

CONF-980713--

To be presented at Microscopy & Microanalysis '98  
 Atlanta, Georgia, July 12-16, 1998 and  
 published in *Proceedings*

## Direct Observation of Threading Dislocations in GaN by High-Resolution Z-Contrast Imaging

Y. Xin,<sup>1,2</sup> N. D. Browning,<sup>2</sup> S. J. Pennycook,<sup>1</sup> P. D. Nellist<sup>3</sup>  
 S. Sivananthan,<sup>2</sup> J.-P. Faurie,<sup>2,4</sup> and P. Gibart<sup>4</sup>

<sup>1</sup>Solid State Division, Oak Ridge National Laboratory  
 P.O. Box 2008, Oak Ridge, Tennessee 37831-6030

<sup>2</sup>Department of Physics, University of Illinois at Chicago  
 Chicago, IL 60607-7059

<sup>3</sup>Cavendish Laboratory, Cambridge University  
 Madingley Road, Cambridge CB3 0HE, UK

<sup>4</sup>CRHEA-CNRS, rue Bernard Gregory  
 06560 Valbonne, France

RECEIVED  
 MAR 30 1998  
 OSTI

"The submitted manuscript has been authored  
 by a contractor of the U.S. Government under  
 contract No. DE-AC05-96OR22464.  
 Accordingly, the U.S. Government retains a  
 nonexclusive, royalty-free license to publish or  
 reproduce the published form of this  
 contribution, or allow others to do so, for U.S.  
 Government purposes."

DISTRIBUTION OF THIS DOCUMENT IS UNLIMITED

MASTER

prepared by  
 SOLID STATE DIVISION  
 OAK RIDGE NATIONAL LABORATORY  
 Managed by  
 LOCKHEED MARTIN ENERGY RESEARCH CORP.  
 under  
 Contract No. DE-AC05-96OR22464  
 with the  
 U.S. DEPARTMENT OF ENERGY  
 Oak Ridge, Tennessee

19980529 035

DTIC QUALITY INSPECTED 1

February 1998

## **DISCLAIMER**

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

# DIRECT OBSERVATION OF THREADING DISLOCATIONS IN GaN BY HIGH RESOLUTION Z-CONTRAST IMAGING

Y. Xin<sup>1,2</sup>, N.D. Browning<sup>1</sup>, S.J. Pennycook<sup>2</sup>, P.D. Nellist<sup>3</sup>, S. Sivananthan<sup>1</sup>, J-P Faurie<sup>1,4</sup> and P. Gibart<sup>4</sup>

<sup>1</sup>Department of Physics, University of Illinois at Chicago, Chicago, IL 60607-7059, USA.

<sup>2</sup>Solid State Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831-6031, USA

<sup>3</sup>Cavendish Laboratory, Cambridge University, Madingley Road, Cambridge CB3 0HE, UK

<sup>4</sup>CRHEA-CNRS, rue Bernard Gregory, 06560 Valbonne, France.

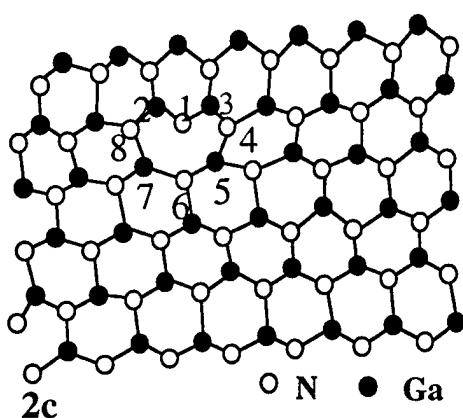
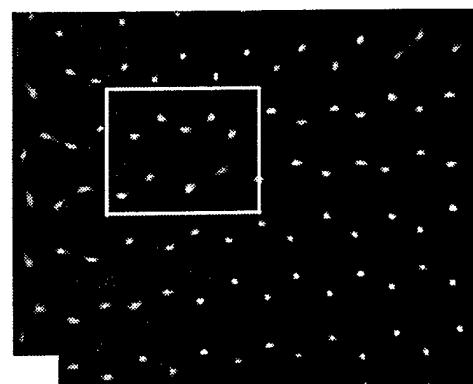
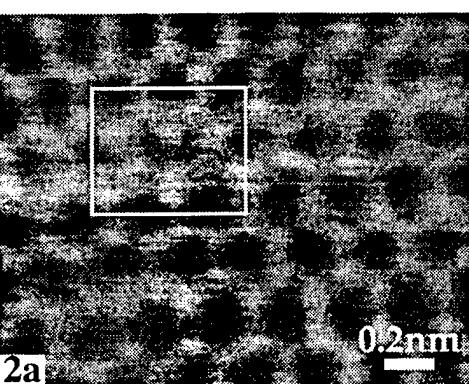
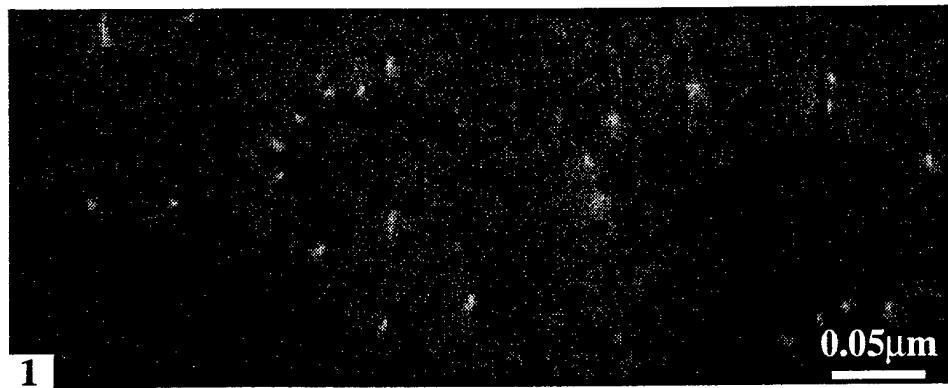
Wide gap nitride semiconductors have attracted significant attention recently due to their promising performance as short-wavelength light emitting diodes (LEDs) and blue lasers<sup>1</sup>. One interesting issue concerning GaN is that the material is relatively insensitive to the presence of a density of dislocations which is six orders of magnitude higher than that for III-V arsenide and phosphide based LEDs. Although it is well known that these dislocations originate at the film-substrate interface during film growth, thread through the whole epilayer with line direction along  $<0001>$  and are perfect dislocations with Burgers vectors of  $\mathbf{a}$ ,  $\mathbf{c}$ , or  $\mathbf{c+a}$ , the reason why they have such a small effect on the properties of GaN is unclear.

To develop a fundamental understanding of the properties of these dislocations, the core structures are studied here by high resolution Z-contrast imaging in a 300kV VG HB603 scanning transmission electron microscope (STEM) with a resolution of 0.13nm. Figure 1 shows a low magnification Z-contrast image of a plan view sample looking down  $<0001>$ , in which dislocations are seen as bright dots (the brightness is a result of diffraction contrast from their strain fields). At higher magnification, the majority of dislocations are seen to be of edge character and have a core structure like the one shown in Figure 2a. As the Z-contrast image is a convolution between the probe intensity profile and the specimen object function, it is possible to obtain more detailed information on the specimen object function, i.e. the structure, through maximum entropy analysis (The maximum entropy technique produces the 'most likely' object function which is consistent with the image). As can be clearly seen in the maximum entropy image (figure 2b), the core structure is just an 8-fold ring, indicated by the numbers 1 to 8 in figure 2c. Comparing with the structure of the  $\{10\cdot10\}$  surface, the central column of the core is similar to a single row of dimers on the surface, as shown in Figure 2d. Such a structure is not expected to have deep levels in the band gap and therefore should be electrically inactive<sup>2</sup>.

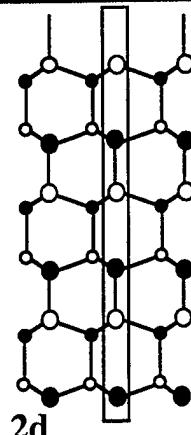
Although the majority of dislocations had the above structure, some dislocations showed no disturbance to the lattice periodicity, as shown in figure 3. These dislocations have no edge component to their Burgers vector, and must therefore be pure screw dislocations with  $\mathbf{b} = \pm\mathbf{c}$ . It is obvious from the image that this screw dislocation has a full core rather than an empty one. In this case, it seems likely that the larger bond distortions at these full core screw dislocations may lead to deep defect states in the band-gap. These observations provide the first direct experimental evidence of the atomic core structures of dislocations in GaN<sup>3</sup>.

## References:

1. S. Nakamura, M. Senoh, S. Nagahama, N. Iwasa, T. Yamada, T. Matsushita, H. Kiyohu, and Y. Sguimoto, Jpn. J. Appl. Phys., **35**, L74 (1996).
2. J. Elsner, R. Jones, P.K. Sitch, V.D. Porezag, M. Elstner, Th. Frauenheim, M.I. Heggie, S. Oberg and P.R. Briddon, Phys. Rev. Lett., **79**, p. 3672 (1997).
3. Research sponsored by DOE under grant number DOE DE-GF02-96ER45610 and contract DE-AC05-96OR22464 with Lockheed Martin Energy Research Corporation, and by an appointment to the ORNL Postdoctoral Research Program administered jointly by ORNL and ORISE.



2b



2d

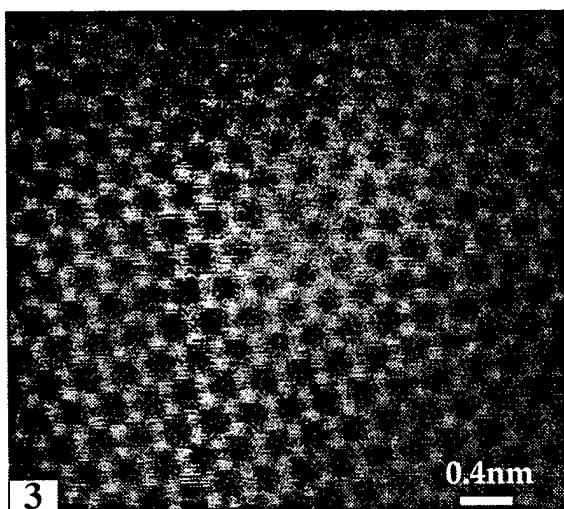


Fig.1 Low magnification angular dark field image along  $<0001>$ . Threading dislocations show as bright dots due to their strain field.

Fig.2(a) High-resolution Z-contrast image of a threading edge dislocation looking down  $<0001>$ .  
 (b) Maximum entropy image of Fig.1(a) showing most probable column positions.  
 (c) Sketch of the core structure determined from the experimental data. (d) dislocation core showing similarity to one dimer row in the  $\{10-10\}$  surface. Smaller symbols denoting the atoms below the surface

Fig.3 High resolution Z-contrast image of an end-on pure screw dislocation showing a full core.

M98004962



Report Number (14) ORNL/CP-97022  
CONF-980713--

Publ. Date (11)

199802

Sponsor Code (18)

DOE/ER, XF

UC Category (19)

UC-400, DOE/ER

DOE