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Breakdown of anomalous channeling with ion energy for accurate strain determination in GaN-based heterostructures

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The influence of the beam energy on the determination of strain state with ion channeling in GaN-based heterostructures (HSs) is addressed. Experimental results show that anomalous channeling may hinder an accurate analysis due to the steering effects at the HS interface, which are more intense at lower ion energies. The experimental angular scans have been well reproduced by Monte Carlo simulations, correlating the steering effects with the close encounter probability at the interface. Consequently, limitations in the determination of the strain state by ion channeling can be overcome by selecting the adequate beam energy. © *2009 American Institute of Physics*. [DOI: 10.1063/1.3202421]

Ion channeling processes are powerful methods to study structural properties of crystalline materials.[1] These phenomena take place when a beam of charged particles moves through a crystal lattice along a high-symmetry direction, reducing the probability of scattering events.[2] The detected yield as a function of the tilt angle shows an elevated sensitivity to any crystal defect, which can be explored with depth resolution when ion channeling is combined with Rutherford backscattering spectrometry (RBS/C).[1] In particular, the detection of strain by RBS/C in a layered system is derived from angular scans across axes which are tilted by the angle θ with respect to the growth direction and within a plane that contains both the layer and substrate axes. The different lattice parameters of the layer and the substrate lead to a change in the tilt angle known as the kink angle, $\Delta\theta = \theta^{\text{subs}} - \theta^{\text{film}}$. In the RBS/C scan this kink angle is reflected in an angular shift between both dips $\Delta\alpha$. It can be directly correlated with the strain state of the film if the relaxed lattice constants of the materials are known. The potential of RBS/C has been proved on several semiconductor heterostructures (HSs), where elastic strain is a main issue affecting band gap and carrier density.[3]

However, this kind of RBS/C studies has shown anomalous behaviors in the angular scans (asymmetries or double dips),[4–6] which decrease the accuracy in the strain determination. The origin of these anomalous channeling processes has been clearly linked to the presence of steering effects (deviation of the projectile due to electrostatic interactions with the target atoms) at the interface of the junction.[5] The thickness of the layer and the strain state strongly influence this behavior since the steering operates when $\Delta\theta$ is smaller or comparable to the critical angle for channeling (ψ_1).[7] In some cases, this error can be corrected by additional Monte Carlo (MC) simulations,[5,7] but in others this approach is not sufficient. However, ψ_1 is given by Lindhard's relation[2] $\psi_1 = (2Z_1Z_2e^2/Ed)^{1/2}$ and, therefore, the beam energy can be tailored to reduce the steering at the interface, which opens an alternative way for the accurate determination of the strain in crystalline HSs.

In this letter, we report an experimental and theoretical evidence of the steering effects breakdown with the increasing beam energy. This is shown in two GaN-based HSs comprising compressive and tensile strain states. RBS/C analysis across the $\langle\bar{2}113\rangle$ axes revealed the influence of the energy on the experimental angular shift $\Delta\alpha$. These RBS/C strain measurements were complemented with reciprocal space maps (RSMs) acquired by high-resolution x-ray diffraction (HR-XRD). Angular scans were compared with MC simulations using the FLUX code.[8]

For the study, quaternary ($Al_{0.02}Ga_{0.90}In_{0.08}N$) and ternary ($Al_{0.86}In_{0.14}N$) layers were grown close to lattice-matched conditions to GaN buffer layer (considered as substrate in the following). Thicknesses were 250 and 130 nm for the quaternary and ternary nitrides, respectively.[9,10] The in-plane (a) and out-of-plane (c) lattice parameters and strain state of both layers were obtained from RSMs around the (0004) and $(10\bar{1}5)$ planes. The scans were measured in a D8Discover diffractometer (Bruker-AXS) using Cu($K\alpha_1$) radiation, an asymmetric two-bounce Ge(220) monochromator, and a scintillation detector.

RBS/C experiments were performed with a 1 mm^2 ^{4}He beam. The probed energy was varied from 2 to 10 MeV using a 5 MV Tandetron accelerator.[11] Backscattered ions were detected by a silicon barrier detector placed at a scattering angle of 170° in the IBM geometry. A three-axes goniometer was employed to control the crystal position with an accuracy of 0.01°. Angular scans across $\langle 0001\rangle$ and $\langle\bar{2}113\rangle$ axes were used to determine the crystalline quality

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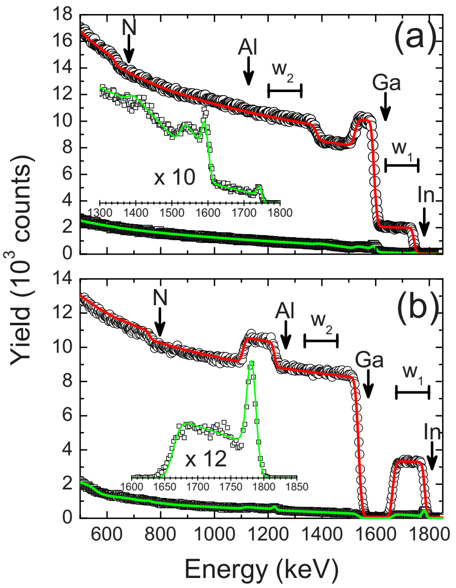

FIG. 1. (Color online) Random and ⟨0001⟩ aligned spectra (circles and squares) and simulation (solid line) from RBS/C experiments at 2 MeV. The insets show the aligned spectrum in detail. Windows of the film (w_1) and the substrate (w_2) signals for the angular scans are also shown.

and the strain state of the films. This $\langle\bar{2}113\rangle$ axis of the wurtzite lattice ($P6_3mc$) is located at $\theta \sim 31.6°$ from the ⟨0001⟩ axis along the $(10\bar{1}0)$ plane as derived from $\tan\theta = a/c$. Steps of 0.05° and 0.1° were employed for the scans of the quaternary and ternary samples, respectively. Random spectra were acquired by rotating the sample up to a dose of 10 μC. Aligned and random spectra were simulated by RBX code.[12]

Figure 1 shows random and ⟨0001⟩ aligned spectra of both HSs from RBS/C experiments. The elemental concentration was determined by the RBX simulation shown in the graph. The fitting was done assuming a two-layer model, keeping a constant composition for both active and buffer layers. Aligned spectra along the ⟨0001⟩ direction (insets in Fig. 1) reveal a minimum yield (relative yield between the aligned and the random spectrum) of $\chi_{\min} \sim 4\%$ for both HSs. This parameter confirms the high crystalline quality of the samples although it is double that typical of GaN substrates and an appreciable dechanneling is visible in the spectra.

The lattice parameters of the active layers obtained from RSMs are summarized in Table I. Considering these data and the relaxed parameters (a_0 and c_0) according to the RBS composition and Vegard's law,[13] the tetragonal distortion of the samples was calculated as $\varepsilon_T = \varepsilon^{\parallel} - \varepsilon^{\perp}$, being $\varepsilon^{\parallel} = (a - a_0)/a_0$ and $\varepsilon^{\perp} = (c - c_0)/c_0$. Results show compressive ($\varepsilon_T < 0$) and tensile ($\varepsilon_T > 0$) strain states, with expected $\Delta\theta$ values of 0.24(4)° and −0.62(3)° for the quaternary and ternary, respectively.

TABLE I. In-plane (a) and out-of-plane (c) lattice parameters from RSMs and derived values for tetragonal distortion (ε_T) and kink angle ($\Delta\theta$).

Sample	a (Å)	c (Å)	ε_T (%)	$\Delta\theta$ (°)
$Al_{0.02}Ga_{0.90}In_{0.08}N$	3.186(2)	5.244(2)	−1.3(1)	0.24(4)
$Al_{0.86}In_{0.14}N$	3.184(1)	5.065(1)	0.70(5)	−0.62(3)

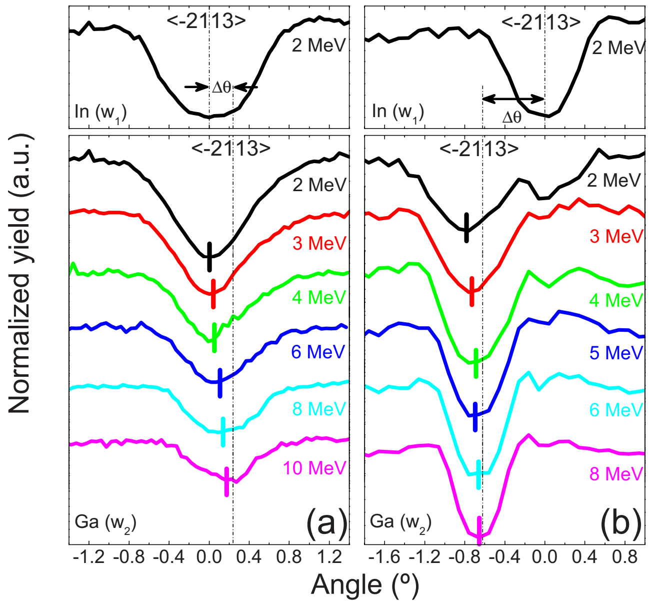

FIG. 2. (Color online) Experimental angular scans across the $\langle\bar{2}113\rangle$ axis for different energies in strained AlGaInN/GaN (a) and AlInN/GaN (b) HSs. As a reference, the angular scan from the active layer (w_1) at 2 MeV is shown (top graphics). The horizontal lines mark the value of the real kink angle for both HSs. The shift from the substrate (w_2) does not match $\Delta\theta$ due to steering effects, which gradually diminish with energy.

For the analysis of the angular scans of the layer and the substrate, the energy regions corresponding to the In (w_1) and Ga (w_2) signals were considered (see Fig. 1). Figure 2 shows the experimental $\langle\bar{2}113\rangle$ scans of the substrate (w_2) for different beam energies. As a reference, the angular scan at 2 MeV is also shown for the layer signal (w_1), being 0° the position where the minimum yield of this first layer is achieved. This position remains constant with the beam energy since ion channeling in the first layer is not disturbed by steering effects. For both samples, the angular shifts between the dips at low energies ($\sim$2 MeV) do not correspond to the real $\Delta\theta$ marked in Fig. 2. In particular, for the quaternary HS, no shift at all ($\Delta\alpha = 0°$) and no asymmetry are observed. For the AlInN sample, $\Delta\alpha$ at 2 MeV is 24% higher than $\Delta\theta$ derived by HR-XRD.

This anomalous behavior ($\Delta\alpha \neq \Delta\theta$) displayed in Fig. 3

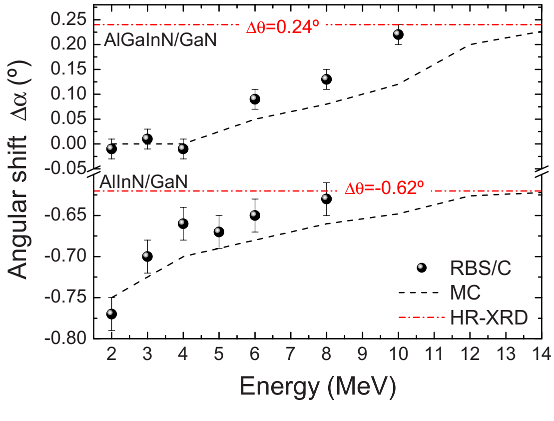

FIG. 3. (Color online) Experimental angular shifts and MC predictions for the HSs analyzed as a function of the probing energy.

is explained by the steering of ions at the GaN interface.[7] The effect is gradually disappearing with the increasing energy and $\Delta\alpha$ converges to $\Delta\theta$. This fact is forced by the decrease in ψ_1 by a factor of 2 or more for the studied energy range. Thus, at low beam energies an appreciable part of the channeled ions can be deflected at the interface and remains channeled in the GaN layer, whereas at high energies ions suffer a significant number of direct scattering events causing dechanneling of the beam. Therefore, features corresponding to the steering effects, such as the additional minimum at 0° in Fig. 2(b) (where the beam is aligned with the film), are progressively removed. The ternary sample reaches the expected value of $-0.62(3)°$ at 8 MeV. However, the scan in the quaternary HS shows an asymmetric dip even at 10 MeV, being the two components (0° for the substrate and 0.24° for the layer) not well resolved yet. Further measurements above 10 MeV to eliminate this artifact were not performed because of the radioactive activation of the sample during the experiment.

MC simulations with the FLUX code were carried out to understand and compare the experimental results. The universal Ziegler-Biersack-Littmark (ZBL) potential was assumed for the individual ion-solid collisions.[14] The incident beam randomly distributed over the unit cell and a total number of 10^5 ions were used to guarantee low statistical error. The simulated angular scans were performed in the $\langle\bar{2}113\rangle$ axis along the $(10\bar{1}0)$ plane of the wurtzite lattice, being the normalized yield derived from the close encounter probability (P) for different angles. A two-layer model was employed comprising the nitride compound and the GaN substrate. The strain state of the top layer was included as an input by means of a rotation matrix with the $\Delta\theta$ value deduced by RSMs. The vibrational atomic amplitudes were 0.08 Å (Al), 0.11 Å (Ga), 0.13 Å (In), and 0.09 Å (N) as in Ref. 7, although the Debye temperature for GaN is still under debate.[15]

The weakening of the ion steering at the GaN interface for higher beam energies is well explained in MC simulations by the increase in P. Indeed, the simulations predict a sharp increase in P from ~0.025 before the interface to 0.44 (0.63, 0.68) at 2 (4, 8) MeV after the interface for an incident angle of 0° (i.e., beam aligned with the axis of the first layer). The changes in P reflect variations of the flux distribution of the ions, which depend on the time that the ion remains channeled in the layer.[16–18] Since this time is also controlled by the particle energy, the change in P can be directly correlated with it.

Figure 3 shows the theoretical results for the angular shift $\Delta\alpha$ obtained from MC simulations in comparison to the experimental results. Both experimental and simulated $\Delta\alpha$ were determined by Gaussian fittings of the dips. The trend of the experimental angular shift is well reproduced by MC simulations, although a slight underestimation is visible for both samples. This means that the experimental $\Delta\alpha$ converges faster than expected to $\Delta\theta$. This fact can be easily explained by the defects in the first layer of the HS, which enhance dechanneling and alleviate the impact of steering effects. A limitation to this approach for very small kink angles is given by the accuracy of the RBS/C technique to determine $\Delta\alpha$ (~0.05°) and the maximum energy of typical tandem accelerators (~15–18 MeV for He^{++}).

In summary, we have demonstrated the influence of the beam energy on the strain determination by ion channeling. The accuracy of RBS/C improves with the increasing energy due to the suppression of steering effects at the interface, in agreement with MC simulations. Thus, limitations in the measurement of strain can be overcome by adapting the beam energy.

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