Atomic resolution microscopy of semiconductor defects and interfaces

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ABSTRACT: The optical arrangement of the scanning transmission electron microscope (STEM) allows formation of incoherent images by use of a large annular detector. Here we show this capability in the imaging of defects in GaN and the interfacial region of an Au/GaAs ohmic contact. A resolution of around 0.15 nm is attained. Such "Z-contrast" images show strong atomic number contrast and allow the probe to be positioned accurately at the defect or interface for the purpose of performing high spatial resolution electron energy-loss spectroscopy (EELS).

1. INTRODUCTION

The ability to routinely determine atomistic and electronic structures of defects and interfaces is one of the goals of contemporary electron microscopy. In semiconductor devices the overall performance is often strongly affected by these regions of the specimen. For instance, the propensity for undesirable electron hole recombination at defects, and the height of Schottky barriers at interfaces are correlated to their electronic structures. As a first step towards understanding these effects at the atomic level, it is desirable to be able to form images of the relevant structure. One method to obtain such atomic resolution images is Z-contrast, high-angle annular dark field (HAADF) imaging (Pennycook *et al* 1997). This requires the microscope to operate in small probe-forming mode: resolution is given by the probe size. For crystalline materials oriented close to a zone axis, the images are generally easy to interpret qualitatively (intensity peaks corresponding to the atomic column locations): strong atomic number (Z) contrast is also shown. The limited information on chemical composition obtained from the image can be greatly augmented by then performing electron energy-loss spectroscopy (EELS). At high spatial resolutions, the optimal probe-forming microscope settings for EELS are identical to those for Z-contrast imaging. Switching between imaging and spectroscopy is therefore easy.

In the case of most semiconductor defects and interfaces, a resolution of between 0.1 nm and 0.2 nm is desirable for clear imaging of the structure. To be able to generate enough current in such a small probe, a high brightness, field emission source is used. Here we demonstrate the formation of Z-contrast images at around 0.14 nm resolution on the 200 kV JEOL JEM-2010F: a widely available instrument with a Schottky field emission source. As illustration, an image of the $\{11\bar{2}0\}$ prismatic stacking fault in GaN is presented. Also, shown are atomic resolution images from an ohmic contact between Au and GaAs showing faceting of the interface on the atomic scale.

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2. SMALL PROBE FORMATION

Figure 1 shows the experimental arrangement for HAADF imaging. A small probe is incident on the specimen and the high angle scattering is collected by a large annular detector. The image is formed serially by displaying collected intensity for each position of the probe as it is scanned in a raster over the specimen. The smallest probe size is determined by four factors: spherical aberration of the probe-forming optics; probe convergence angle; incoherent broadening due to finite brightness of the electron source; and incoherent broadening due to electrical and mechanical instabilities. The microscope we used has a spherical aberration coefficient (when the lenses are set to form a probe) experimentally determined to be 0.57 mm (James *et al* 1998). From wave optical calculations, the optimum aperture size at 200 kV is then 12 mrad and a probe size at Scherzer focus of around 0.13 nm is expected. In general though, it is the incoherent probe broadening effects that dominate the final probe size. However, if a large demagnification of the electron source is set, using the condenser lenses and electrostatic gun lens, we find it is possible to largely avoid this limitation on an unmodified JEM 2010F and approach the Scherzer limit of 0.13 nm, still with enough probe current for imaging (James and Browning 1999).
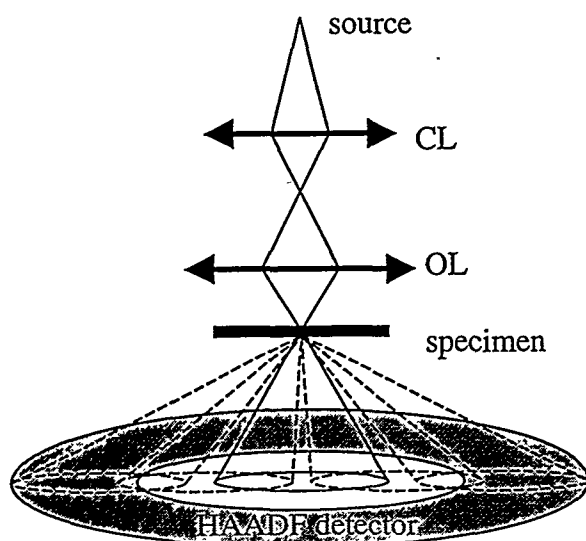

Fig. 1: Schematic illustration of the optical arrangement for HAADF imaging. CL=condenser lens system OL=objective lens pre-field ·
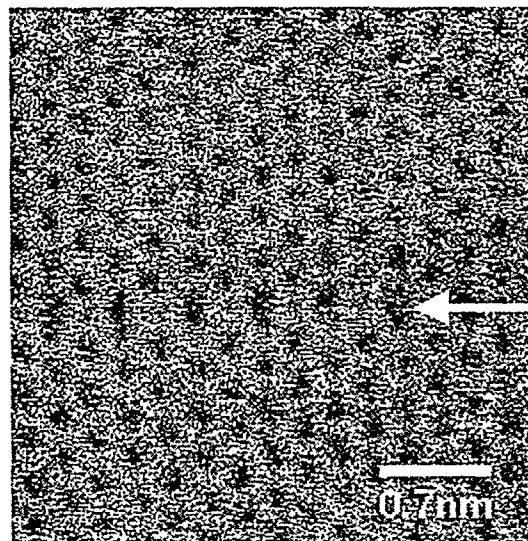

Fig. 2: Prismatic stacking fault in GaN viewed down <0001>

3. IMAGES OF SEMICONDUCTOR DEFECTS AND INTERFACES

Figure 2 shows the image of a prismatic stacking fault in GaN, with the beam oriented parallel to the <0001> zone axis. The specimen was grown by MBE on a GaP (111) substrate. The electronic structures of these faults, which lie on $\{1\bar{1}20\}$ planes, and also of threading dislocations, which are present with a high density, are currently under investigation since it is desirable to know if they act as electron hole recombination sites and impede the light emitting efficiency of GaN devices (Natusch *et al* 1998). Figure 2 is a raw image with a 4.3 s acquisition time and shows the structure as previously directly observed in the 300 kV STEM (Nellist *et al* 1997) and as predicted by the analysis of Cherns *et al* (1998).

The second structure imaged was the interface in a sample of Au grown on n-type GaAs (001) by MBE. This ohmic contact was alloyed at 420°C for 15 seconds after growth. The interface region exhibits spiking with Au protruding approximately 50 nm into the GaAs. The Au grains are aligned with the $(1\bar{1}0)$ plane approximately parallel to the interface. Figure 3a shows a Z-contrast image at relatively low magnification showing one of the Au spikes, and the atomic resolution structure of the interface 50 nm away from the spike is shown in Fig. 3b. The 256×256 image was acquired in 4.3 s. The image shows Au terminating on the $(1\bar{1}0)$ plane which results in a lattice mismatch of 2.5% with respect to the (001) terminated GaAs. An atomic step in the interface is present near the image center and the resolution here is approximately 0.15 nm. In Fig. 3c an enlarged section of one of the protruding spikes is shown. The Au forms a (111) tilt boundary with GaAs (the angle is
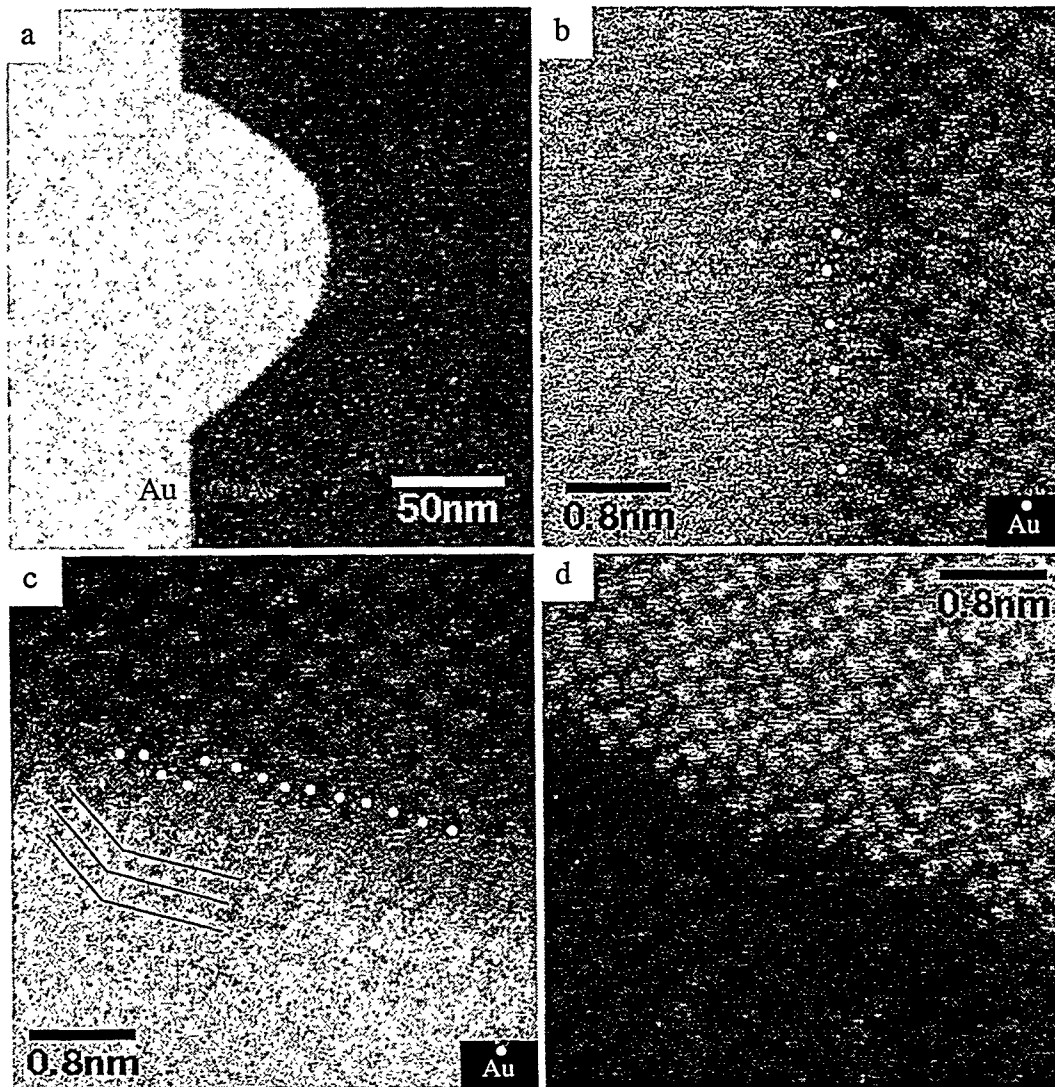

Fig. 3: (a) Raw Z-contrast image at low magnification showing Au metal deposited on the GaAs substrate and the occurrence of spiking. (b) Raw Z-contrast image of the Au/GaAs interface at approx. 0.15 nm resolution (c) Raw atomic resolution Z-contrast image from the Au spike upper region. A (111) tilt boundary is formed with the GaAs with regularly spaced dislocation cores along the interface. (d) Raw Z-contrast image of the lower spike region. Here the Au interface is faceted along the close packed {111} planes.

approximately 18°) and a twin boundary is seen in the bulk Au where the angle of the interface changes. Dislocation cores are visible in the raw image, lying at the interface approximately every 0.5 nm along the interface. Finally, Fig. 3d shows a third example of the interface structure along one side of a spike. Au is faceted along the close packed {111} plane with steps every one to two atomic columns.

4. DISCUSSION AND CONCLUSIONS

Atomic resolution HAADF imaging is possible on a 200 kV transmission electron microscope fitted with a standard Schottky field emission gun and an annular dark field detector. Defect structures in GaN and the atomistic nature of an Au contact to GaAs, in the vicinity of an Au spike, have been imaged at a resolution of around 0.15 nm.

The inelastic scattering signal sampled by EELS is mainly confined to low angles: therefore, it can be collected simultaneously with or immediately following Z-contrast image acquisition. Using the image as a map, the probe can then be stopped at a particular position (such as at a dislocation core or site at an interface) and a spectrum acquired with the same microscope settings. Typically, most of the scattering not collected by the dark field detector is used, in order to approach incoherent EELS conditions.

Our JEM-2010F instrument is equipped with a Gatan imaging filter. In a 0.2 nm probe we observe a current of approximately 15 pA: an energy resolution of around 1 eV is obtainable (a measurement of the full-width-half-maximum of the zero-loss peak). This performance is sufficient to begin examining fine structure details for a number of core-loss edges at atomic spatial resolution. Work is under way to investigate the electronic structure of GaN threading dislocations and the role of Ni in Ni/Au/Ge contacts to GaAs.

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