrate, although these dislocations do not propagate inside the island. In order to estimate the degree of plastic relaxation in the heterostructures, a cross sectional study was done along the $\langle 11\bar{2}0\rangle$ directions in areas containing the interface between the GaN substrate and InN quantum dots. In Fig. 1, a HRTEM micrograph of this interface is shown, and in the inset, a Fourier filtered image of the same area is

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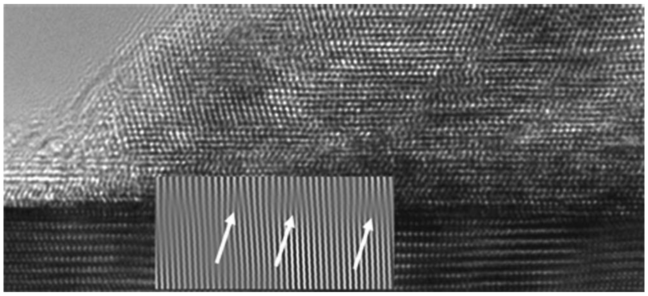

FIG. 1. High resolution XTEM micrograph of an uncapped InN quantum dot along $[11\bar{2}0]$. The inset is a Fourier filtered image of the interface where an array of MDs is observed.

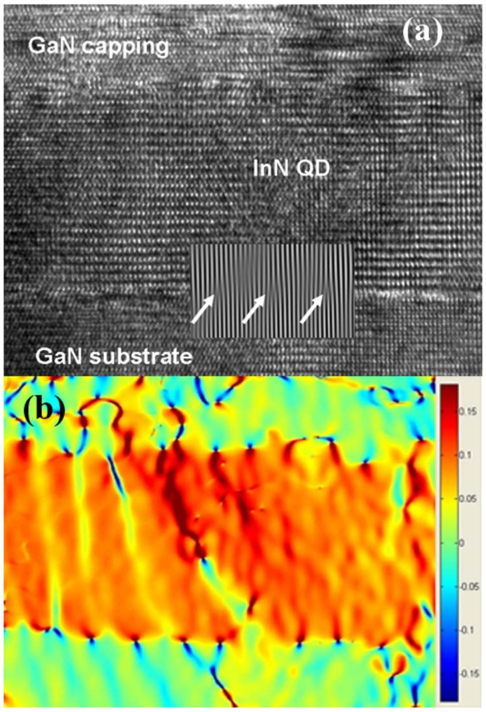

FIG. 2. (Color online) (a) High resolution XTEM micrograph of a capped InN quantum dot taken along $[11\bar{2}0]$. The inset is a Fourier filtered image of the interface where an increase of the distance between MDs after the capping process is observed. (b) Strain mapping of the image, showing the MD networks at both InN/GaN interfaces.

shown in which only one set of $\{10\bar{1}0\}$ planes is displayed. This shows that an average of one misfit dislocation is introduced every 9.5 planes of InN (or equivalently 10.5 planes of GaN). This results in a distance between misfit dislocations of $\lambda_d=2.9$ nm and an interplanar spacing in this direction of $d_{\mathrm{InN}}^{\mathrm{un}}=0.3053$ nm. This distance can also be expressed as $\lambda_d=|\mathbf{b_r}|/\delta$, where $|\mathbf{b_r}|$ is the edge component of the Burger vector at the interface plane perpendicular to the $\langle 11\bar{2}0\rangle$ directions [in this case $|\mathbf{b_r}|=(\sqrt{3}/2)a_{\mathrm{GaN}}=0.276$ nm] and δ is the plastic relaxation. Substituting, we obtain $\delta=(-)0.0952$. Since the theoretical lattice mismatch for this heterosystem is $f=(-)0.0971$, we can conclude that 98% of the initial compressive strain is relieved by the introduction of the misfit dislocation network. This result is in good agreement with previous work, where the degree of plastic relaxation was estimated from the analysis of moiré fringes in PVTEM.[10]

After the LT-GaN capping process, strain state changes can be seen. From the analysis of HRTEM micrographs of the interface between the GaN and the capped InN QD [Fig. 2(a)], we observe an increase in the distance between the MDs to every 10.2 $\{10\bar{1}0\}$ planes of InN (or equivalently 11.2 planes of GaN), and therefore, $\lambda_d^{\mathrm{cap}}=3.2$ nm and an interplanar spacing in this direction of $d_{\mathrm{InN}}^{\mathrm{cap}}=0.3031$ nm. Applying again Eq. (1), we obtain a plastic relaxation of $\delta^{\mathrm{cap}}=89\%$. However, in this case, a second MD network may be expected at the interface between the GaN capping layer and the InN QD. To clarify the density and position of both MD networks, we have constructed strain maps by applying the geometric phase algorithm (GPA),[11] which allows a quantitative measurement of the strain distribution at high spatial resolution. In Fig. 2(b), the MD networks at both interfaces (InN/GaN and GaN/InN) are visible, consisting of regularly spaced blue and red lobular shapes that correspond to the strain distribution around the edge component of a misfit dislocation. The strain map shows clearly that both MD networks have opposite Burger vectors, where the compressive fields (blue lobe) are located at the bottom and top of the GaN/InN and InN/GaN interfaces, respectively. Fourier filtered images are used again to estimate the strain state of the GaN capping layer. For the upper interface, a MD is introduced every 10.4 $\{10\bar{1}0\}$ planes of InN, and taking in account the value of $d_{\mathrm{InN}}^{\mathrm{cap}}$ and applying Eq. (1), we deduce that the LT grown GaN in the capping layer is ~99% relaxed. Therefore, in the final configuration, the capping layer is fully relaxed by the introduction of a misfit dislocation network while the quantum dot increases its residual strain. We thus do not expect changes in the strain state of the InN QD with any increase in the thickness of the GaN capping layer.

In the ideal case, a perfect correspondence in the location and density of both MD networks might be expected.[12] In an unstressed InN layer, the lower MD network would be replicated at the upper interface with opposite Burger vectors; this would generate a GaN capping layer with a similar stress state to the GaN substrate. However, the generation of MDs during epitaxial growth is gradual, depending mainly on the thickness of the capping layer, and therefore, the first GaN capped monolayers exert an additional compressive stress on the buried InN QD. As a result, a small increase in the residual strain of the InN QDs is energetically favorable since it decreases the strain in the GaN capped layers; i.e., a stress balance can occur between the layers. This is observed experimentally as a reconfiguration of the MD network at the InN/substrate interface towards lower MD densities.

To date there are few studies on the exact configuration of MD networks in large-mismatch systems.[13] The methodology shown above, although it is the most widely used, provides an incomplete characterization of the MD network since many relevant features such as changes in the line direction of the dislocations or interactions between them remain unknown. Thus, there is a variety of different models for the dislocation network that could accommodate the lattice misfit in the case of interfaces formed by close-packed planes such as (111) and (0001) for face centered cubic and compact hexagonal systems, respectively.[14] These models vary from different kinds of hexagonal honeycomb networks to a net of independent lines that could form various mosaic structures. PVTEM observations would answer this question, but in heterosystems with a high difference in lattice parameter such as InN/GaN, the MDs are so closely spaced that

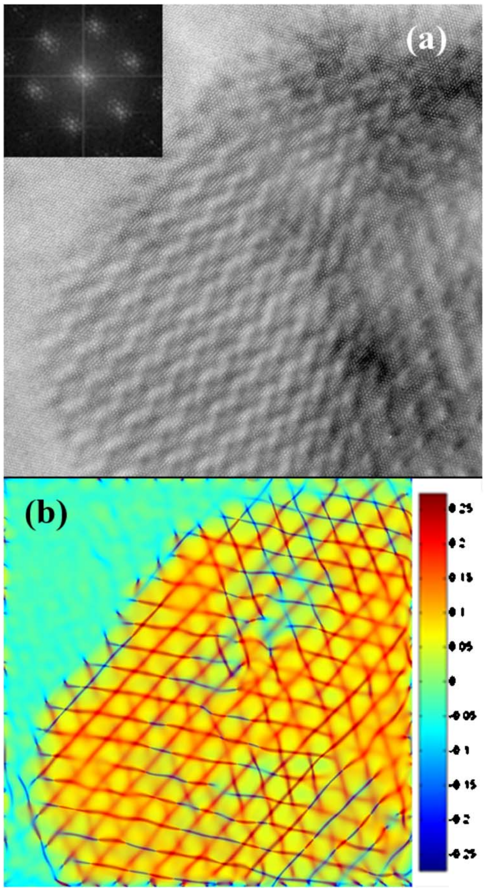

FIG. 3. (Color online) (a) Plan-view HRTEM image along the [0001] axis of an uncapped InN QD. The top-left inset shows the diffractogram. (b) Strain mapping showing the three families of 60° misfit dislocations.

the image width of the dislocation in diffraction contrast is larger than that of the spacing between MDs. However, in the present case, we have carried out a full characterization of the MD network on the atomic scale in a highly mismatched interface by applying the GPA to HRTEM images obtained in the plan view orientation. In Fig. 3(a), a PV-HRTEM micrograph of an InN quantum dot taken along the ⟨0001⟩ direction and the corresponding Fourier transform is displayed. To analyze the image, a Wiener filter was applied in order to reduce the noise in the image. Subsequently, Bragg masks were applied around the $(10\bar{1}0)$ peaks corresponding to InN and GaN separately, excluding the double diffraction spots that would lead to the formation of the moiré fringes. The phase images were obtained taking the fully relaxed GaN substrate as a reference. Figure 3(b) shows the superposition of the obtained strain maps, where the red lines correspond to higher strained zones and therefore are related to three different sets of regularly spaced misfit dislocations lying along the main $\langle 11\bar{2}0\rangle$ directions. As can clearly be observed, these dislocations do not interact, so no dislocation nodes are created; they form a regular "David's star" distribution, with pseudomorphic interfaces in both the hexagonal and triangular areas. This shows that despite of the high density of misfit dislocations, no threading dislocations are generated inside the quantum dots being an important result to consider in the future fabrication of InN QDs-based optoelectronic devices.

We have established that a MD network is formed in the uncapped QDs by independent MDs without node formation. The nonexistence of nodes must facilitate the rearrangement of the MDs observed in the capped QDs, keeping their linearity. Unfortunately, the existence of the capping layer that provides an extra thickness and the two MD networks have not allowed us up until now to obtain HRTEM micrographs with enough information to carry out a complete description of the MD network at the InN/GaN interface in capped QDs. Actually, the lateral movement of the MDs at this interface is an open question because the MDs would not be expected to glide in the basal plane (0001) in wurtzite systems due to biaxial stress from the lattice misfit.[15] The high atomic mobility and temperature instability of InN may be the main reasons for the rearrangement of the MD network during the growth of the capping layer. Further investigations are needed in order to clarify the mechanisms of the rearrangement of the MD network.

In conclusion, the uncapped InN QDs are almost fully relaxed—98% of the initial strain due to lattice mismatch—by the introduction of a MD network in the InN/GaN interface. A characterization of this network by applying the GPA shows that it consists of a set of three families of 60° misfit dislocations lying along the three main directions $\langle 11\bar{2}0\rangle$, without interaction between them or generation of threading dislocations. The introduction of a low temperature GaN capping layer induces a rearrangement of the misfit dislocations at the first InN/GaN interface, with an increase of the distance between them and the subsequent lessening of the plastic relaxation. The InN/GaN capped interface shows a second MD network giving fully relieved misfit strain of the GaN capping layer. This result suggests that changes in the strain state of the QDs are not expected during subsequent growth over the heterostructure.

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