InN{0001} polarity by ion scattering spectroscopy

M. Walker[1], **T. D. Veal**[1], **Hai Lu**[2], **W. J. Schaff**[2], and **C. F. McConville**[*1]

[1] Department of Physics, University of Warwick, Coventry, CV4 7AL, UK
[2] Department of Electrical and Computer Engineering, Cornell University, Ithaca, New York 14853, USA

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The polarity of a wurtzite InN thin film grown on a c-plane sapphire substrate with GaN and AlN buffer layers has been investigated by co-axial impact collision ion scattering spectroscopy (CAICISS). Time of flight (TOF) spectra of He^+ ions scattered from the surface of the InN film were taken as a function of the incident angles of the primary 3 keV He^+ ions. From the TOF spectra, the polar angle-dependence of the In scattered intensity was obtained. Comparison of the experimental polar-angle dependence of the In CAICISS signal intensity with simulated results for the various volume ratios of (0001)- and (000$\bar{1}$)-polarity domains indicated that the InN film is approximately 75 % In-polarity and 25 % N-polarity.

1 Introduction Since the discovery that high quality epitaxial InN [1, 2, 3] has a narrow band gap [4, 5, 6], several unusual electronic properties of this material have been discovered. Effects such as the non-parabolicity of the conduction band [7] and the existence of surface electron accumulation [8, 9] make the electronic properties of InN more akin to those of InAs than its III-nitride counterpart GaN.

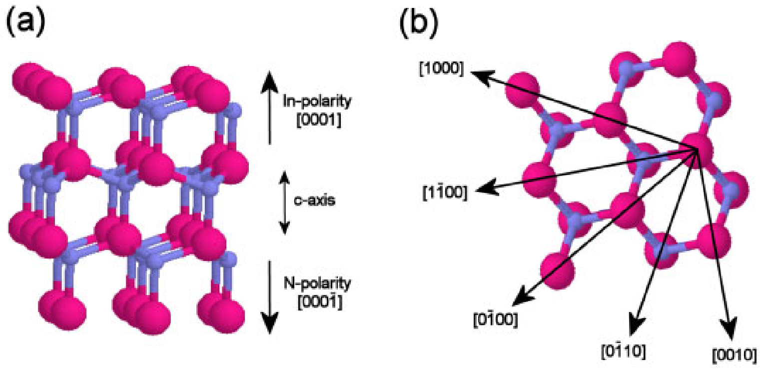

Fig. 1 Ball and stick model, illustrating (a) the In-polarity [0001] and N-polarity [000$\bar{1}$] directions of wurtzite InN and (b) the different azimuthal directions on the (0001) surface. The large deep-pink balls represent In atoms and the small medium-purple balls represent N atoms.

However, when it comes to epitaxial growth, several properties are common to both InN and GaN. One major concern in wurtzite III-N growth is crystal polarity. Unlike zinc-blende crystals, where the (001) and

* Corresponding author: e-mail: C.F.McConville@warwick.ac.uk

$(00\bar{1})$ crystallographic directions are equivalent, in wurtzite crystals the (0001) and $(000\bar{1})$ directions are different. This inequivalence of the In-polarity (0001) and N-polarity $(000\bar{1})$ is shown in figure 1(a). The In-polarity (N-polarity) is defined as the direction along the c-axis that the single bond of the In (N) atom is normal to and directed towards the surface [10]. The In (N) atom is also bonded to three N (In) atoms in the direction away from the surface. The upper surface of the model in figure 1(a) is the In-termination of the In-polarity crystallographic direction (0001), while the lower surface is the In-termination of the N-polarity crystallographic direction $(000\bar{1})$. The N-termination of each polarity is obtained by removing a single layer of In atoms from the particular surface.

While co-axial impact collision ion scattering spectroscopy (CAICISS) has been used extensively to probe the polarity of GaN [11], studies of InN polarity have been less common [12, 13]. In the CAICISS study of Saito *et al.*, CAICISS spectra were collected directly from the InN epilayers, but no analysis of these spectra was performed. Instead, GaN cap layers were grown on InN to infer the polarity of the InN layer. Experimental CAICISS spectra from these GaN cap layers were interpreted by comparison with simulations of CAICISS spectra of Ga- and N-polarity GaN [12]. This work relied upon the assumption that polarity inversion does not occur during GaN growth on InN. Xu and Yoshikawa have used *in situ* CAICISS to determine the polarity of InN films, but no CAICISS data or simulations were shown [13]. In this article, we report the results of a direct investigation of the polarity of InN using *ex situ* CAICISS.

2 Experimental The experiments were carried out in a UHV chamber equipped with low energy electron diffraction (LEED), a dual anode X-ray source, a 100 mm concentric hemispherical electron energy analyzer, and a *bolt-on* CAICISS system (described elsewhere [14]). The data presented here are of the polar scans of the [1000] azimuth. The two-dimensional periodicity of the InN surfaces was determined by LEED and also enabled azimuthal alignment of the sample to be achieved for the CAICISS experiments.

The InN{0001} samples used in this study were grown at 500 °C to a thickness of 1500 nm by migration enhanced gas source molecular beam epitaxy (MBE) on a 220 nm GaN buffer layer on a 10 nm AlN buffer layer on a c-plane sapphire substrate. Details of the growth can be found elsewhere [15]. The samples were transferred through air to the CAICISS instrument. Prior to CAICISS analysis, the InN surface was prepared *in situ* by atomic hydrogen cleaning (AHC). Molecular hydrogen was thermally cracked with $\sim$ 50 % efficiency using a TC-50 atomic hydrogen source (OAR Ltd, UK). The AHC process consisted of two 10 kL doses of H_2, the first at room temperature and the second at 175 °C. Finally, the sample was annealed without exposure to hydrogen at 300 °C for 2 h. This surface preparation resulted in the sharp (1×1) LEED pattern shown in the inset of figure 2. Sample cleanliness was confirmed by X-ray photoelectron spectroscopy (XPS) - there was no observable intensity in the C 1s or O 1s regions and no oxide components were apparent in the In 3d or N 1s regions, indicative of complete removal of the native oxides and the hydrocarbon contamination.

3 CAICISS results The CAICISS data and simulations are shown in figure 2. From the variation of the energy and flux of the scattered ions as a function of incidence or azimuthal angle, it is possible to analyze the structure of the epilayer. To enable accurate interpretation of the data, trial structures have been simulated for each data set using the FAN simulation program developed by Niehus [16] until agreement is achieved between the simulated intensity as a function of polar angle and the experimental data.

With reference to figure 2, three distinct changes are observed in the In intensity profile as the proportion of N-polarity material is increased in the model structure. Firstly, an increase in the intensity of the feature at 46°; secondly, a decrease in the intensity of the feature at 76°; and finally, the profile in the 55° to 65° region changes, with the trough becoming more shallow as the proportion of N-polarity material is increased. Comparison of these three features in the simulated spectra with those in the experimental spectrum indicates that the InN film studied has mixed polarity, with 75 % In-polarity and 25 % N-polarity. Further investigations to establish the effects of buffer layers are currently ongoing, including studies of InN films grown on an AlN buffer layer and directly on to the c-sapphire substrate.

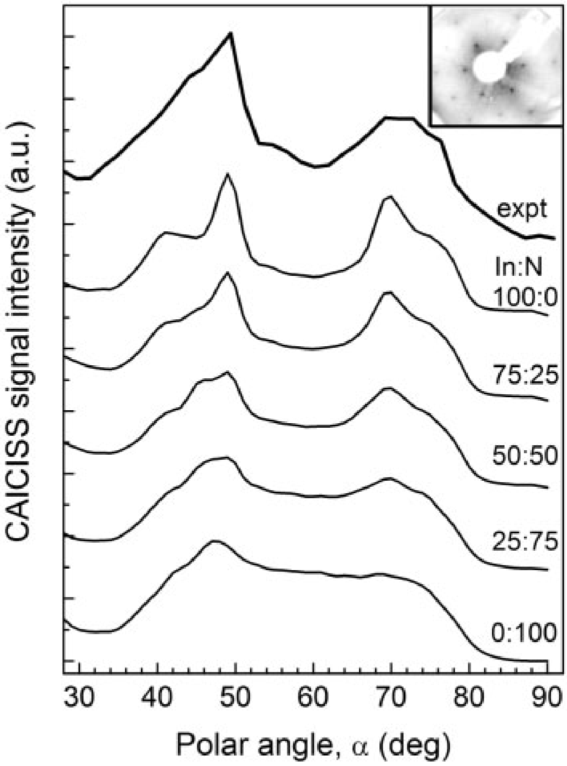

Fig. 2 Experimental CAICISS signal intensity as a function of polar scattering angle for the [1000] azimuth. Simulated CAICISS spectra are also shown for various volume ratios of In-polarity (0001) and N-polarity (000$\bar{1}$) domains. A (1×1) LEED pattern recorded from an InN{0001} surface using an electron beam energy of 168 eV is shown in the inset.

The determination of the polarity of InN epilayers is important both to further the understanding of InN epitaxial growth and to the development of potential device applications. The presence of polarity-dependent internal spontaneous polarisation fields in these uniaxial wurtzite semiconductors brings new challenges, but also new possibilities for the design of devices [17]. The internal polarisation may give rise to additional interface charge of up to several 10^{13} e/cm^2; the In-face (N-face) is expected to have negative (positive) internal polarisation. In combination with charge residing in surface and interface states, a detailed understanding of charge balance at the interfaces is required to understand contact formation, band offsets and achieve reliable device simulation schemes.

4 Conclusion The polarity of InN{0001} grown by MBE at 500 °C on a GaN buffer on an AlN buffer on a c-plane sapphire substrate has been studied directly using *ex situ* CAICISS. Simulation of CAICISS data collected in the [1000] azimuth indicates a majority of In-polarity material, but also shows the presence of approximately 25 % N-polarity material.

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