Study of strain and composition in semiconductor nanostructures by x-ray spectroscopy and anomalous diffraction, in grazing incidence

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Introduction

Thanks to synchrotron radiation facilities, grazing incidence x-ray scattering is at present widely used for quantitative strain, structure and morphology analysis of nanoobjects. Yet, the nano-sizes, lattice mismatches and possible intermixing cause large overlapping of the scattered signals. Accordingly, discriminating the substrate, nanoobjects and capping layers contributions is often impossible. Anomalous scattering can bypass that difficulty. In this paper we address the issue of the strain state and composition in small-size QDs under gradual capping. The discussion will focus on the GaN/AlN QDs system, that potentially span a large range of optoelectronic applications from visible to ultraviolet.

Methods and Materials

The samples studied in this work were grown by plasma assisted molecular beam epitaxy on 6H-SiC(0001) substrates heated at 740°C. A 5 nm thick AlN buffer was first deposited. Four GaN MonoLayers (ML) were then grown under Ga-rich conditions, which led after the Ga excess evaporation under vacuum to GaN QDs surrounded by a 2 ML thick GaN wetting layer. Following their nucleation, the QDs were let to evolve under vacuum during one minute, before being capped with various AlN deposits, namely 2, 4, 8, 11, 18, and 20 ML. Atomic Force Microscopy (AFM) carried out on an uncapped sample revealed typically 30 nm - 4 nm QDs, with a $6.10^{10}cm^{-2}$ in-plane density.

Results

To achieve high surface sensitivity we fixed the incident angle of the x-ray beam to 0.15°. Figure 1(a) shows the scattered intensity measured along the *h* reciprocal space direction, close the (30-30) reflection, as a function of the AlN coverage. For uncapped QDs, the position of the GaN peak lies close to the position for bulk GaN, indicating a large in-plane strain relaxation in the dots. As the AlN deposit increases, a progressive shift towards higher *h* values is observed, together with a large overlapping of the scattering from the dots and the material below the dots. Further analysis was made possible by distinguishing the GaN and AlN contributions, using Multiwavelength Anomalous Diffraction (MAD) measurements [1]. Figure 1(b) shows some of the 12 scattered intensities measured for increasing AlN deposit, across the Ga K-edge, taking advantage of the Ga anomalous effect to localize the Ga contribution along *h*. Figure 1(c), shows the extracted Ga contribution, $\|F_{Ga}\|$. The $h=h_{Ga}$ position of the QDs scattering peak is inversely proportional to the in-plane average strain ε_{xx}.

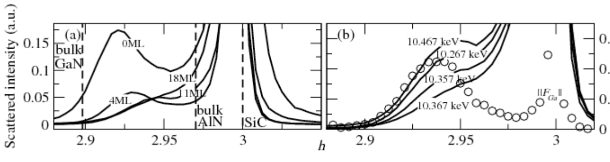

Fig.1

We measured Extended Diffraction Anomalous Fine Structure (EDAFS) oscillations at the maximum of the $\|F_{Ga}\|$ scattering contribution to quantitatively characterize the local environment of the Ga atoms, specifically in the dots. The local environment of Ga atoms includes short-range order information regarding the ε_{xx} and ε_{zz} in- and out-of-plane strains and the possible occurrence of Al in the dots. The ε_{xx} strain was set to the value provided by the MAD analysis. A supercritical grazing incidence angle of 0.3°. The analysis was performed using a first order approximation, EXAFS-like path formalism of EDAFS [1]. Figure 2(a,b) shows the EDAFS contribution to the diffracted intensity, plotted in the *k* photoelectron wave number space and in the *R* real space. The fit was performed in *R* space using theoretical standards provided by the FEFF8 code [2] and the Artemis interface to the IFEFFIT fitting package [3].

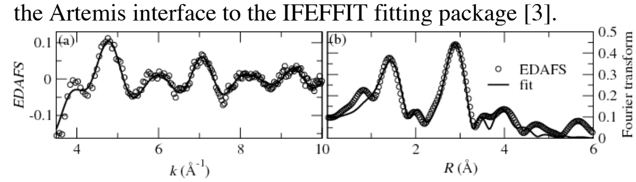

Fig.2

Discussion

Figure 3 shows in- and out-of-plane strains deduced from MAD and EDAFS, as compared with pseudomorphic biaxial GaN on AlN. The low, biaxial like out-of-plane strain relaxation for small AlN deposits presumably originates from the low aspect ratio, roughly 0.13, of the dots, as deduced from the AFM analysis of uncapped QDs. For larger deposits, the selective growth of AlN in between the dots [1] may result in extra in-plane compression of the GaN cells in the dots, and consequently extra out-of-plane expansion, which is consistent with the observed non biaxial behavior. From the EDAFS analysis, the Ga-N first shell in-plane and out-of-plane distances show to be very close to each other, within the fit errors (0.001 nm), in agreement with previous studies. At last, the Al content was systematically found very small, as an evidence that no intermixing takes place in the QDs as expected for the Al/Ga species.

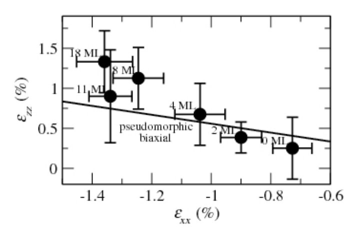

Fig.3

[1] J. Coraux *et al*, Phys. Rev. B **73**, (2006), in press.
[2] A. L. Ankudinov *et al*, Phys. Rev. B **58**, (1998), 7565
[3] M. Newville *et al*, Physica B **208-209**, (1995), 154