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Ion beam characterization of $GaAs_{1-x-y}N_xBi_y$ epitaxial layers

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Abstract

Incorporation of Bi in $GaAs_{1-x}N_x$ epitaxial layers represents a significant interest as Bi compensates the lattice parameter reduction caused by the N incorporation while contributing to the reduction of the band gap energy. $GaAs_{1-x-y}N_xBi_y$ epitaxial layers were grown on GaAs wafers by molecular beam epitaxy. The quality of the films as well as the concentration and lattice location of Bi and N were characterized by channeling Rutherford backscattering spectrometry and nuclear reaction analysis using 2 and 3.72 MeV He beams, respectively. The amount of nitrogen in the film was measured by means of the $^{14}N(\alpha, p)^{17}O$ endothermic nuclear reaction and elastic recoil detection. The results indicate that high quality epitaxial layers were obtained, with $y = 1.8\%$ Bi incorporated into the layer. Angular scan along the main axes showed no strain in the film and indicated that most of Bi atoms are located at substitutional sites. Nitrogen lattice incorporation is more difficult to establish because of the presence of Bi in the layer, but we estimate the substitutional fraction to be $71 \pm 6\%$.

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1. Introduction

$GaAs_{1-x}N_x$ has been studied for more than a decade due to its potential applications for optoelectronic devices [1,2]. Because of giant bowing coefficient, $GaAs_{1-x}N_x$ alloy simultaneously lower both the lattice constant and the band gap. However, due to the large size mismatch between N and As, the growth of high-quality $GaAs_{1-x}N_x$ on GaAs substrate is difficult. In order to overcome this problem, a coalloying approach has been proposed [3]. By substituting a large-type atom like Bi, the new alloy GaAsNBi can be made lattice-matched to GaAs while mitigating the undesirable effects produced by N.

$GaAs_{1-x-y}N_xBi_y$ as a potential candidate for band gap material that is lattice matched to GaAs has been studied theoretically [4]. The coalloying

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of Bi with N in GaAs can significantly lower the N concentration required to reduce the alloy band gap. The strain compensation between the small-sized N and the large-sized Bi also reduces the alloy formation energies. $GaAs_{1-x}Bi_x$ has been successfully grown using metal-organic vapor phase epitaxy (MOVPE) [5,6] and most recently prepared by molecular beam epitaxy (MBE) [7,8]. So far, however, there is no experimental report on the structural characterization of $GaAs_{1-x-y}N_xBi_y$ epitaxial layer.

Recently, successful measurements were made on $GaAs_{1-x}N_x$ with a nitrogen fraction of a few percents in both random and channeling modes combined with Rutherford backscattering spectrometry (RBS) and nuclear reaction analysis (NRA) [9]. However, the presence of Bi in the layers makes the technique more difficult to apply. In this paper, we present for the first time the characterization of $GaAs_{1-x-y}N_xBi_y$ epitaxial layers prepared by MBE using RBS/channeling, Elastic recoil detection by time-of-flight (ERD-TOF) and NRA/channeling techniques.

2. Experimental methods

$GaAs_{1-x-y}N_xBi_y$ samples were grown in a VG-V80H MBE deposition system on semi-insulating (0 0 1) GaAs substrates at 380 °C with a growth rate of 0.8 μm/h. The details of sample preparation can be found elsewhere [7,10]. Two samples were grown with the following nominal structure: one 180 nm thick with $x = 0.010$ and $y = 0.018$ (r1316) and the other 300 nm thick with $x = 0.015$ and $y = 0.013$ (r1378).

The ion beam characterization was performed on the 1.7 and 6 MV tandem accelerators at Université de Montréal. For RBS and NRA, the incident beam was defined by a $\varnothing$1 mm aperture. The typical beam currents were 5 nA He^+ for RBS/channeling and 15 nA He^{2+} for NRA. Each time, the current on the target was confirmed by a current measurement in a Faraday cup. The outcoming particles were detected by a 360° movable standard passivated implanted planar silicon (PIPS) detector with a ~15 keV energy resolution. The sample-detector distance is 122 mm and the solid angle of detection is 6.69 mSr. For the ERD-TOF, a description of the setup can be found in [11].

RBS studies were performed with a 2 MeV He^+ beam in both random and aligned modes with detector placed at 170° backscattering angle. The lattice location of Bi was further characterized by angular scan along the $\langle 0\,0\,1\rangle$ and $\langle 0\,1\,1\rangle$ directions. The strain in the layers was investigated by angular scan along $\langle 0\,1\,1\rangle$ direction.

Several nuclear reactions can be used to characterize nitrogen, including $^{14}N(d, \alpha)^{12}C$, $^{14}N(d, p)^{15}N$ and $^{14}N(\alpha, \gamma)^{18}F$. However deuterium beam activation will induce long-term radiation background in the setup. Instead, the N content and its lattice location was investigated using the $^{14}N(\alpha, p)^{17}O$ endothermic nuclear reaction with a 3.72 MeV He^{2+} beam [12] where the proton was detected at 160° with the beam direction. The width of this reaction (~60 keV) corresponds approximately to the energy loss in the 180 nm layer. Seven layers of 2.54 μm mylar foil with total thickness of 17.78 μm were placed in front of the detector to stop the elastically scattered α particles. Such a large thickness was required since the Bi in the layer produced higher-energy backscattered α particles. In principle, the total N content in the layers can be extracted from NRA spectra. For this purpose, a thick kapton foil with a known N concentration was measured as a reference under the same experimental conditions, and the ratio of the number of particles detected at the peak of the reaction was calculated. For each measurement, the total collected charge was 100 μC. The NRA/channeling spectra were also collected with the sample first aligned using a 2 MeV He^+ beam without the stopping foil.

3. Results and discussion

Fig. 1 shows the RBS spectra of sample r1316 collected in random, $\langle 0\,0\,1\rangle$ and $\langle 0\,1\,1\rangle$ directions as well as a simulation of the random spectrum using RUMP [13]. The quality of the epitaxial layer is evidenced by the low χ_{min} for both GaAs (6.1%) and Bi (5.2%). On the other hand, it is observed that Bi is not homogeneously distributed in the

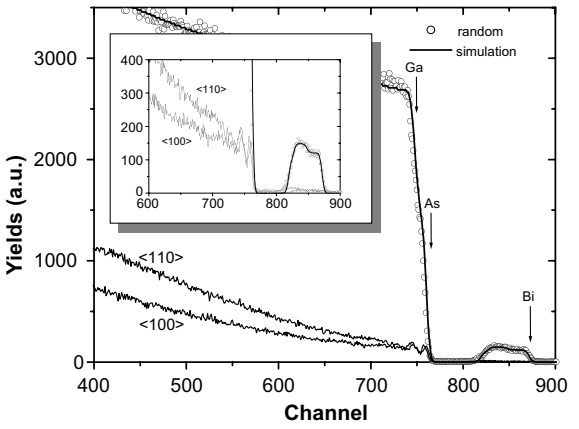

Fig. 1. RBS spectra for sample r1316 in the random, ⟨0 0 1⟩ and ⟨0 1 1⟩ directions as well as the simulation of the random spectrum; the inset shows an enlarged portion of spectra.

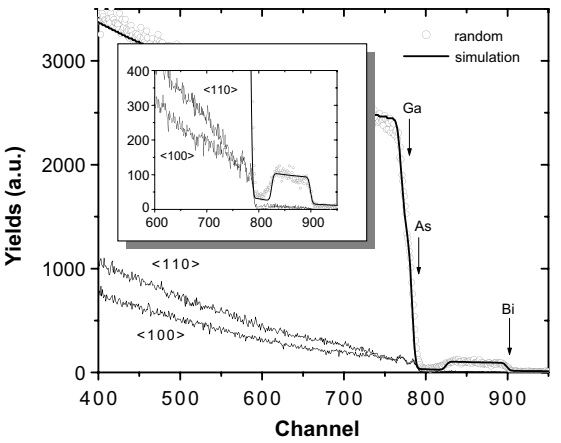

Fig. 2. RBS spectra for sample r1378 in the random, ⟨0 0 1⟩ and ⟨0 1 1⟩ directions as well as the simulation of the random spectrum; the inset shows the enlarged portion of spectra.

layer. This is clear from the inset of Fig. 1 where the left part of the peak, corresponding to the deeper part of the layer, has a higher intensity. The best simulation gives the following structure: GaAs (substrate)/$GaAsBi_{0.011\pm0.001}$ (27 ± 5 nm)/$GaAsBi_{0.017\pm0.001}$ (67 ± 5 nm)/$GaAsBi_{0.014\pm0.001}$ (79 ± 5 nm). The thickness was estimated using the atomic density of GaAs crystal since the contents of Bi and nitrogen are low. The interface layer was added to fit the low energy tail. For channeling spectra, the yield of GaAs in the layer is slightly higher along ⟨0 1 1⟩ and ⟨0 0 1⟩ directions. ERD-TOF measurements show that the N concentration is a little smaller than the nominal value with $x = 0.007 \pm 0.001$.

Fig. 2 shows the RBS spectra for sample r1378. Again the quality of the layer is good. The distribution of Bi in r1378 is more homogeneous than that of sample r1316. Taking into account pileup effects, a uniform layer of $GaAsBi_{0.012\pm0.001}$ (237 ± 5 nm) was obtained from simulation of the random spectrum. From ERD-TOF measurements, the nitrogen content is estimated to be $x = 0.011$, again smaller than the nominal value.

Compared with the spectra of sample r1316, the channeling spectrum of GaAs along ⟨0 1 1⟩ direction does not show a higher yield in the region corresponding to the epitaxial layer. It is not clear whether the higher yield observed is a result of an inhomogeneous composition or because the Bi and N concentrations are not optimized to minimize the lattice compensation. This requires further investigation.

The strain in this sample was examined by angular scan along the ⟨0 1 1⟩ direction in the (1 0 0) plane. Fig. 3 shows the angular scans obtained from sample r1378. It is seen that the Bi and GaAs curves fully overlap, which could be an indication that Bi is substitutional within the sensitivity limit. There is no angle shift between the

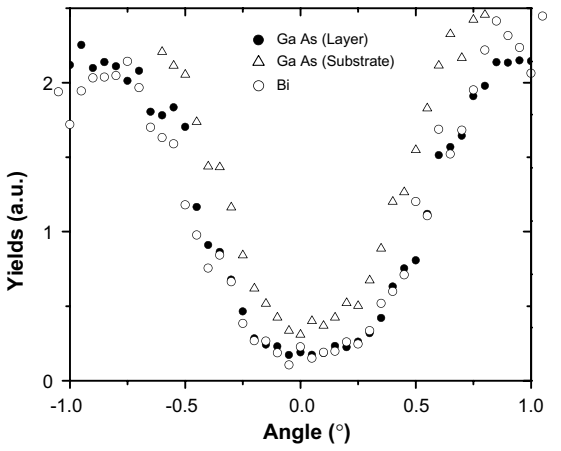

Fig. 3. Angular scan along ⟨0 1 1⟩ in the (0 0 1) plane for the layer and substrate of sample r1378.

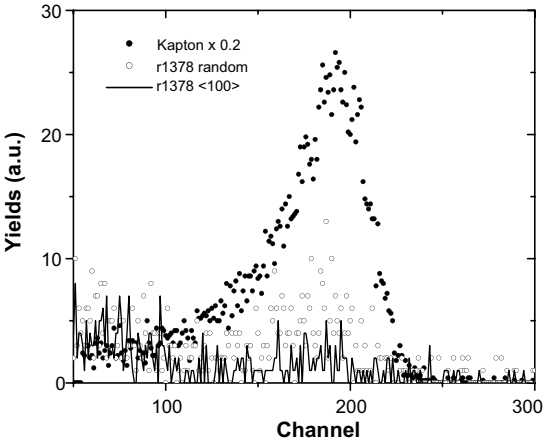

Fig. 4. NRA spectra in the random and ⟨0 0 1⟩ channeling directions for sample r1378, compared to the spectrum obtained from a kapton foil.

GaAs yields in both layer and substrate or shoulder on the angular scan. This indicates that the layer is not strained.

The nitrogen content of sample r1378 was also measured by NRA. Fig. 4 shows the NRA spectra of this sample and the reference kapton foil. The content of N is low, but a weak peak centered near channel 190 can be observed. The low energy tail comes from α particles backscattered by Bi, reducing the sensitivity for the nitrogen detection. Comparing the peak intensity with the one obtained from a kapton foil, a nitrogen concentration of $(1.9 \pm 0.6) \times 10^{20}$ at./cm^3 is obtained, i.e. $x = 0.004$. The discrepancy might namely be due to the straggling in the thick stopping foil. According to SRIM simulations [14], it contributes to spread the energy by another 50 keV, widening the detected peak and thus decreasing its maximum value.

Comparing channeled versus random yields must however result in a reliable estimate of the lattice site incorporation of nitrogen. Channeled NRA spectra were collected with the samples first aligned using 2 MeV He^+ without the stopping foil in front of the detector. Again, due to the low concentration of N in the layer, it is hard to quantify the proportion of substitutional nitrogen, although we observed that the yield in channeling spectrum is significantly smaller than that in the random spectrum. From the ratio of the peak area and considering a χ_{min} of 6.1% from the GaAs channeling, the substitutional N fraction is estimated to be $71 \pm 6\%$. Larger detector, and methods to better separate the backscattered α particles from the protons produced by the nuclear reaction will be required in the future to increase the detection efficiency, and make angular scans foreseeable.

4. Conclusion

In summary, the structure of $GaAs_{1-x-y}N_xBi_y$ epitaxial layers grown by MBE can be well characterized by RBS/channeling. The results indicate that good quality layers were grown. Bi is well located at substitutional sites. But the presence of Bi requires thicker stopping foil in the NRA measurement, reducing the sensitivity to nitrogen compared, for example, to GaAsN layers. There is no measurable strain between the layer and the substrate based on angular scans.

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