PARSEM

3rd Workshop

25-28 March 2008

Selwyn College, Cambridge

PARSEM 3rd YEAR WORKSHOP / MEETING
Selwyn College, Grange Road, Cambridge, 25-28 March 2008

3rd Workshop on III-Nitride heterostructures – nanostructures

Programme

Tuesday, 25th March

On arrival go to the Porters' Lodge at the front of Selwyn College, collect keys to room and go to room.

19:00 – 21:00 Registration and Buffet Supper in Chadwick Room

Wednesday, 26th March

08:00-08:45 Breakfast in Hall

09:00-09:15 Welcome: Philomela Komninou, Colin Humphreys

Plenary Session

09:15-10:15 Tom Foxon (University of Nottingham)
Growth of group-III Nitrides by Plasma-assisted Molecular Beam Epitaxy (Invited Speaker)

10:15-10:45 *Coffee Break*

10:45-11:45 Jesús Zúñiga Pérez (CNRS-CRHEA)
ZnO epitaxial films and nanostructures (Invited Speaker)

11:45-12:45 Philippe Vennéguès (CNRS-CRHEA)
Microstructure of Non-polar and Semi-polar GaN and ZnO heteroepitaxial films (Invited Speaker)

12:45-14:15 *Lunch* (not included in price. Available in self-service cafeteria in Hall, £10 per person, or in pubs/restaurants nearby)

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Session: Theory and Modelling

14:15-14:35	L. Lymperakis and J. Neugebauer (University of Paderborn, Germany) **Thermodynamics and Adatom Kinetics of Non-polar GaN Surfaces**
14:35-14:55	D. Holec and C.J. Humphreys (University of Cambridge, UK) **Precise Modelling of Electron-energy-loss Near Edge Structure of III-Nitrides**
14:55-15:15	H. Lei, J. Chen, P. Ruterana and G. Nouet (Caen, France) **Simulation of Indium Distribution in InGaN/GaN quantum wells**
15:15-15:35	A. Belkadi, G.P. Dimitrakopulos, J. Kioseoglou, G. Jurczak, T.D. Young, P. Dluzewski and Ph. Komninou (Aristotle University of Thessaloniki, Greece & IPPT, Poland) **A Method for Atomistic/Continuum Analysis of large HRTEM Images**
15:35-15:55	T.D. Young (IPPT, Poland), S.-L. Sahonta and Ph. Komninou (Aristotle University of Thessaloniki, Greece) **Statistical Electronic Density-Functional Theory: Structural Properties of $In_yX_{1-y}N$ Randomly-ordered Alloys**
15:55-16:20	*Coffee Break*
16:20-16:40	E. Kalessaki, J. Kioseoglou, L. Lymperakis, G. P. Dimitrakopulos, Ph. Komninou, and Th. Karakostas (Aristotle University of Thessaloniki, Greece& University of Paderborn, Germany) **Atomistic modeling of (Al,In)N/GaN interfaces**
16:40-17:00	M. Petrov, L. Lymperakis, J. Neugebauer, R. Stefaniuk and P. Dluzewski (University of Paderborn, Germany & IPPT, Poland) **Multi-scheme *ab-initio*-finite Element Calculation of III-Nitride Based Quantum Dots Electro-mechanical Properties**
17:00-17:20	O. Marquardt, T. Hickel and J. Neugebauer (University of Paderborn, Germany) **Optical Properties of Semiconductor Nanostructures Including Strain and Pie**

17:20-17:40	A. Belabbes, J. Kioseoglou, G. P. Dimitrakopulos, Ph. Komninou, and Th. Karakostas (Aristotle University of Thessaloniki, Greece) **Magnesium adsorption and incorporation at InN (0001) and (000-1) surfaces: A first-principles study**

Session: Nanostructures

17:40-18:00	H. Kirmse, I Häusler, W. Neumann, S. Kret, P. Dluzewski, E. Janik, G. Karczewski and T. Wojtowicz (HUB, Berlin, Germany & IPPT, Poland) **Defect Formation in Semiconductor Nanowires**
18:00-18:20	L. Lari, R.T. Murray, T. Bullough, P.R. Chalker, C. Cheze, L. Geelhaar and H. Riechert (University of Liverpool, UK & PDI, Berlin, Germany) **Aluminium Incorporation Studies in AlGaN and GaN/AlGaN Core/shell Nanowires**
18:20-18:40	C. Cheze, L. Geelhaar, W. Weber, H. Riechert, Ph. Komninou, T. Kehagias and T. Karakostas (Paul-Drude-Institute [PDI], Berlin, Germany & Aristotle University of Thessaloniki, Greece) **Catalyst-free and catalyst-induced Growth of GaN-nanowires by MBE**
19:00	*Pre-dinner Drinks reception*
19:30	*Conference Dinner in New SCR*

Thursday, 27th March

08:00-08:45	Breakfast in Hall

Plenary Session

9:00-10:00	Robert Martin (University of Strathclyde, Scotland, UK) **Investigations of AlGaN-GaN Heterostructures** (Invited Speaker)
10:00-11:00	Phil Dawson (Manchester University, UK)

Optical Properties of Nitride-based Quantum Well Structures (Invited Speaker)

11:00-11:30 *Coffee Break*

11:30-12:00 Dietmar Schmitz (Aixtron, Germany)
Epitaxial Reactor Technology: Material Production for Solid-State Light Emitters (Invited Speaker)

12:00-14:30 *Punting on River Cam* (or tourist bus tour of Cambridge if weather is not permitting)
Packed Lunch included.

Session: Growth and Characterization

14:30-14:50 O. Gourmala, A. Trassoudaine, Y. André, J. Tourret, R. Cadoret, D. Castelluci and E. Gil (LASMEA University Blaise Pascal Clermont II, France)
Experimental Conditions Influence on Growth Rate and Quality of GaN Layers by Standard and ELO HVPE

14:50-15:10 R. Chmielowski, T. Guehne, G. Nataf and Philippe Vennéguès (CNRS-CRHEA, Valbonne, France)
Transmission Electron Microscopy Investigation of the Influence of the Si/N Treatments on the Structural Defects in the Non-polar and Semi-polar MOVPE-grown GaN Films

15:10-15:30 C. Salcianu, C. McAleese, E.J. Thrush and C.J. Humphreys (Aixtron & University of Cambridge, UK)
Influence of Carrier Injection on the Electroluminescence properties of GaN-based LEDs

15:30-15:50 J. Smalc-Koziorowska, G.P. Dimitrakopulos, Ph. Komninou, S.-L. Sahonta, G. Tsiakatouras and A. Georgakilas (FORTH, Microelectronics Research Group, Heraklion, Crete, Greece & AUTH, Greece)
Epitaxial Orientations of GaN grown on Nitrided R-Plane Sapphire by Molecular Beam Epitaxy

15:50-16:20 *Coffee Break*

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16:20-16:40	S.-L. Sahonta, A. Adikimenakis, Ph. Komninou, G.P. Dimitrakopulos, E. Iliopoulos, A. Georgakilas and Th. Karakostas (AUTH, Greece & FORTH, Heraklion, Crete, Greece) **Structural Characterization of PAMBE-grown InAlN Films on Sapphire (0001) by Transmission Electron Microscopy**
16:40-17:00	P. Manolaki, I. Häusler, A. Mogilatenko, H. Kirmse and W. Neumann (Humboldt University [HUB], Berlin, Germany) **Analysis of TEM Diffraction contrast of (InGa)N/GaN Nanostructures**
17:00-17:20	A. Mogilatenko, W. Neumann, E. Richter, M. Weyers, B. Velickov and R. Uecker (Humboldt University, Berlin, Germany) **Structure of Polar and Non-polar GaN Layers Grown on $LiAlO_2$**
17:20-17:40	I. Häusler, H. Kirmse and W. Neumann (Humboldt University, Berlin, Germany) **Composition Analysis of Ternary Semiconductors by Combined Application of Conventional TEM and HRTEM**
17:40-18:00	T. Guhne, P. De Mierry, M. Nemoz, S. Chenot, E. Beraudo and G. Nataf (CNRS-CRHEA, Valbonne, France) "Semipolar (Ga, In)N Blue-Green Light-Emitting Diodes on *M*-Plane Sapphire"
19:00	Assemble outside Porters' Lodge (Selwyn Main Entrance) to walk to *The Anchor Public House* for *Dinner* (Cost of Dinner included in registration fee but drinks are to be purchased individually)

PARSEM 3rd YEAR WORKSHOP / MEETING
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PARSEM MEETING

Friday, 28th March

08:00-08:45 Breakfast in Hall

Work Package Results, Plans and Discussions

09:00-10:30 **Work Package meetings**
Discussion on PARSEM's 4th year plans: organization of collaborations, timetable, and deliverables

10:30-11:00 *Coffee Break*

11:00-12:30 **Presentation of WP results/deliverables and the 4th year planning**

- **WPI** C.J. Humphreys
- **WP2** A. Georgakilas
- **WP3** A. Trassoudaine
- **WP4** H. Riechert
- **WP5** W. Neumann

12:30-13:30 **Discussion and planning for the next possible Marie Curie project**

13:30 **Close of Meeting**

Growth of group-III Nitrides by Plasma-Assisted Molecular Beam Epitaxy

Tom Foxon

School of Physics and Astronomy, University of Nottingham, Nottingham NG7 2RD

Abstract

In this talk I will discuss the growth of group III-Nitrides using plasma-assisted molecular beam epitaxy (PA-MBE). I will first briefly explain the growth of conventional semiconductor materials by MBE. I will then consider the special requirements for the growth of nitride-based semiconductors by MBE, which relate to the difficulty of finding a source of active nitrogen and problems related to the lack of suitable lattice-matched substrates.

In practise, there are only two options for supplying active nitrogen, ammonia can be thermally decomposed on the surface during the growth process, but this approach is limited to films grown at temperatures above ~500^{o}C. For In-containing films this is not suitable, due to the high Indium vapour pressure giving rise to loss by re-evaporation from the surface. The alternative approach, which I will describe in detail, uses active nitrogen from a plasma source. Two different commercial sources are available, activated by either RF or ECR radiation. The former approach is now used by most groups using the PA-MBE method. I will describe the operation of an RF plasma source and present optical spectroscopy from a typical commercial system, which shows evidence for both atomic nitrogen and excited molecular nitrogen, both of which may react on the surface to form group III-Nitrides.

I will then discuss the growth of GaN by PA-MBE, as a function of substrate temperature and V:III flux ratio. In particular I will explain why, unlike conventional MBE, we use group III-rich growth conditions to obtain higher quality films. I will then discuss the influence of the lack of lattice matched substrates, which results in the incorporation of a high concentration of extended defects. I will also show that using low-defect density GaN substrates grown by a high pressure process, defect free films and low-dimensional structure can be prepared. I will then present data for the growth of AlGaN and InGaN alloys, which can be grown over the entire composition range by PA-MBE.

Group III-Nitrides normally grow in the wurtzite (hexagonal) form, but using Arsenic as a surfactant we have been able to produce the meta-stable zinc-blende GaN polytype, which has a distinctly different band gap and due to symmetry avoids the electric fields present in (0001) oriented wurtzite structures arising from the spontaneous polarisation and piezo-electric effects. Recently, we have shown that it is possible using PA-MBE to produce free-standing cubic GaN substrates, with potential applications in UV emitters and other devices. I will also show data for the growth of GaN using the stable N_{15} isotope, resulting in NMR activity. Finally I will show examples of defect-free GaN nano-columns grown by PA-MBE under strongly N-rich conditions.

ZnO epitaxial films and nanostructures

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Centre de Recherche sur l'Hétéro-Epitaxie et ses Applications (CRHEA-CNRS), Rue Bernard Gregory, Sophia Antipolis, 06560Valbonne, France.

In the last years ZnO has raised a worldwide research effort due to its possibilities in fields such as spintronics, optoelectronics and, especially, in nanotechnology. This talk will address the reasons for such interest on ZnO, the problems encountered, and the contributions of CRHEA to each of them.

After introducing ZnO properties, I will highlight the seminal papers that around 2000 made the materials science community "rediscover ZnO once again" (C. Klingshirn). In particular:

1st **Spintronics**: It has been predicted that ZnO doped with magnetic ions, such as Mn or Co, could show under certain conditions a Curie temperature as high as 300K, paving the way for spintronic devices at room temperature. Even though several groups have published such an achievement, a big controversy remains about the origin of the observed ferromagnetism. CRHEA, in collaboration with other groups, has shown that the study of the magnetic anisotropy of these materials offers simple criteria, both experimental and theoretical, for the identification of the intrinsic ferromagnetism.

2nd **Optoelectronics**: Due to its large bandgap and exciton binding energies (3.3 eV and 60 meV, respectively) one of the main interests on ZnO arises from the field of optoelectronics, where it is supposed to become an alternative to GaN. Although some reliable reports on stable *p*-type doping have appeared, the main problem for the development of a ZnO-based technology is still *p*-type doping. Furthermore, the fact that ZnO crystallizes in the wurtzite structure, whereas CdO and MgO -which are used for lowering and increasing ZnO bandgap, respectively- crystallize in the cubic rocksalt structure, renders difficult the growth of quantum heterostructures.

Nevertheless we have achieved the growth of ZnO/ZnMgO quantum wells along both the polar [0001] and the nonpolar [11-20] directions; this enabled us to proof the existence of longitudinal electric fields induced by spontaneous and piezoelectric polarizations in ZnO, similar to GaN; besides, we have verified that the solution employed in GaN for avoiding the effect of these electric fields does also apply for ZnO. In parallel, CRHEA has fabricated ZnO/nitrides microcavities to profit of the ZnO huge oscillator strength and to demonstrate strong exciton-polariton coupling at room temperature on ZnO-based microcavities.

3rd **Nanostructures:** The never-ending list of ZnO nanostructures (nanobelts, nanowires, nanoribbons, nanosheets, nanohelices, etc.) grows almost every week. Most of these structures can be explained in terms of electrostatic energy minimisation and, some of them, exploit the effects of surface charges in piezoelectric field effect transistors or nanogenerators. A brief introduction to the advantages and problems of these nanostructures will be given, paying special attention to the electrical contacts at the nanometer scale.

Microstructure of Nonpolar and Semipolar GaN and ZnO heteroepitaxial films

P. Vennéguès

CRHEA-CNRS, Rue Bernard Grégory, Sophia Antipolis, 06560 Valbonne, France

The wurtzite III-nitrides and ZnO wide-gap semiconductors are, most of the time, grown along the polar <0001> direction. With such an orientation, internal electric fields resulting from both spontaneous and piezoelectric polarizations markedly affect the physical properties of quantum heterostructures. The interest of growing thin films along non-polar and semi-polar directions has recently increased in order to avoid these polarization effects.

Homoepitaxy on GaN platelet-like substrates or on ZnO bulk substrates is a very interesting approach. High efficiency homoepitaxial non-polar light emitting III-nitrides devices have already been demonstrated. But, GaN platelet-like substrates are sliced from thick <0001>-oriented halide vapor phase epitaxy (HVPE) self-supported substrates and their sizes remains small (a few mm^2). On the other hand, the availability of commercial ZnO nonpolar substrates is still not verified. Therefore, heteroepitaxial growth on foreign substrates should also be considered.

The purpose of this presentation is to describe and compare the structures and the microstructures of nonpolar and semipolar GaN and ZnO heteroepitaxial films grown on R and M-plane sapphire and on A-plane 6H-SiC. The epitaxial relationships and the strain relaxation processes will be described. The nature and densities of crystalline defects will be also studied.

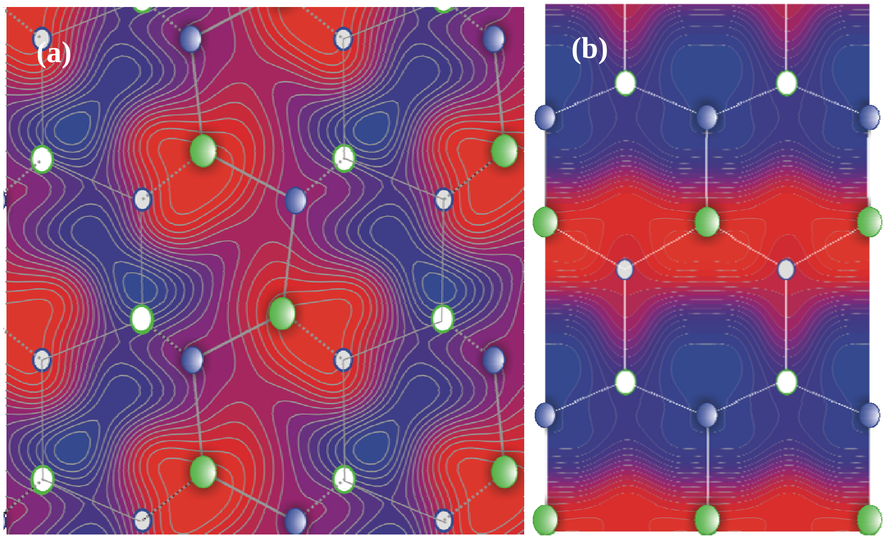
THERMODYNAMICS AND ADATOM KINETICS OF NON-POLAR GAN SURFACES.

LIVERIOS LYMPERAKIS, JÖRG NEUGEBAUER

Max-Planck-Institut für Eisenforschung, Max-Planck-Strasse 1, 40237,Düsseldorf, Germany

III-Nitride based nanowires have recently attracted considerable interest due to their potential applications for novel nano-optoelectronic devices. The shape and size of the nanostructure as well as the quality of the grown material depends strongly on the atomistic mechanisms taking place on the facets of the nanowires during growth. GaN nanowires usually grow having the c-axis as axial direction while the side facets are expected to exhibit non-polar surfaces. While extensive and detailed theoretical studies on the thermodynamics and kinetics of the polar *c*-plane GaN surfaces exist, a detailed analysis which will combine thermodynamics and kinetics of the non-polar *a*- and *m*-plane surfaces is still lacking. We have therefore performed planewave pseudopotential calculations within the density functional theory in order to study the thermodynamics and the adatom kinetics on *a*- and *m*- plane GaN surfaces.

Based on our calculations we derive surface phase diagrams for both non-polar surfaces. In accordance to previous ab-initio calculations we find that for growth under N rich conditions the bare surface which consists of Ga-N dimmers is the thermodynamically most stable configurations. On the other metal rich surfaces consisted of 4 ML of Ga are energetically favourable for Ga-rich growth. The mapping of the potential energy surface for the Ga adatoms (minority species for N rich growth) reveals a strong anisotropy for the diffusion barriers for both *a*- and *m*-plane surfaces. For N adatoms (minority species for Ga rich growth) our results show a subsurface diffusion channel which becomes activated already at low growth temperatures. Based on these results we have been able to explain recent experimental observations on the in-plane growth anisotropy of GaN non-polar surfaces as well as on the growth of GaN nanowires.



Potential energy surface for Ga adatom diffusion on the (a) *a*-plane and (b) *m*-plane GaN surfaces. Green filled (open) balls correspond to first (second) layer Ga atoms and blue filled (open) balls to first (second) layer N atoms respectively. The dashed rectangles denote the corresponding ×surface unit cells.

PRECISE MODELLING OF ELECTRON ENERGY LOSS NEAR EDGE STRUCTURE OF III-NITRIDES

DAVID HOLEC and COLIN J. HUMPHREYS

Department of Materials Science and Metallurgy, University of Cambridge, CB3 2QZ Cambridge, UK

In this paper we present results of N K-edge electron energy loss near edge structure (ELNES) calculations for III-nitride ternary alloys. In particular, we focus on $Al_xGa_{1-x}N$ alloy. Such calculations are needed for correct interpretation of experimental data that can now be obtained with a high spatial and energy resolution in modern transmission electron microscopes. It is known that better agreement with experiments is obtained for simulations using core-holes and especially partial core-holes [1]. Eventhough a partial core-hole with only a fraction of electron charge does not correspond directly to any physical situation, it is believed that it constitutes a good approximation to the excitation process. However, there is no universal rule for what charge of the core-hole should be taken and thus this can be estimated only by a thorough comparison with experimental data.

We used a full potential `Wien2k` code [2] which treats all electrons explicitly and thus allows a straightforward implementation of core-holes. Moreover, the `Telnes` program allowing direct calculation of ELNES spectra is a part of the `Wien2k` package.

Ab initio calculations are very time expensive when high numbers of atoms are used. Therefore, we use 2 × 2 × 2 supercells (32 atoms in total) to model various compositions. Atomic positions in the supercells were derived using special quasi-random structures methodology [3]. A detailed analysis of available experimental data and calculated N K-edges of AlN and GaN proved that a partial core-hole of 0.5 e is an ideal compromise for the whole range of compositions of $Al_xGa_{1x}N$.

We also studied variations of ELNES spectra with different neighbourhoods of nitrogen atoms. Our results imply that the four nearest neighbours of a N atom have a principal influence on the ELNES. This conclusion justifies the use of the 2 × 2 × 2 supercells which are usually regarded as too small (see for example the discussion in [4]). We showed that in our case, the supercell of this size is capable of a successful reproduction of the ELNES N K-edge evolution with composition x, and at the same time remains computationally affordable.

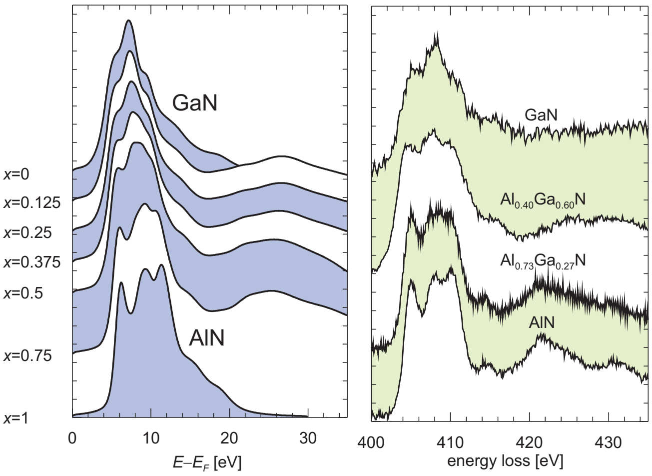


Figure 1: Simulated and measured N K-edge of $Al_xGa_{1-x}N$.

In the last part of our paper we present preliminary results of N K-edge evolution in other important III-nitride ternary alloys, namely $In_xGa_{1-x}N$ and $Al_xIn_{1-x}N$.

In summary, we present a reliable way for modelling ELNES spectra of ternary III-nitride alloys. ELNES spectra are regarded as fingerprints of material electronic structures and together with their precise simulations (such as these presented here) allow for experimental studies of their electronic structures.

References

[1] J. Luitz. *Simulation of core level spectra using Density Functional Theory*. PhD thesis, Technischen Universitt Wien, 2006.

[2] P. Blaha, K. Schwarz, G. Madsen, D. Kvasnicka, and J. Luitz. `Wien2k`, an improved and updated version of ab initio calculation package originally published as: P. Blaha, K. Schwarz, P.I. Sorantin, S.B. Trickey, Full-potential linearised augmented plane wave programs for crystalline systems, *Comput. Phys. Commun.* **59** (1990) 399–415., 2000.

[3] S.-H. Wei, L.G. Ferreira, J.E. Bernard, and A. Zunger. Electronic properties of random alloys: Special quasi random structures. *Phys. Rev. B*, **42**(15):9622–9649, 1990.

[4] D. Holec, P.M.F.J. Costa, P.D. Cherns, C.J. Humphreys, Electron energy loss near edge structure (ELNES) spectra of AlN and AlGaN: a theoretical study using the `Wien2k` and `Telnes` programs, *Micron*, 2007, doi:10.1016/j.micron.2007.10.013, in press.

Simulation of indium distribution in InGaN/GaN quantum wells

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The issues of indium distribution are important in order to explain the luminescence mechanism of InGaN/GaN quantum wells (QW). Early experimental studies have shown chemical fluctuations with formation of nanoscale indium-rich clusters due to the thermodynamic instability of InGaN alloys. However, the calculated phase diagram (S.Y. Karpov, MRS Internet J. Nitride Semicond. Res. 3, 16 (1998)) indicated that the strain may suppress the formation of In phase separation for low indium concentration. Actually, controversial results are obtained from the experimental data. In order to clarify the problems about indium distribution at low concentration, we have systematically calculated the deformation energy and micro-structures properties of InGaN/GaN QW for different indium concentrations, In-rich cluster sizes and quantum barrier thicknesses. The calculations are based on the Stillinger-Weber empirical potential.

At first, pure In-clusters are embedded in pure GaN quantum wells. The QW deformation energy increases with the cluster sizes. The metal-N bond lengths slightly fluctuate within clusters and in the GaN matrix and they steeply change at the interface between the two regions.

For a random distribution of indium atoms in the InGaN QW, the QW deformation energy increases as the indium concentration. The distribution of the bond lengths of In-N and Ga-N in the QW are centered on each mean value, respectively. The variation of the bond lengths also depends on the GaN barrier thickness, specially the behavior of Ga-N bonds is inverted if the barrier thickness exceeds a critical value. This change can be explained by a model based on the force balance.

At last, the pure indium clusters are constructed in In random distribution InGaN quantum wells. The results indicate that the increase of cluster size raises the deformation energy for a constant indium concentration in the whole InGaN quantum wells. The bond lengths of In-N inside and outside of clusters are different and behave distinctly with the variation of the barriers thicknesses and cluster sizes. Even in the same region, the behavior of bond lengths of Ga-N and In-N varies as a function of the barriers thicknesses and cluster sizes.

At present, I am calculating the electronic properties of threading dislocations and their induced strain field in binary and ternary compound materials with SIESTA.

A METHOD FOR ATOMISTIC/CONTINUUM ANALYSIS OF LARGE HRTEM IMAGES

A. Belkadi[1], G. P. Dimitrakopulos[2], J. Kioseoglou[2], G.Jurczak[1],
T. D. Young[1], P. Dluzewski[1], and Ph. Komninou[2]

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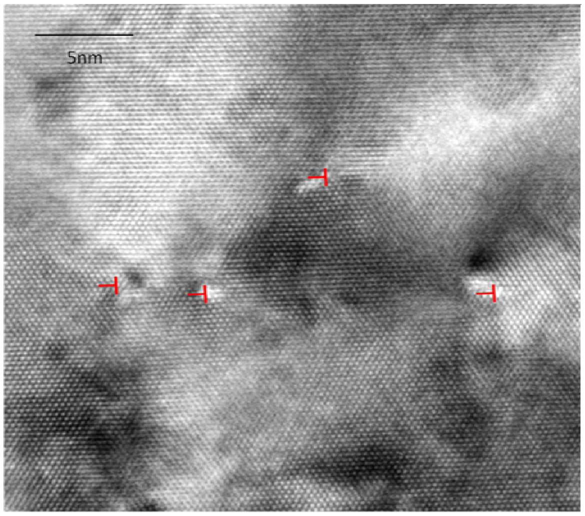
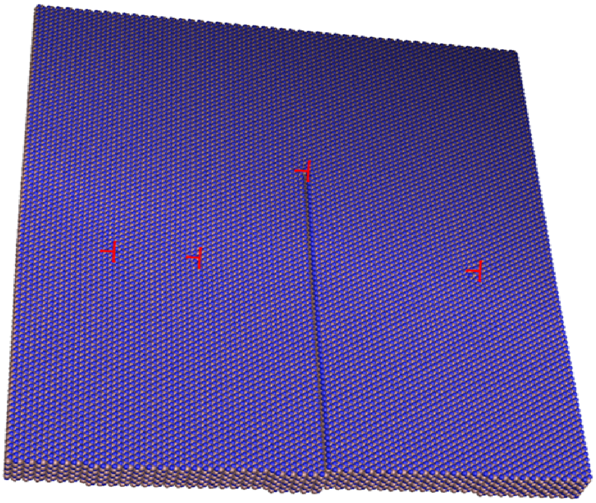
[2]Solid State Physics Section, Department of Physics, Aristotle University of Thessaloniki, GR-54124 Thessaloniki, Greece

The capability to extract continous lattice distortion fields from High Resolution Transmittion Electron Microscopy (HRTEM) images is invaluable for treating a large number of material problems; and methods, such as Geometrical Phase Analysis (GPA) or peak-finding have been employed for this purpose. However, it is difficult to use such methods to obtain experimental strain maps from HRTEM images of large areas containing many dislocations due to localized changes of the defocus conditions imposed by the strain fields or by variations of the specimen thickness (see figure 1). In this work we propose another method for the investigation of large area dislocation structures and their strain maps. In the first step, the atomic structure including all dislocations visible on the HRTEM image is generated. Independently of the atomic structure the maps of the lattice distortion tensor are then generated and the stress equilibrium configuration is determined by using a nonlinear finite element method for anisotropic nonlinear elastic structure. The stress/force equilibrium configuration of the lattice is determined both for the respective continuum problem and for the atomic structure. Using the atomic structure in a state of self-equilibrium a virtual HRTEM image is generated and compared with the `real' one. By the method proposed here, problems induced on the HRTEM observation due to lattice curvature and foil effects can be accounted for and analysed. Also the residual stress induced by these dislocations embedded in an anisotropic non-linear elastic structure are calculated. Compared to two-dimensional approaches such as the GPA and peak-finding, this method has the advantage of yielding three-dimensional fields surrounding the dislocations, which is significant in the case of mixed-type dislocations. Furthermore, this method conveniently overcomes the `size-problem' in the analysis of HRTEM images as it is applicable to large volumes of material with many dislocations trapped inside.





STATISTICAL ELECTRONIC DENSITY-FUNCTIONAL THEORY: STRUCTURAL PROPERTIES OF $In_YX_{1-Y}N$ RANDOMLY-ORDERED ALLOYS

TOBY D. YOUNG[1], *SUMAN-LATA SAHONTA*[2], *and PHILOMELA KOMNINOU*[2]
[1]*Department of Computational Science, Institute of Fundamental Technological Research, Polish Academy of Sciences, ul Swietokryska 21, 00-49 Warsaw, POLAND*
[2]*Solid State Physics Section, Department of Physics, Aristotle University of Thessaloniki, 54124 Thessaloniki, GREECE*

Investigations in applied physics concerning ordered InXN alloys (X{Al,Ga}) have recently focused on $In_yX_{1-y}N$ alloys in which the In molar fraction is $y \neq 0.5$, and the possibility for an inhomogeneous distribution of indium in the bulk crystal may arise [1,2]. Varying the In molar fraction augments the physical response of the optical and electronic properties of the crystal according to the desired device applications. In theoretical modelling of electronic systems first principles calculations are often employed to investigate their structural and thermodynamic properties, usually owing to the relatively high degree of accuracy found when referred back to empirical observations. The most widely used of these is in the form of an electronic density-functional theory. The application of electronic density-functional theory to randomly-ordered alloys however is at its best very difficult, due to the vast computational costs required for large many-body systems.

The large systems considered here are “randomly-ordered” in the sense that locally (by unit cell) the atomic molar fraction is random, however due to the usage of periodic boundary conditions, the global (bulk) system is well ordered. From probability theory it can be easily shown that the number of possible ways of arranging atoms in substitutional alloys, say for a 2 x 2 x 2 zinc-blende or wurtzite conventional unit cell, is daunting. This is impossible to handle holistically starting from a standard first-principles electronic density functional theory. To overcome this, we turn to a statistical “parasol” approach known as the Connolly-Williams method [3]. The Connolly-Williams method of statistically averaging over a number of carefully chosen states of ternary (or quaternary) alloys has been shown to be time-wise cost effective while maintaining a satisfactory link between substance and attributes of the system under investigation. We consider the effect that this approach has on our interpretation of the metaphysics of randomly-ordered alloys.

An application to $In_yX_{1-y}N$ in the zinc-blende phase (conducted by other authors) is presented [4]. Although here our computations pursue applications within particle electronic density-functional theory, relations within the frameworks of virtual crystal approximation, molecular statics and valence force-field models are also considered. A tentative and analogical application of the Connolly-Williams statistical method to randomly-ordered $In_yX_{1-y}N$ in the wurtzite phase is then given in order to clarify the behaviour of its structural properties as a function of fractional In molar content, where we expect deviations from Vegard's law to be largest (see for example [5,6]). We employ the usual assumptions pertaining to electronic density-functional theory cast within the local density approximation.

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ATOMISTIC MODELING OF (Al,In)N/GaN INTERFACES

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Interfaces play an important role in semiconductor device applications, such as LEDs and laser diodes, since the later are actually based on epitaxially grown heterostructures.

Based on our experimental observations of (0001) InN/GaN (Fig.1c) and AlN/GaN interfaces, and the increasing interest of the scientific society on the structural properties of group III nitrides, we studied the aforementioned interfaces focusing on their structural and electronic characteristics.

At first, we implemented Tersoff interatomic potential calculations in order to handle the 15.000 and 144.000 atoms configurations, for InN/GaN (Fig.1) and AlN/GaN respectively, resulting from the fact that we wanted to take into account the existence of misfit dislocations in these heterostructures due to their lattice mismatch (10.9 % for InN/GaN and 2.4% for AlN/GaN).

In the case of AlN/GaN (Fig.2) we also performed ab initio calculations assuming pseudomorphic growth of AlN on GaN motivated by the "good fit" areas observed on the relaxed supercells of our first calculations. We considered all three possible cases; imposing the average basal lattice constant on both AlN and GaN or AlN's lattice constant in GaN and vice versa.

Three main criteria were taken into account concerning the structural characterization: a) polarity, b) interfacial stacking sequence and c) interfacial plane; cutting of single or double bonds. Band structure study was performed concerning the electronic properties of the AlN/GaN heterostructures.

Our empirical calculations for InN/GaN as well as AlN/GaN interfaces suggest that III polarity – cutting single bond interfaces are preferable, but no certain conclusion can be extracted for the favorable stacking sequence. Density functional theory calculations on AlN/GaN interfaces confirm our former results but also lead us to the conclusion that the wurtzite stacking is preferable in comparison to the zinc blende, and the interfacial energy difference ($\Gamma_W - \Gamma_{ZB}$) increases proportionally to the basal lattice constant of the pseudomorphically adjusted thin layers.The band structure calculations performed at this point suggest that the band gap increases while the compressive strain increases (Fig.3), thus a linear dependence of $E_g^{AlN/GaN}$ on the lattice constant is evident. However, biaxial strain is found to flatten this linear variation considerably.

Acknowledgment

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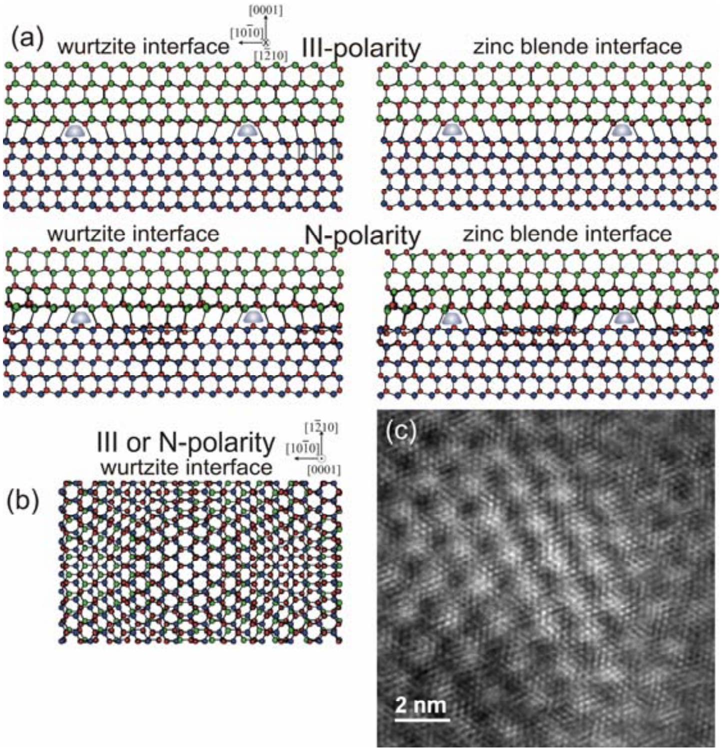

Figure 1. (a) Relaxed InN/GaN type 1 (cutting single bonds) interfaces for wurtzite and zinc blende interfacial structures viewed along [$1\bar{2}10$] and (b) projection of the interface along [0001] direction. The two polarities are non distinguishable when viewed along [0001]. (c) HRTEM image along the [0001] direction of InN/GaN interface. The moiré pattern reveals the regions of "good" and "bad" fit.

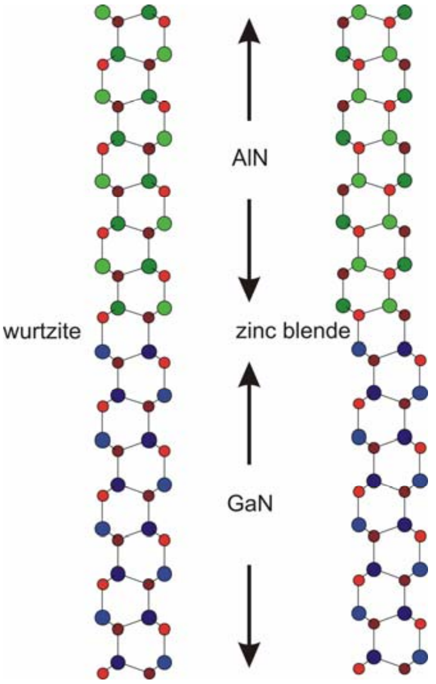

Figure 2. Atomistic unrelaxed models of the supercells having wurtzite and zinc blende interfacial stacking.

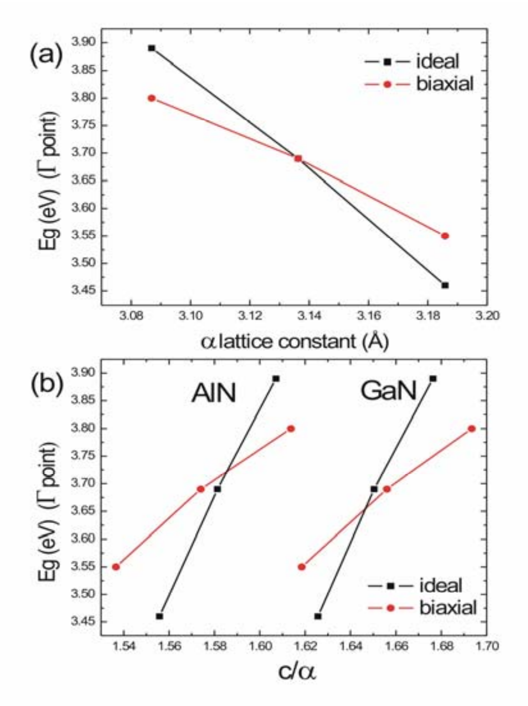

Figure 3. Band gap of wurtzite AlN/GaN as a function of the imposed lattice constant *a* (a) and *c*/*a* ratio (b) for the "ideal" and the biaxially strained case.

MULTI-SCHEME *AB-INITIO* – FINITE ELEMENT CALCULATION OF III-NITRIDES BASED QUANTUM DOTS ELECTRO-MECHANICAL PROPERTIES

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The knowledge of properties of nanostructures like III-Nitrides based quantum dots (QD) are becoming important as their usage for optoelectronic devices is rising. In this work we combine ab-initio and Finite Element Method (FEM) calculations, which were used to study the electro-mechanical properties of a GaN QD embedded in AlN matrix. The calculations have been performed in two steps: In a first step the linear and non-linear elastic properties for AlGaN alloys were calculated by means of first principle calculations. The elastic properties were computed with respect to the composition and strain measure alteration while the anisotropic hyperelasticity has been also taken into account [1]. Our calculations show that linear dependence of the elastic constants on the alloy composition can be assumed.

In a second step we perform FEM calculations and solve the electro-mechanically coupled non-linear boundary problem of the strain and polarization constitutive equations. Our calculations show the significant variation of the charge distribution along the QD growth direction. This distribution is expected to result to spatial localization of the carriers and thus to induce inherent dipole moment. Among the interesting result is as well the fact that implementation of the elastic non-linearity does not qualitatively affect the charge distribution. Nevertheless, it results in quantitative differences of the order of about 5%.

OPTICAL PROPERTIES OF SEMICONDUCTOR NANOSTRUCTURES INCLUDING STRAIN AND PIEZOELECTRIC EFFECTS

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Optical properties of semiconductor nanostructures such as quantum dots and wires are a direct consequence of their shape, size and material composition. The $\boldsymbol{k}\cdot\boldsymbol{p}$ formalism provides a real space approach to compute relevant parameters of nanostructures as e.g. needed to simulate optoelectronic devices such as light and laser emitting diodes. We have reformulated this approach into a mixed real/reciprocal space formalism and have implemented it into our plane-wave DFT-package S/Phi/nX. This allowed us to make efficient use of the existing highly optimized minimization routines as well as the efficient preconditioner techniques in a plane-wave basis set.

In the present work we present an 8-band description where the effects of strain and piezoelectricity are explicitly taken into account. In a first step these additional contributions are calculated by minimizing the strain free energy using the second-order elastic constants. Moreover, calculations based on the simpler 6-band plus effective mass description as well as tight-binding calculations which fully resolve the atomistic structure have been performed in order to verify the validity of our approach. Our results show an excellent agreement with the atomistic tight-binding calculations. Moreover, they show that the accuracy of the 6-band model along with the effective mass description of electron states is not sufficient. Finally, we show that the spin-orbital splitting, which is commonly neglected in III-Nitride materials calculations due to its small value, lifts the artificial degeneracy of the hole states.

MAGNESIUM ADSORPTION AND INCORPORATION AT InN (0001) AND (000-1) SURFACES: A FIRST-PRINCIPLES STUDY

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We present first principles calculations of Mg incorporation at InN (0001) and InN (000-1) surfaces under various Mg coverage conditions obtained within the framework of density functional theory by using plane wave pseudopotential techniques.

We find significant differences in Mg incorporation between In- and N-polar surfaces; Mg incorporation is easier at the N-polar surface than the In-polar one. For In-polarity high Mg coverage is found to cause flattening of the InN bilayers while Mg atoms are substituting In atoms below the surface. It is also found that on In polarity InN the diffusion barrier for Mg and In adatoms is decreased for small doses of Mg doping.

For N polarity InN the In adlayer and consequently the In rich conditions facilitate the diffusion of In and Mg adatoms. At the N-polar surface, the preferred configurations at all coverages are those with all Mg atoms just below the terminating InN bilayer or In adlayer. Finally the Mg incorporation is favoured under In-rich and Mg-less than rich conditions.

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DEFECT FORMATION IN SEMICONDUCTOR NANOWIRES

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Semiconductor nanowires very often exhibit planar defects. The knowledge of the nature of these defects provides access to the control of their formation and even to their prevention.

In this work, we analyse planar defects formed in ZnTe nanowires. This II-VI semiconductor material can be applied to fabricate various devises in the field of, e.g., optoelectronics, spintronics, and detection of molecules. The nanowires were grown on (001)-oriented GaAs substrate by molecular beam epitaxy at a temperature of 400 °C. The 1-dimensional growth of the nanowires was induced by a gold-gallium eutectic droplet at the tip of the individual nanowire.

The defects are observed in all nanowires investigated by transmission electron microscopy (TEM). High-resolution TEM images of the nanowires clearly show different orientations of thin lamellae oriented perpendicular to the nanowire axis. The thickness of the lamellae ranges from 2 to 6 monolayers (MLs).

In order to analyse the type of the defects the stacking sequence as concluded form the HRTEM images was compared with that of intrinsic as well as extrinsic stacking faults. For both types a disagreement was found.

Alternatively, a formation of rotational twins was assumed where an 180° rotation around the {111} nanowire axis was applied. In this case, the atomic structure agrees exactly. In order to generate lamellae, a multiple twinning has to be considered.

The twinning in favour of stacking fault (SF) formation can be understood by analysing the stacking sequences of the three defects: extrinsic SF, intrinsic SF and rotational twin.

Stacking faults parallel to the {111} plane always cause a modification of the coordination number from initially 4 to 6 for the Zn atom placed at the position (¼ ¼ ¼) of the unit cell. Altering the stacking sequence for sphalerite AaBbCcAa to AaBb*AaBb*CcAa (extrinsic SF) or to AaBb*AaCc*Aa (intrinsic SF) results into a 6-fold coordination for the layers marked by an underscore.

In contrast to that, the Zn atom at (¼ ¼ ¼) is always coordinated by 4 Te atoms for the twin configuration. The stacking sequence of a twin lamella of 2 MLs thickness reads: AaBb*CaBc*Aa. The layers denoted by *italic* letters form the twin. Hence, the twin configuration maintains the initial coordination of the Zn atom. This fact justifies the twinning in favour of the formation of stacking faults.

ALUMINIUM INCORPORATION STUDIES IN ALGAN AND GAN/ALGAN CORE/SHELL NANOWIRES

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Growth of GaN nanowires (NW) by molecular beam epitaxy (MBE) has been already demonstrated on sapphire substrates with the use of nickel a seed as promoter of the NW growth. In addition, preferential NW radial or axial growth can be selected through the control of growth parameters, particularly the group III to group V ratio (N-rich or Ga-rich conditions) [1]. The next challenge is the controlled growth of NW heterostructures incorporating both GaN and AlGaN. The achievement of this step will open the way to device development, such as nanowire-based FETs, which have been already obtained with other materials. A critical issue is the control of aluminium incorporation in AlGaN NWs and AlGaN/GaN NW heterostructures.

In this work is reported a compositional analysis of two III-nitride NW samples grown by MBE on c-sapphire substrates at the same temperature. The first is a nominally uniform composition AlGaN sample, grown in N-rich conditions. The second sample is a radial heterostructure with a GaN core grown in N-rich condition, and an AlGaN “shell” grown subsequently in Ga-rich condition. In both cases Al and Ga beam fluxes were designed to obtain AlGaN material with nominally 10 at% Al.

Analysis was undertaken using electron energy loss spectroscopy (EELS) and energy dispersive X-ray analysis (EDX) techniques on the North West STEM facility at the University of Liverpool. This is a VG HB601UX scanning transmission electron microscope operating at 100 keV with a cold-field emission source and a optimum spot size of 1 nm. It is also equipped with a Gatan Enfina parallel channel EELS acquisition system and a windowless Si(Li) EDX spectrometer by Oxford Instrument. EELS line scans and point analysis were quantified assuming a single power law decay for the background subtraction. The electronic partial cross sections for inelastic scattering were calculated using the Hartree-Slater model for each specific core loss feature [2]. The calculated mean free path for all inelastic scattering in the material fulfilled the condition of thin samples, allowing plural scattering to be neglected. EDX spectra were processed using thin film approximation with calculated K factors with both Zaluzec and Mott/Massey models [3].

For the nominally uniform AlGaN NWs, the aluminium content was found to decrease along the NWs with distance away from the sapphire substrate. Al was not detected at the tip of AlGaN NWs. In comparison, EDX line scans across the radial NW structures with GaN core and AlGaN shell showed AlGaN surrounding the GaN core only near the growth tip, with a decrease of Al content towards the NW root at the substrate.

The observation are compared with previous studies made on GaN nanowires [4] and discussed in terms of different Al incorporation mechanisms. Elemental intensities of EDX line scans are discussed using geometric models appropriate for the NW structures.

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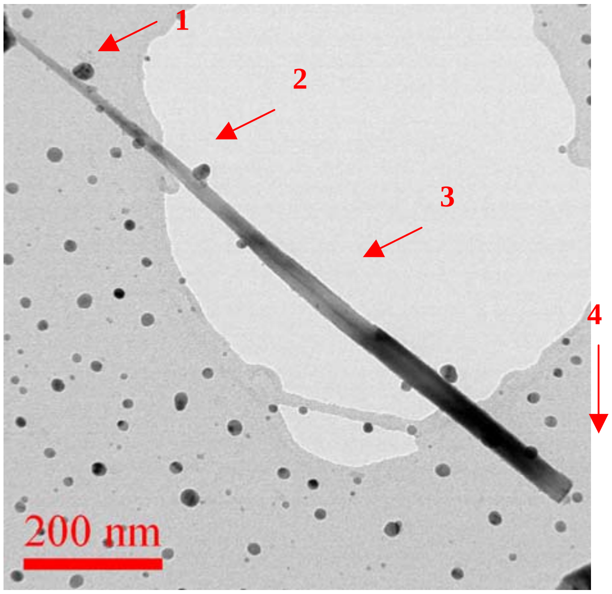

FIG. 1. STEM bright field image, the arrows indicate the EELS point analyses positions. Quantified analysis of Al distribution along the length of NW are reported in the table below:

Position	Distance from tip	NW diameter	Al at%
1	150 nm	10nm	0±3
2	350 nm	20nm	14±4
3	700 nm	35nm	25±4
4	1100 nm	35nm	34±5

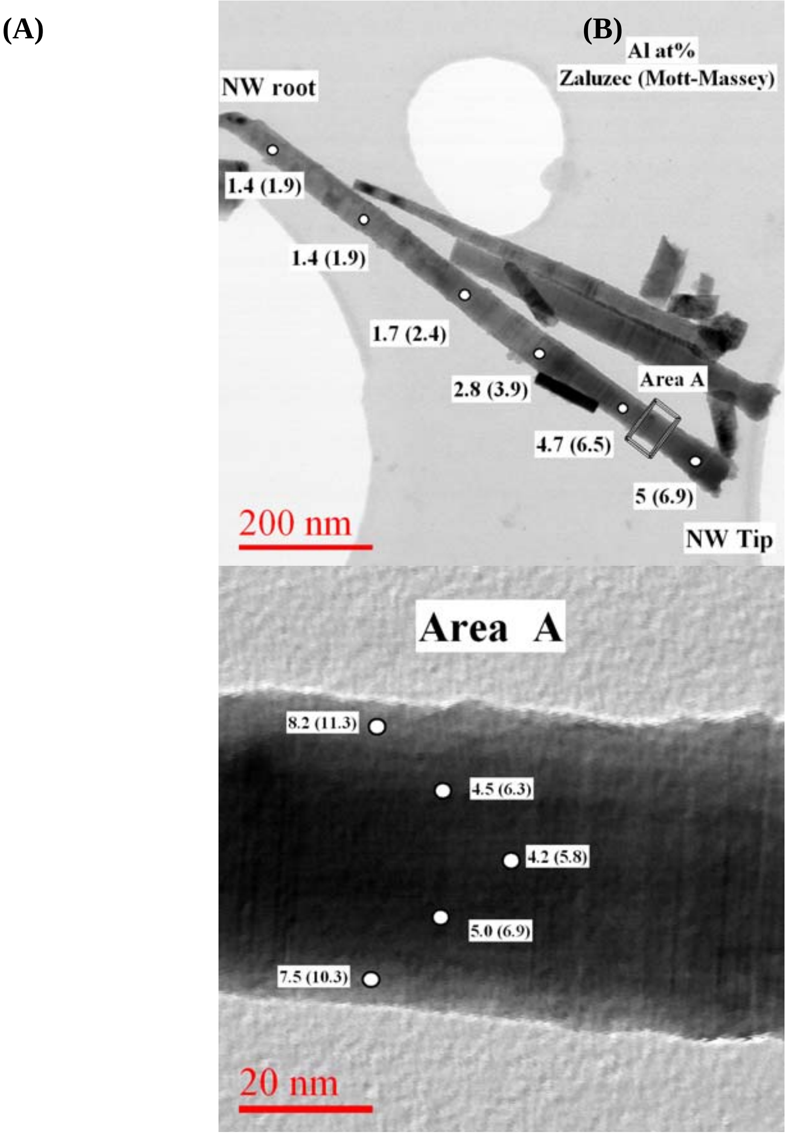

FIG. 2. (A) STEM bright field image of GaN/AlGaN core/Shell NW heterostructure. Results report Al at% from EDX point analysis quantification using Zaluzec (Mott-Massey) cross-section models. (B) Variation of Al at% across the NW diameter consistent with a core/shell structure.

CATALYST-FREE AND CATALYST-INDUCED GROWTH OF GAN-NANOWIRES BY MBE

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GaN Nanowires (NWs) have already demonstrated their amazing potential for photonic and electronic applications. In the bottom up approach, various methods have been successfully developed to initiate their formation: catalyst particles, nucleation layers, and self-organisation without any catalyst. In the present work GaN NWs were grown by solid source molecular epitaxy (MBE) with and without catalyst under very similar conditions, enabling thus a direct comparison of their growth mechanisms and characteristics.

Apart from the type of substrate, growth parameters were identical for all these experiments. On any substrate, NWs form only under N-rich conditions. Whether a catalyst is necessary to induce the formation of NWs is determined by the type of substrate. On c-plane sapphire (c-Al_2O_3), NWs grow only when Ni seeds are deposited on the substrate before GaN-growth. Transmission electron microscopy revealed particles at the tips of these NWs, suggesting that NWs form in a way similar to the vapour-liquid-solid[1] mechanism. In contrast, on both Si(111) and Si(100) NWs form in a self-induced way, and there is not any indication of particles or droplets at their tips. The deposition of Ni seeds on Si substrates does not change NW growth, and there are still not any particles at the NW-tips. Ni-induced NWs on c-Al_2O_3 are fairly homogeneous in length and diameter, while growth on bare Si resulted in shorter NWs that have a much broader distribution of diameters and lengths. These NWs do not exhibit any extended defects, but the Ni-induced NWs contain numerous stacking faults. Furthermore, the growth rate of the NWs was systematically investigated in dependance on the growth parameters temperature, N-rate, and Ga-rate. Surprisingly, in the case of catalyst-assisted growth, the NW growth rate amounts to the effective N-rate. This evidences that growth is limited by atomic N impinging on the NW tip and occurs under locally Ga-rich conditions as suggested in ref [2]. In the case of catalyst-free growth, only a small amount of NWs grow with a growth rate approaching the N-rate. Apparently, nucleation processes are more complicated in this case.

Acknowledgements

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Investigations of AlInN-GaN heterostructures

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The ternary semiconductor $Al_{1-x}In_xN$ has received much less attention than its close relations $Al_{1-x}Ga_xN$ and $In_xGa_{1-x}N$, yet promises a variety of important niche applications. This is in large part due to two factors: the wide range of achievable band-gaps covering energies from 6.2 eV (for x=0) to 0.7 eV (for x=1) and the possibility to lattice match the alloy to GaN at an InN mole fraction near 0.17. These allow strain-free III-nitride heterostructures where the benefits of low dislocation density, free-standing GaN substrates can be maximised.

A range of AlInN epilayers and GaN/AlInN quantum well structures grown by metal-organic vapour phase epitaxy have been characterised using optical spectroscopy. The substrates used include c-plane sapphire, low-dislocation GaN-on-sapphire templates and free-standing GaN. Photoluminescence (PL) and PL excitation spectra reveal how the emission peak energies and energy gaps of the AlInN layers vary with InN mole fraction. The composition dependence of the Stokes shift can then be determined and compared to data from the other ternary III-nitrides. PL spectra from the quantum wells show how the emission peak energy varies with quantum well width due to the spontaneous polarisation fields that exist in these structures, even when lattice-matched. Screening of these fields is investigated by varying the intensity of the exciting laser spot and demonstrates a well-width dependent behaviour. Analysis of all the optical data provides extensive information on the properties and growth of AlInN materials.

Optical Properties of Nitride based Quantum Well Structures

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Over the last fifteen years or so the optical properties of nitride quantum well structures have been studied extensively, and most of this work has concentrated on structures grown on polar substrates. Compared with the detailed spectroscopy that can be performed on the more "traditional" quantum well structures such as GaAs/AlGaAs the spectroscopy of polar nitride based structures is much less informative.

In this talk I will discuss reasons for this behavior and show that even in nitride based structures, under certain circumstances the traditional techniques of photoluminescence and photoluminescence excitation spectroscopy can be very revealing. This is especially the case for quantum well structures grown on semi-polar and non polar substrates.

Epitaxial Reactor Technology
Material Production for Solid-State Light Emitters

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The main factors determining the Success of the approach applying Solid State Light Emitters for General lighting are the capability of producing the required material quality for high efficiency and durability of the devices and the provision of commercially attractive prices for such. In the strive of reaching these goals it is the task of a supplier of tools for the production of these materials to stay with the development of the equipment close to the state of art in materials science.

The material quality demand is inextricably depending on the device structures developed for high efficacy lighting. The development of crystal growth tools for this task requires a very deep insight into the growth chemistry to allow combinations favourable for the designed results.

The second requirement to obtain commercially attractive pricing for the lighting devices is an even higher enabling factor for the future of this emerging application of semiconductor materials. Regarding this the production cost represented by the “Cost of Ownership (Coo)” of the used production tools, here specifically the MOVPE reactor, is a significant factor. This being influenced by throughput and the yield of the process, hence the target for tool development is keeping both maximized.

One strategy is the increase of the wafer area per run. Coming from single wafer reactors for III-N “production” about a decade ago typically modern reactors for III-N materials today can carry up to 42x2 inch wafers. The development for such tools as well requires a very detailed knowledge about the growth chemistry as well as all factors enabling growth on large wafer areas.

As examples the content of this presentation will introduce the basic functional principles as well as the development background of today’s leading MOVPE technologies provided by AIXTRON.

Besides such production volume oriented development work there are approaches to optimize the substrates used either on the quality or on the use of alternative solutions.

Bulk growth techniques for thick GaN layers or even boules are introduced and technical details discussed as well as results on large area Si substrates by MOVPE technology.

Results on layers and structures provided from the described technologies for industrial applications are demonstrated and discussed.

EXPERIMENTAL CONDITIONS INFLUENCE ON GROWTH RATE AND QUALITY OF GaN LAYERS BY STANDARD AND ELO HVPE

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Robert CADORET, Dominique CASTELLUCI, Evelyne GIL

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To produce 2 inch large GaN substrates having low dislocation density, there is an approach which consists mainly in the growth of thick layers of GaN on sapphire and subsequently to remove the template to get a free-standing GaN layer. Thus, Hydride Vapour Phase Epitaxy (HVPE) seems to be the efficient method for this kind of process; it remains the technique which provides the highest growth rate capabilities, up to hundred of microns per hour, and a perfect intrinsic selectivity. By combining with epitaxial lateral overgrowth (ELO), which consists in a structurally controlled GaN growth in line patterns and dot patterns substrates followed by thickening, the dislocation density can be significantly reduced in thick GaN layers (up to 6×10^{6} cm^{-2} [1]). In fact, GaN templates can be grown in a single HVPE process, after the ELO growth and controlled coalescence of stripes and further thickening by altering the experimental conditions to favour a high vertical growth.

In this work, we have first investigated the HVPE growth process of GaN layers via various experimental parameters such as: the influence of the parasitic deposit on the growth rate [1], the variation of the NH_3 flow rate during the growth, the growth temperature, the carrier gas composition and the V/III ratio on the growth rate. All these experiments were performed on GaN-MOCVD templates provided by UCAM.

The next step was the investigation of the selective growth. The goal is to control the epitaxial morphologies via the vertical and the lateral extensions with the variation of the carrier gas composition, the growth temperature, the V/III ratio, the type of the substrate (Sapphire or GaN MOCVD) and the stripes orientation (<11-20> or <1-100>). These experiments were performed on sapphire and on UCAM GaN-MOCVD templates after the pattern process performed by the CRHEA.

From these results, in order to favour lateral extensions, ELO HVPE was carried out on heavily-dense patterned substrates in order to coalesce the stripes and to produce GaN films. Indeed coalescence of growth structures was favoured and a uniform GaN layers about 10 µm thick were successfully grown directly on low cost sapphire substrates [2]. These 10 µm of GaN were grown on sapphire substrate pattern processed by the CRHEA. After this first successful coalescence, we are trying to optimise the coalescence with the variation of other experimental conditions.

All these experiments were correlated with a phenomenological GaN model that has been developed by R.Cadoret [3]. This theoretical approach still be a powerful method for the analysing and predicting near-equilibrium HVPE experiments. It is based on physical analysis including thermodynamical and kinetic modelling. The growth process of the model is a surface process involving the adsorption of NH_3 molecules, the adsorption of N atoms resulting from NH3 decomposition, and then the adsorption of GaCl molecules on the N atoms and finally the chlorine desorption [3,4,5]. The goal of the comparison between this theoretical model and the experimental results is first the comprehension of the growth mechanisms predominant at different growth conditions and secondly the comparison between the results obtained by standard HVPE and ELO HVPE.

Scanning electron microscopy (SEM) images were performed at the CRHEA. Dislocation density measurements of standard HVPE GaN layers and atomic force microscopy (AFM) of standard HVPE and ELO HVPE GaN layers characterisations are in progress (AUTH).

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We are grateful to Menno Kappers from CAMBRIDGE for GaN-MOCVD templates, to the CRHEA (UPR CNRS N°10) for patterned GaN/sapphire and sapphire substrates and to Philippe Vennéguès and Luan Nguyen from CRHEA for their help during SEM investigations.

TRANSMISSION ELECTRON MICROSCOPY INVESTIGATION OF THE INFLUENCE OF THE SI/N TREATMENTS ON THE STRUCTURAL DEFECTS IN THE NON-POLAR AND SEMI-POLAR MOVPE-GROWN GaN FILMS

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GaN is generally deposited on the basal plane (0001) sapphire. Epitaxy over this polar orientation results in strong internal electric field. This polarization reduces the energy and intensity of the optical emission from quantum wells. The growth along a non-polar or semi-polar direction is a promising option to eliminate or reduce this effect and obtain more efficient devices.

The microstructures of non-polar and semi-polar GaN films deposited on sapphire substrate are dominated by the presence of I_1 type basal stacking faults (BSFs). These BSFs are either terminated by partial dislocations (PDs) or connected by prismatic stacking faults (PSFs). Different growth techniques (3D growth induced by Si/N treatment [1], Epitaxial Lateral Overgrowth [2]) have been developed to reduce the densities of defects in c-oriented GaN films. In this study, the influence of similar Si/N treatments on the microstructures of non-polar (11-20) and semi-polar (11-22) GaN films grown by metalorganic vapor phase epitaxy on R- and M-plane sapphire respectively are investigated by transmission electron microscopy. Three kinds of samples are investigated: without any Si/N treatment, with a single and a double Si/N treatment. The first Si/N treatment is performed on the sapphire substrate whereas the second one is performed at an intermediate stage of the GaN film growth. Figures 1a and 1b show different investigated orientations in non- and semi-polar samples, respectively.

Dark field images presented in figures 2a and 2b show the microstructure of the non-polar sample without any Si/N treatments viewed along [-1100] and [2-1-10] zone axis, respectively. The PDs are on contrast and the BSFs are out-of contrast when the diffraction vector is g = 11-20 (Fig 2a). Both types of defects are imaged using the diffraction vector g = 01-10 (Fig 2b). One can see that the PDs and the BSFs are perpendicular to the interface GaN/sapphire. The densities of the PDs and BSFs are very high 5.10^{11} cm^{-2} and 6.10^{5} cm^{-1} respectively (measured in plan-view). The effect of both kinds of Si/N treatments is to induce a three-dimensional growth mode. Thanks to lateral growth, growth islands coalesce and the resulting films have a smooth surface. Dark-Field images taken with (Fig. 3a) g = 11-20 and (Fig. 3b) g = 1-100 show the microstructure of the non-polar sample with double Si/N treatment. The main observed effect of Si/N treatments on the microstructure of non-polar films is the bending of PDs and the formation of internal voids. After a double Si/N treatment the density of the PDs is only slighty lower than 2.10^{10} cm^{-2} and the density of BSFs is similar to the reference sample without Si/N treatment (5.10^{10} cm^{-1}). After the first Si/N treatment more voids than after the second one are observed. The PDs which are not longer perpendicular to the interface have tendency to regroup in triangular forms above these voids.

In the case of the semi-polar samples the effects of the Si/N treatments are similar. Figures 4a and 4b show the microstructures of the semi-polar sample with double Si/N treatment. A high density of defects is observed in the inclined c-planes. Basal stacking faults are out-of-contrast in the g = 0002 dark field image and the observed defects are PDs (Fig 4a). The BSF are on-contrast in the g = 11-20 dark-field image. After the second Si/N treatment the density of PDs decreases (Fig. 4a and 4b). This effect is also clearly seen in the [11-23] zone axis. Due to the first Si/N treatment a three-dimensional growth has induced disoriented grains indicated by white stars (Fig. 5). Above these grains a zone with a low density of defects is observed, pointed by red arrows. Statistic measurements of the densities of defects will be done on the semi-polar samples.

Transmission electron microscopy investigation shows that Si/N treatments in non-polar GaN do not strongly reduce the densities of PDs and BSFs. Although the statistic measurements in semi-polar samples have not been made, it is expected that the reduction of the density of defects in these samples will be very similar.

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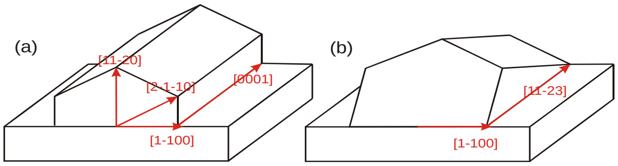

Fig. 1. Investigated orientations in (a) non-polar and (b) semi-polar GaN

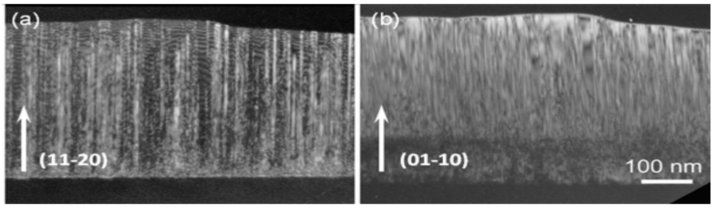

Fig. 2. Dark field images of the microstructure of the reference non-polar sample without any Si/N treatment, (a) PDs are imaged using g = 11-20 close to [1-100], (b) BSFs and PDs are imaged using g = 01-10 close to [2-1-10]

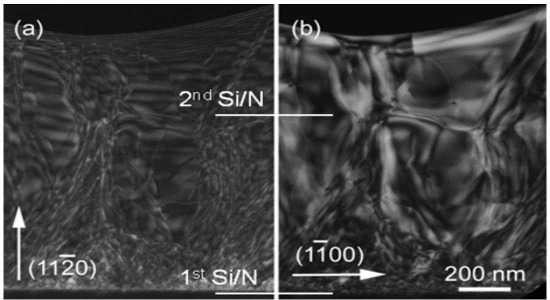

Fig. 3. Dark-field cross-section images taken with (a) g = 11-20 and (b) g = 1-100 near the [0001] zone axis of a nonpolar sample grown with double Si/N treatment, showing the bending of the PDs.

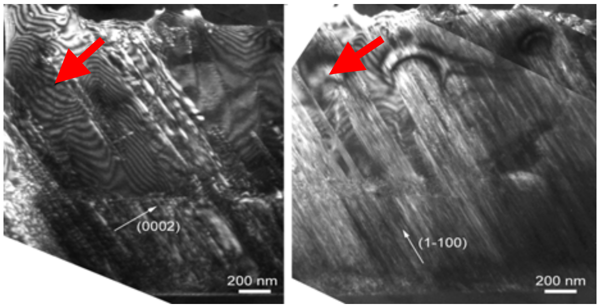

Fig. 4. Dark field cross-section images of the microstructure of a semi-polar sample with double Si/N treatment close to the [1-100] zone axis, (a) PDs are imaged using g = 0002, (b) BSFs and PDs are imaged using g = 1-100; the red arrows show the zone with a

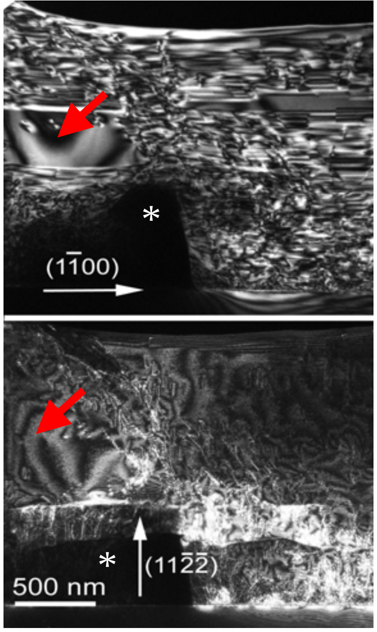

Fig 5. Dark-field cross-section images of a semipolar sample with double Si/N treatment close to the [11-23] zone axis. Disoriented grains (white stars) and zone with low density of defects (red arrows) are imaged.

INFLUENCE OF CARRIER INJECTION ON THE ELECTROLUMINESCENCE PROPERTIES OF GaN-BASED LEDs

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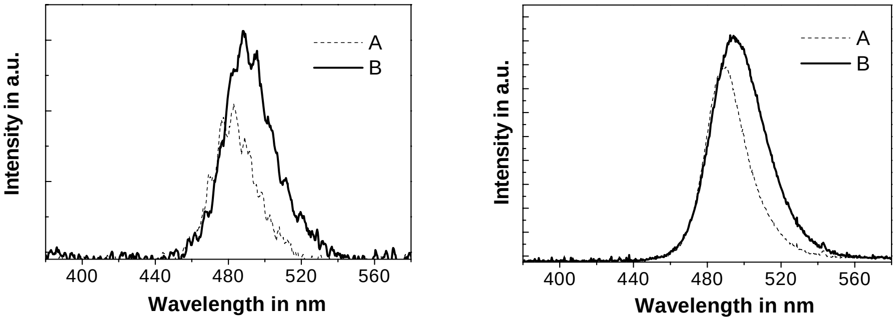
Environmentally friendly and low power consumption light sources have significant potential applications in traffic lights, full-colour displays, and solid-state lighting. An important factor that hinders the uptake of LEDs into the general lighting market is their price and there remains many aspects of fabrication that need to be explored and improved. Non-destructive characterisation of LED structures prior to the fabrication of LED-chips can play an important role in reducing the overall cost by limiting effort-intensive device processing to material of proven quality.

Photoluminescence (PL) is primarily used to assess the optical properties of the LED structures, but these measurements only provide a rough guide to how the active layer will perform optically when driven by current injection, as in a LED, and moreover do not account for the electrical properties of the whole structure. A more appropriate method to assess material intended for use in LEDs is to electrically inject electrons and holes into these structures and to compare the resulting electroluminescence (EL) spectra and I/V characteristics of the wafers under test.

This paper presents wafer scale optoelectronic data obtained using point-contact current injection and their comparison to the conventional measurements taken after the structures have been processed into devices. At similar current injection densities, the results in terms of relative light intensity, FWHM and emission wavelength are in good agreement (Figure 1). These results show that the wafer-level electroluminescence method is a fast and non-destructive tool to assess the quality of light emitting structures at low injection currents prior to their processing into devices.



a. Wafer-level electroluminescence spectra b. Chip-level electroluminescence spectra

Figure 1. Comparison of electroluminescence spectra measured at the wafer scale (a) and at the chip-level (b) showing good agreement between the two sets of results for two structures A and B having different QW-based active regions.

EPITAXIAL ORIENTATIONS OF GALLIUM NITRIDE GROWN ON NITRIDED R-PLANE SAPPHIRE BY MOLECULAR BEAM EPITAXY.

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Nitride-based devices are recently being grown along non-polar crystallographic orientations, such as $\{1\underline{1}00\}$ (m-plane) or $\{11\underline{2}0\}$ (a-plane), to eliminate the high interface charge densities and spatial separation of carrier wave functions in quantum well structures, which are effects of the built-in polarization along the [0001] direction of the wurtzite structure. One important foreign substrate for the growth of a-plane III-nitride layers is r-plane (i.e. $(1\underline{1}02)$) sapphire. Growth of a-plane GaN and AlN layers on r-plane sapphire, both by MOCVD and MBE, has already been reported. In the present, work the structural quality of the GaN epilayers grown on $(1\underline{1}02)$ sapphire by rf plasma-assisted MBE is investigated using transmission electron microscopy techniques. It is found that the substrate nitridation has a significant effect on the epitaxial orientation of the epilayer. In particular, in addition to the well-established $[0001]_{\text{III-N}}$ // $[\underline{1}101]_{\text{sapphire}}$ and $(11\underline{2}0)_{\text{III-N}}$ // $(1\underline{1}02)_{\text{sapphire}}$ epitaxial orientation (Fig. 1 a), a secondary epitaxial relationship (Fig. 2 a), promoted by specific interfacial structural features was also observed. This relationship is described as $<0\underline{1}10>_{\text{III-N}}$ // $[\underline{1}101]_{\text{sapphire}}$ (also visible in Fig. 1 a) and $\{0001\}_{\text{III-N}}$ // $\{11\underline{2}3\}_{\text{sapphire}}$, and is attributed to GaN nucleation on $\{11\underline{2}3\}$ facets of bunched steps on the r-plane sapphire surface, probably formed during sapphire nitridation. The geometric atomic configuration between the semipolar islands and the $(2\underline{11}3)$ step on the r-plane sapphire is proposed (Fig. 2 c). Although low misfit is ensured for both epitaxial relationships, the growth of the a-plane epilayer is locally destroyed by grains of the secondary orientation. Furthermore, pockets of sphalerite structure are promoted as a result of the superposition of intrinsic stacking faults along the [0001] growth direction of these grains (Fig. 2 a). In addition, crystallographically equivalent variants of the secondary orientation also lead to the introduction of twinning. The coexistence of different orientation grains with the principal GaN orientation creates grain boundaries inside the a-plane epilayer. However, these phenomena are confined relatively close to the epilayer/substrate interface since the dimensions of the misoriented GaN islands do not usually exceed a thickness of 10 nm and are quickly overgrown by the a-plane GaN layer. On the other hand, a succession of interfacial steps in vicinal substrates could promote the secondary orientation, as has been observed by other authors [1].

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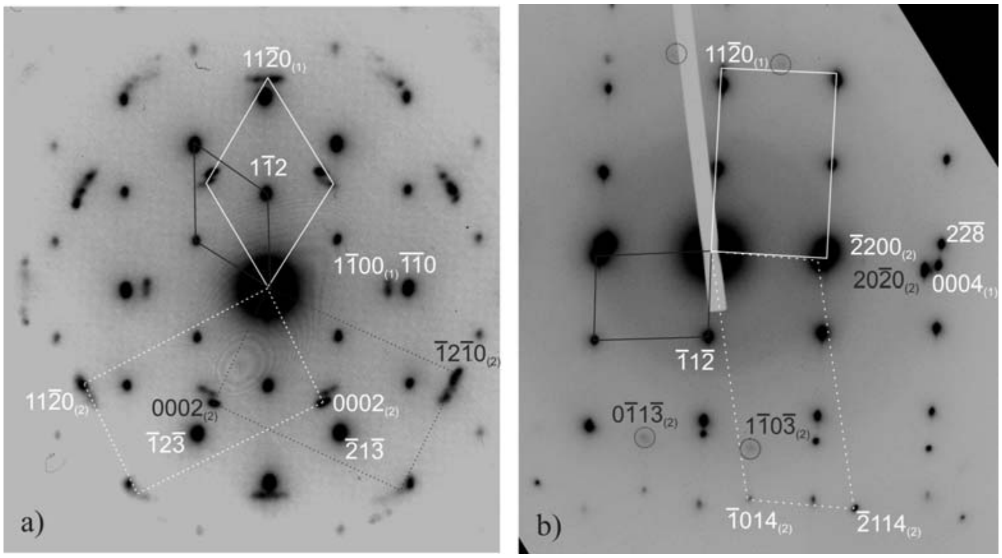

Figure 1 Selected-area diffraction patterns common to four crystal elements (indices of sapphire reflections are indicated in three-axis notation) a) taken along $[\underline{1}101]$ Al_2O_3 (dark solid line) // [0001] nonpolar GaN (1) (light solid line) zone axes and along $[1\underline{1}00]$ GaN (2) (light dashed line) and $[\underline{1}010]$ GaN (2) (dark dotted line) of semipolar islands, b) taken along $[\underline{11}20]$ Al_2O_3 (dark solid line) // $[1\underline{1}00]$ nonpolar GaN (1) (light solid line) zone axes and taken along $[\underline{44}8\underline{3}]$ GaN (2) (light dashed line) and $[1\underline{2}11]$ GaN (2) (reflection indicated with dark dotted circles) zone axes of semipolar islands.

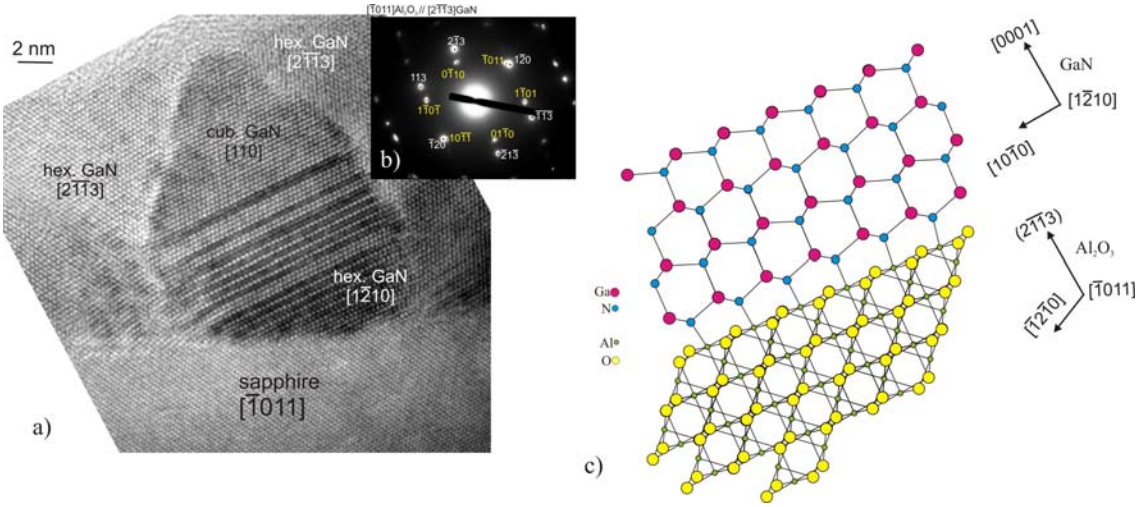

Figure 2 a) Cross-section HRTEM image of the interfacial area between GaN epilayer and sapphire substrate viewed along $[2\underline{11}3]$ wurtzite // $[1\underline{2}10]$ wurtzite // [110] sphalerite // $[\underline{1}011]$ sapphire zone axes; b) Diffraction pattern taken along $[2\underline{11}3]$ wurtzite and $[\underline{1}011]$ sapphire zone axes (indices of sapphire reflections are indicated in three-axis notation); c) Geometric atomic configuration between semipolar GaN island and $(2\underline{11}3)$ step on the r-plane sapphire.

STRUCTURAL CHARACTERISATION OF PAMBE-GROWN InAlN FILMS ON SAPPHIRE (0001) BY TRANSMISSION ELECTRON MICROSCOPY

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Nitride materials such as AlGaN are advantageous in the fabrication of high electron mobility transistors (HEMTs) due to the natural piezoelectric and spontaneous polarizations across the GaN/AlGaN/GaN heterostructures, which give high 2DEG densities at the heterointerfaces. Addition of high Al content AlGaN films in the barrier increases the carrier density due to the difference in band gap between GaN and AlGaN in the heterojunction, however increasing the Al content also increases the heterointerfacial lattice mismatch, causing high defect densities which have a deleterious effect on the carrier mobility. This problem can be addressed by the use of the ternary alloy InAlN, which may be grown with a chosen In content to provide almost lattice matching to GaN, whilst providing very high sheet carrier densities due to the high spontaneous polarization. However the growth of InAlN is problematic due to the very different relative growth temperatures of InN and AlN films, and the high bond strength of Al-N which causes In to desorb from the surface of the growing films. Studies of the microstructure and morphology of InAlN are therefore essential to optimise the crystal quality of heteroepitaxial films, in order to fabricate transistors with the greatest performance.

In this work, plasma-assisted MBE was used to grow a variety of InAlN films on AlN/sapphire (0001) and GaN/sapphire (0001) substrates with varying In content to allow near-lattice matching with underlying GaN or AlN templates. These heteroepitaxial systems were investigated by conventional and high resolution transmission electron microscopy. It was observed that in all cases the InAlN films were deposited as hexagonal columnar grains which appeared to have coalesced in the early stages of film growth whilst maintaining distinct grain boundaries, occasionally lined with threading dislocations. The misfit dislocation density in the films was low with very few threading dislocations observed, the vast majority of which were pre-existing edge-type dislocations which propagated from the substrate/template interface.

Plan view observations revealed that the hexagonal columns had predominantly {11-20} and {1-100}-type facets, and the crystal grain size was on average 20 nm in diameter. TEM mass contrast suggests that there is In depletion at the column grain centres and In accumulation at the edges of the columns. Such composition modulations in the InAlN layer may be attributed to the relative weak bond strength of In compared to Al, arising in a tendency for In to be incorporated at low N-coordination sites like edges, steps and facets. Also the intermediate growth temperature may encourage desorption of In from the growing crystal and may result in its apparent accumulation at grain boundaries and facets. The non-uniformity of th In distribution may also be driven by strain fields at morphological features such as column edges and growth steps. With In-rich edges of the columns, carriers in the film will be attracted to potential minima in between the columns, and not in the column centres, creating a 2DEG that is interrupted by grain boundaries and defects that may lie within them, reducing the carrier density in the heterojunction. These three mechanisms of In diffusion and their effect on the electric fields present in the different heterojunctions studied are discussed.

ANALYSIS OF TEM DIFFRACTION CONTRAST OF (In,Ga)N/GaN NANOSTRUCTURES

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Nanostructures of III-N semiconductors have a great commercial potential due to their optoelectronic properties. The structural and chemical characteristics of such structures determine the performance of the light-emitting devices. Transmission electron microscopy can be used to determine these characteristics at a nanometer scale. For determination of the chemical composition several analytical methods available in transmission electron microscopy (TEM) can be applied. Here we focus on the evaluation of the composition utilizing chemical sensitive TEM diffraction contrast imaging.

The applicability of the method was tested using (In,Ga)N/GaN nanostructures generated by a two-step growth procedure. First a GaN buffer layer was grown by metal organic chemical vapour deposition on sapphire (0001). In a second step 7 (In,Ga)N layers of a nominal In content of 27 at.% were grown by molecular beam epitaxy. The nominal thickness of the (In,Ga)N quantum wells (QWs) was 3 nm separated by a 7 nm thick GaN barrier layer. The growth temperature for the (In,Ga)N QWs and the GaN barriers was 600 °C. Finally the structure was capped by a 30 nm thick GaN layer.

The sample was prepared for TEM by mechanical preparation comprising face-to-face gluing, formatting, mechanical polishing, dimpling, and final ion milling. Structural analysis was performed on a TEM Hitachi H-8110 operating at 200 kV. The values of the intensity of the diffracted beams were simulated using the EMS-online software (Stadelmann) chosing as parameters the In concentration of the (In,Ga)N and the sample thickness.

Experimental TEM dark-field images alternatively using the 0002 (Fig. 1a) and 0001 (Fig. 1b) reflections show a striking different contrast behaviour for (In,Ga)N which has wurtzite structure. This behaviour is similar to that of sphalerite materials like (In,Ga)As where a chemically-sensitive 002 and a strain-sensitive 004 reflection exist. In order to understand the different contrast regimes in case of wurtzite materials, one has to calculate the intensity I_g of the different diffracted beams g by means of the kinematical theory which is analogous to the square of the structure factor [1]. I_{0002} being a function of the sum of the squares of the atomic scattering amplitudes of the group III and the group V element is found to be strain-sensitive. Inspecting the 0002 dark-field image (Fig.1a) it is obvious that the image intensity is dominated by the strain. The undulated strain contrast of the QWs hints to the formation of quantum dots (QDs).

Although the 0001 beam is forbidden according to the kinematical theory, it is dynamically excited. The dark-field image of Fig. 1b clearly shows the contrast behaviour of a chemical sensitive reflection. The QWs appear brighter, indicating an In enrichment compared to the GaN spacers. The inhomogeneities of the In distribution in the QWs are visible as well. The strain contrast is suppressed.

For explaining the contrast behaviour of the 0001 beam, its intensity in dependence on the In content was calculated for different sample thickness by the Howie-Whelan equation (Fig. 2a). It was found, that there is a strong dependency of the 0001 intensity of both composition and thickness. All of the curves shown in Fig. 2a exhibit an intensity maximum which is advantageous for quantitative composition analysis. For a clearer visualization, these findings were applied to a virtual (In,Ga)N layer containing 16 at.% of In embedded in GaN. Moreover, a Gaussian distribution of the In composition was taken into account. In Fig. 2b the 0001 intensity profiles across the layer are presented. The thickness ranges from 20 to 120 nm for the different curves. The profiles exhibit a transition from double maximum to single maximum shape and to double maximum again.

Conclusively, the In content of (In,Ga)N layers embedded in GaN can be determined from a series of 0001 dark-field images for different thickness.

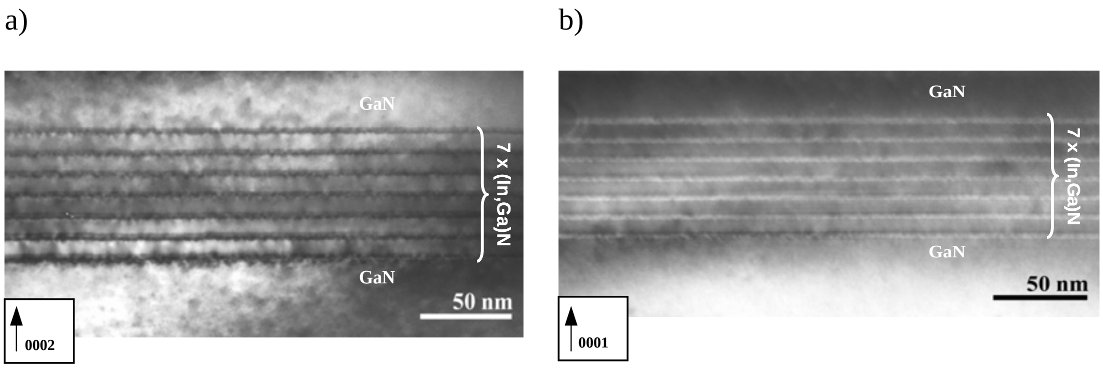

Fig. 1: Diffraction contrast imaging of multiple (In,Ga)N quantum wells:

a) strain-sensitive 0002 dark-field image, b) composition-sensitive 0001 dark-field image.

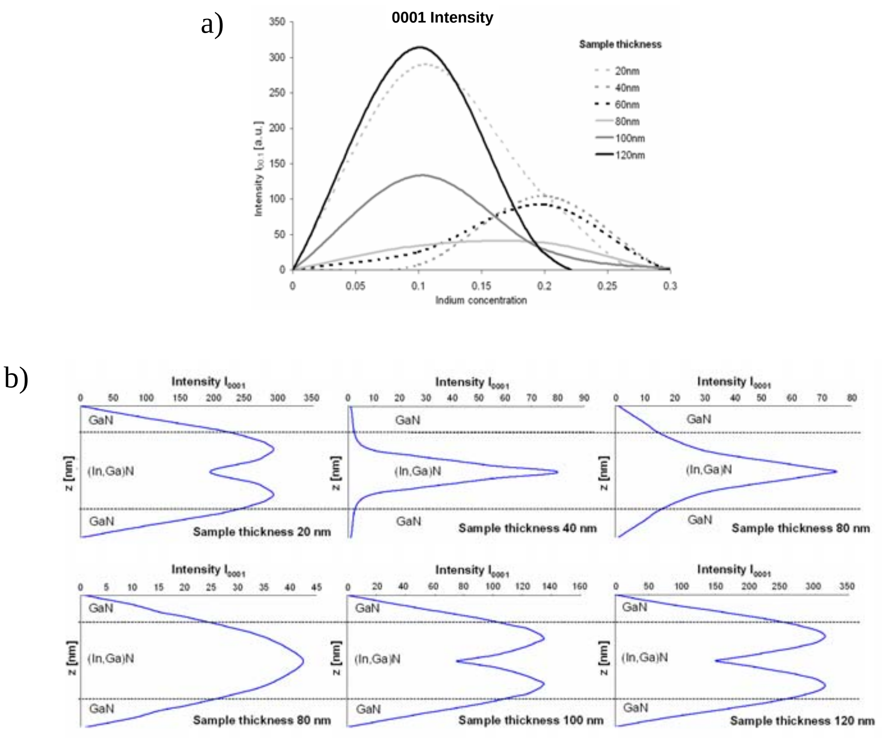

Fig. 2: Diagrams of the simulated intensities of the 0001 beam of (In,Ga)N:

a) 0001 intensity as a function of the In concentration for different sample thickness,
b) simulated thickness series of 0001 intensity profiles across the (In,Ga)N layer with a nominal In content of 16 at.%.

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STRUCTURE OF POLAR AND NON-POLAR GaN LAYERS GROWN ON $LiAlO_2$

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In the last years several research groups succeeded to grow epitaxial GaN layers on single crystalline (100)γ-$LiAlO_2$ substrates [1, 2]. The main advantage of (100)$LiAlO_2$ compared to the commonly used sapphire substrates is the possibility to grow GaN layers in both a non-polar [1-1.0] (so-called m-plane GaN) and the polar [00.1] (c-plane GaN) growth directions with a relatively small lattice mismatch. The m-plane oriented GaN layers show absence of internal polarisation fields along the growth direction which is advantageous for fabrication of optoelectronic devices with high performance [3]. On the other side, the growth of c-plane GaN is primarily attractive for fabrication of thick GaN wafers which can be used as substrates for subsequent GaN homoepitaxy [4]. For this purpose the use of $LiAlO_2$ might be advantageous over the other substrates because $LiAlO_2$ separates spontaneously from thick GaN films during post-growth cooling down. The self-separation of the substrate is caused by $LiAlO_2$ decomposition at elevated growth temperatures as well as a large difference in thermal expansion coefficients between $LiAlO_2$ and GaN [5].

The present study shows that despite a relatively small lattice mismatch between the (100)$LiAlO_2$ face and the (1-100)GaN as well as the (0001)GaN growth planes, the films of both orientations contain a large number of defects. Understanding the origin of the defect formation would allow the growers to tune the growth conditions in order to improve a layer quality and correspondingly a device performance.

The defect structure of the obtained layers was analysed by transmission electron microscopy. Freestanding thick c-plane oriented GaN layers show the presence of GaN regions, which appear brown in colour in the colourless GaN matrix and have a shape of inverse pyramids. These regions contain 12-sided v-pits. TEM inspection of GaN layers, which still adhere to the substrate, suggests that the v-pits are formed at the top of N-polar inversion domains, which appear in the Ga-polar matrix. It seems that the incorporation of impurities (presumably Li_2O as a product of the substrate decomposition) is enhanced in the N-polar GaN regions, which results in the brownish colour of GaN.

In contrast, no inversion domains have been observed in the m-plane oriented layers gown by metalorganic vapour phase epitaxy. However, m-plane GaN contains a complex net of prismatic grain boundaries and a large number of intrinsic basal plane stacking faults. Some of the stacking faults nucleate at the GaN/$LiAlO_2$ interface. Besides that, the grain boundaries enhance the fault formation acting as additional nucleation sites for the basal plane stacking faults.

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COMPOSITION ANALYSIS OF TERNARY SEMICONDUCTORS BY COMBINED APPLICATION OF CONVENTIONAL TEM AND HRTEM

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The tailoring of electronic and optical properties of nanostructured semiconductor materials for device applications requires the characterisation of the structure and the chemical composition.

In order to analyse the composition of ternary layers a new method was developed basing on transmission electron microscopy techniques (TEM). The method combines the analysis of chemically sensitive dark-field images (DF) with quantitative high-resolution TEM (HRTEM). For this characterisation the material system has to fulfil the following preconditions. First, the structure must show a chemically sensitive reflection. Second, the matrix material adjacent to the ternary layer has to contain only atomic species of the layer. This method will be demonstrated for the $GaAs_{1-x}Sb_x$/GaAs heterostructure system.

For this purpose Ga(As,Sb) were deposited on (001)-oriented GaAs substrate by means of metal-organic chemical vapour deposition (MOCVD). The pure material (GaAs, GaSb) as well as the alloyed ones ($GaAs_{1-x}Sb_x$) crystallize in the zincblende structure with a space group $F\bar{4}3m$. The misfit of about 8% between GaAs and GaSb leads to strained tetragonal Ga(As,Sb) unit cells with a space group $I\bar{4}m2$ and to a formation of 3-dimensional quantum dots (Stranski-Krastanov growth mode). Ga(As,Sb) has a chemical sensitive 002 reflection for both the unstrained and the tetragonal strained structure. This reflection was used for the compositional analysis. The 002 reflection intensities I^{002} were calculated depending on the Sb concentration x by the program jems [1].

For analysing 002 dark-field images the intensity curve must be normalized by a known concentration which is determined by quantitative HRTEM. For this purpose HRTEM images were digitally analysed using DALI (Digital Analysis of Lattice Images [2]) for visualising the strain distribution across the Ga(As,Sb) wetting layer. Using the displacement field $\vec{u}_z$ it was possible to measure the antimony concentration inside the wetting layer.

This method can be applied to analyse conventional DF-TEM images as an alternative way to the application of analytical TEM methods, particularly for the analysis of nanosized structures and radiation sensitive materials.

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SEMIPOLAR (Ga, In)N BLUE-GREEN LIGHT-EMITTING DIODES ON *M*-PLANE SAPPHIRE

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Nitride based light-emitting diodes (LEDs) are generally grown along the polar [0001] crystallographic direction (*c*-axis). As a consequence, the (Ga,In)N quantum wells (QWs) which are compressively strained on GaN, exhibit a strong piezoelectric field and a corresponding Quantum Confined Stark Effect (QCSE) which decreases the internal quantum efficiency of the LED. This effect can be partially or totally suppressed if the LED structure is grown along a semipolar or nonpolar direction, i.e, when the *c*-axis is tilted with respect to the growth direction. Although the performances of such devices are still strongly affected by the huge density of structural defects [1], semipolar (11-22) nitride LEDs on *m*-plane sapphire were recently achieved [2].

In this work, we present a comparative study of semipolar (11-22) (Ga,In)N/GaN LEDs and polar (0001) (Ga,In)N/GaN LEDs grown *silmutaneously* in the same run, by Metalorganic Vapor Phase Epitaxy (MOVPE). These structures were grown on half 2 inchs-GaN templates with 2 distinct (11-22) and (0001) orientations. Also the templates were grown formerly by MOVPE, from (10-10) *m*-plane and (0001) *c*-plane sapphire substrates, respectively.

The LED structures consist of a 1.5 µm-thick Si doped n-type GaN layer, five (Ga,In)N QWs with nominal thicknesses of 3 nm, separated by 12 nm-thick GaN barriers, followed by a 12 nm-thick Mg-doped $Al_{0.2}Ga_{0.8}N$ electron-blocking layer and finally a 0.2 µm-thick p-type GaN:Mg layer. Planar LEDs were processed by standard clean-room techniques i.e. UV-lithography and reactive ion etching.

Two pairs of semipolar / polar LEDs were grown, using two different QW growth temperatures. For each pair, electroluminescence (EL) evidenced a systematic red-shifted emission wavelength for the semipolar LEDs, suggesting a higher indium content in the semipolar QWs. Complementary measurements of X-ray diffraction (HRXRD) and Energy dispersive X-ray spectroscopy (EDS) on thick (~60 nm) (Ga,In)N layers grown on (11-22) and (0001) GaN templates confirmed this hypothesis. Surprisingly, the semipolar LEDs showed a strong blueshift under increasing forward DC injection. In the case of polar LED structures, this blueshift is traditionally associated with the screening of the piezoelectric field by carriers in the QWs, and with the filling of localised states formed by indium composition fluctuations in the QWs. Since our semipolar LEDs exhibit a reduced piezoelectric field, the observed blueshift is mainly due to the localised states filling by carriers. This latter result stresses the importance of In composition fluctuations in (Ga,In)N QWs on both polar and semipolar orientations.

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Effect of growth conditions on the morphology and optical properties of GaN nanowires spontaneously grown on (111) Si by molecular beam epitaxy

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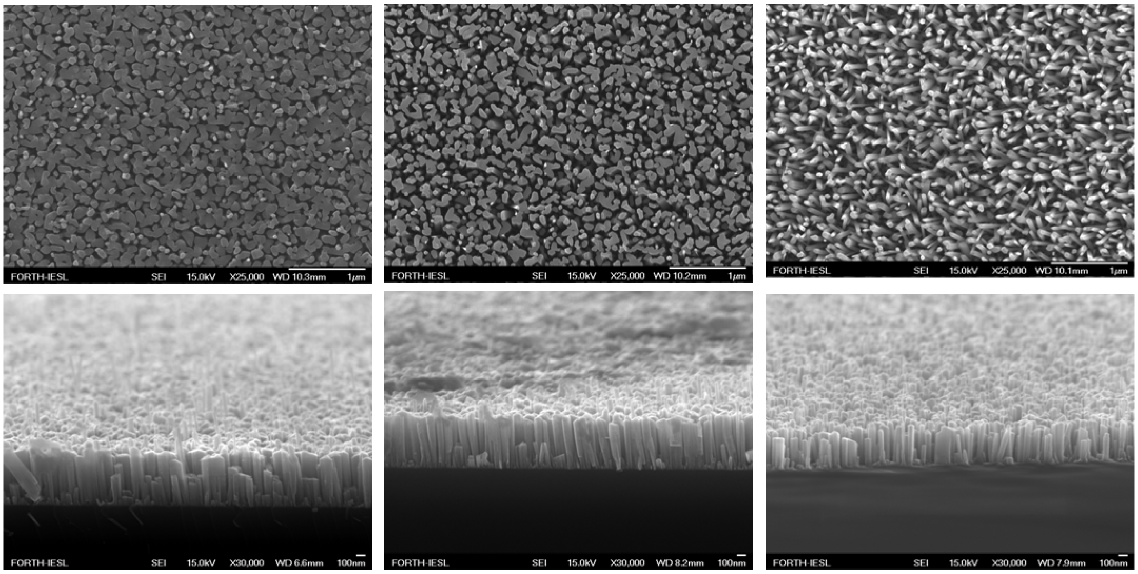
III-nitrides are promising semiconductor materials because of their application in optoelectronics and high power electronic devices. One of the major problems of III-nitride materials hetroepitaxial growth is a high density of threading dislocations, of the order of 10^8–10^{10} cm^{-2}, which adversely affect the device performance. Nanodimensional nitrides such as nanowires (NWs) / nanopillars are attractive materials for the reduction of the dislocation density. In addition to the reduction of threading dislocations, the NW geometry also allows the device dimensions to be scaled down. Different techniques such as metal-organic chemical vapor phase epitaxy, molecular beam epitaxy (MBE), chemical beam epitaxy, and laser ablation have been used to grow a variety of semiconductor NWs with high crystalline quality. It has also been reported that the GaN NW morphology is affected by the N/Ga flux ratio and the substrate temperature. However, it is desirable to independently control the rod-like morphology of NWs in order to optimize their crystalline quality. The catalyst-free growth and the optoelectronic properties of GaN NWs grown on (111) Si substrates by plasma-assisted molecular beam epitaxy have been investigated. The GaN NWs grown on Si generate from the lattice mismatch strain on Si and the high surface energy of the nitrogen stabilized (0001) GaN surface. At constant N/Ga flux ratio, the NW morphology, density and growth rate are controlled by the substrate temperature, which affects the gallium adatom diffusion length before desorption. A change in substrate temperature from 700^{o}C to 800^{o}C resulted in reduction of the average diameter, density and growth rate of NWs from 90nm to 70nm, 9.0x10^{9}cm^{-2} to 2.6x10^{9}cm^{-2}, and 210nm/h to 144nm/hr, respectively. The reduction of the GaN NW growth rate at 800^{o}C is attributed to a reduced residence time (τ) of Ga adatoms on the substrate surface. When growth temperature is increased, diffusion coefficient increases but residence time is decreased and the overall effect is a reduction in the Ga adatom diffusion length before desorption, hence less Ga is transferred from the uncovered substrate area to the NWs. Furthermore, it was found that the nucleation density can be changed by changing the Ga flux for a constant nitrogen flux. A four times reduction of the Ga flux resulted in a reduction of nucleation density from 9x10^{9}cm^{-2} to 1x10^{9}cm^{-2}. Low temperature photoluminescence spectra at 20 K revealed that PL intensity ratio of donor-bound exciton peak (D^oX at 3.470eV) with defect related peak (Y_2 at 3.445eV) increased in the smaller diameter NWs and a free excitonic peak at 3.472eV was observed at the shoulder of the spectra. PL and Raman spectra showed that the GaN NWs are completely stress-free irrespective of the growth conditions.



700°C 750°C 800°C

Figure 3: SEM images of surface and cross-sectional view of GaN NWs grown on (111) Si with V/III ratio of 5 at different temperature 700°C, 750°C, and 800°C.

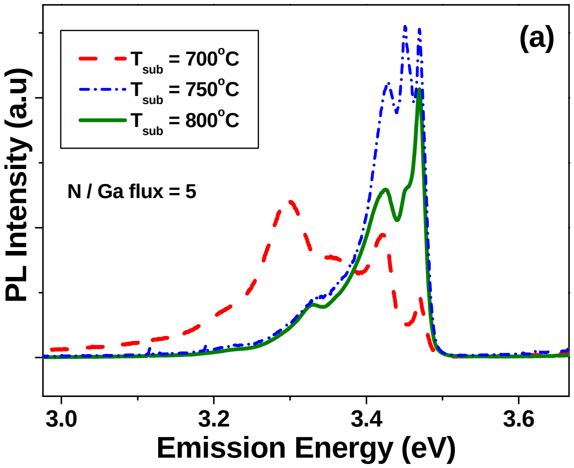


Figure 2: LT-PL spectra at 20K of the GaN NWs on (111) Si grown (a) At different substrate temperature keeping the N/Ga flux ratio of 5.

FORMATION OF A PERIODIC ARRAY OF STEPS ON THE r-PLANE SAPPHIRE SURFACE AND ITS INFLUENCE ON a-PLANE GaN NUCLEATION

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Non-polar heterostructures are very promising because of the lack of the quantum confined Stark effect caused by polarization-induced built-in electric fields. Today the growth of a-plane GaN on r-plane sapphire is still challenging and many issues have to be addressed in order to achieve a good structural quality. Two important steps of the growth are the nitridation of the r-plane sapphire and the nucleation of a-plane GaN. The nitridation procedure is expected to modify the surface of Al_2O_3 by O to N anion exchange, converting a substrate surface layer from Al_2O_3 to AlN. The nucleation procedure should optimize the morphology and structure of an initial GaN layer on sapphire, allowing the subsequent growth of a compact and smooth epilayer with low defect density. In this work, the r-plane sapphire nitridation and a-plane GaN nucleation by nitrogen rf plasma source MBE (RFMBE) have been investigated.

Nominally on-axis (1-102) r-plane sapphire substrates were used. Sapphire nitridation experiments were carried out in a wide range of experimental parameters, such as substrate temperature, nitridation time and active nitrogen flux. Initial sapphire nitridation experiments were monitored by in-situ RHEED observations, whilst AFM was used to observe the morphology of the nitrided sapphire surface. A transition of the RHEED pattern from a streaky to a spotty one indicated the roughening of the nitrided surface. The time needed for the surface roughening transition increased monotonically with the substrate temperature in the range of 200-800°C. Subsequent nitridation experiments were limited in time duration preserving the smoothness of the nitrided sapphire surface. In this case, AFM revealed that a periodic array of steps is formed on the r-plane sapphire surface, along the projection of the sapphire [0001] direction on the substrate surface plane (Fig. 1a). The periodic arrays of steps are related to small unintentional miscut angles of the r-plane sapphire substrates in the range of 0.01-0.2 degrees. A comparative study revealed that the step height reduces and the terrace width increases with the increase of nitridation temperature from 200°C to 600°C (Fig. 1b).

The nucleation of GaN on nitrided surfaces with periodic arrays of steps was studied for substrate temperatures from 350°C to 800°C. In all cases, GaN growth followed a 3D growth mode and r-plane GaN islands were formed on the sapphire surface. The periodic array of steps on the substrate surface (Fig 2a) became even more evident with GaN nucleation at temperatures higher than approximately 500°C (Fig 2b-d). AFM revealed that the distance of steps remained constant and the increased contrast was due to nucleation of 3D GaN islands at the sapphire steps (Fig. 2c). The preferential nucleation at the step edges on wide terraces could be used for the spontaneous formation of one-dimensional GaN structures along the <1-100> GaN direction (Fig. 2b-d).

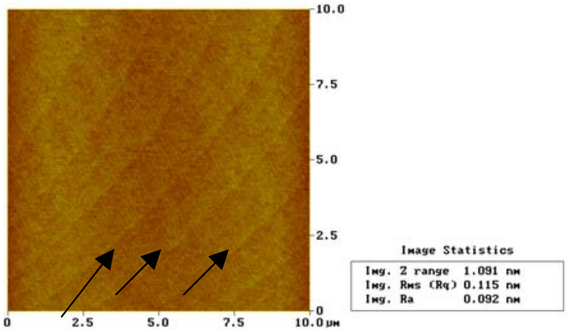

Figure 1a: AFM image for nitrided sapphire surface exhibiting an array of periodic steps (see arrows)

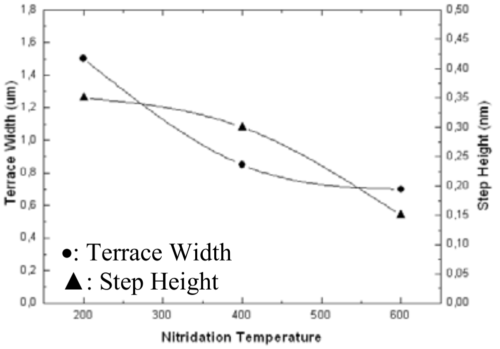

Figure 1b: Dependence of terrace width and step height on nitridation temperature

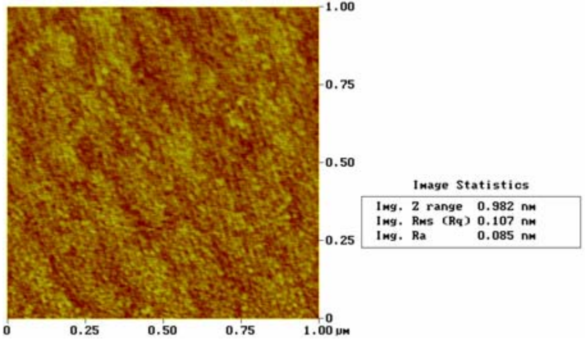

Figure 2a: Periodic array of steps on the nitrided substrate surface

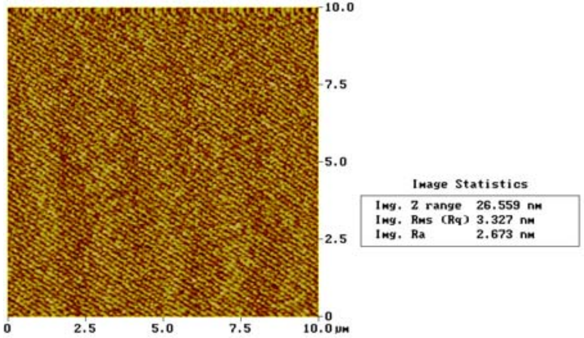

Figure 2b: Periodic array of steps on GaN nucleation layer grown at temperature higher than 500°C

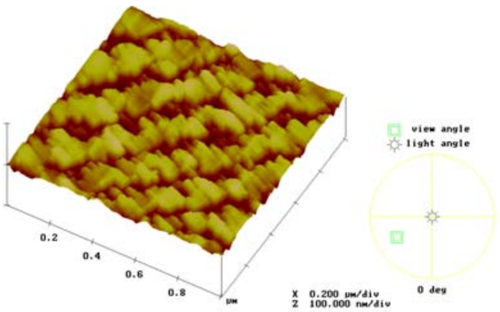

Figure 2c: 3D AFM image showing the periodic array of steps on GaN nucleation layer grown at temperature higher than 500°C

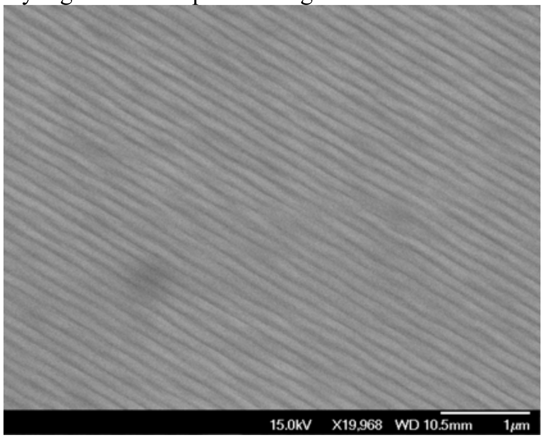

Figure 2d: SEM image of the periodic steps on GaN nucleation layer grown at temperature higher than 500°C

The Department of Materials Science & Metallurgy

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We hope you have enjoyed your stay and wish you a safe trip back home.