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Atomic Resolution Imaging of Dislocations in AlGaN and the Efficiency of UV LEDs

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Hatsujiro Hashimoto pioneered the imaging of single atoms in an electron microscope [1], developed an aberration-free electron microscopy technique [2], and was one of the first to image dislocations in an electron microscope [3]. This paper builds upon his brilliant achievements and reports the use of atom-resolving aberration-corrected electron microscopy to study the dislocation structure of AlGaN, a key material for UV LEDs and lasers.

A puzzling problem with III-nitride LEDs is why an external quantum efficiency of InGaN-based blue LEDs of over 80% can be achieved [4], whereas that of AlGaN-based deep UV LEDs is less than 10% [5]. A related puzzle is why the efficiency of InGaN-based blue LEDs is remarkably insensitive to a high density of dislocations [6] whereas the dislocation density appears to be an important factor limiting the efficiency of AlGaN-based LEDs [7]. The atomic structure of the dislocation core in GaN and InGaN has been widely studied [for example, refs 8, 9] because of the potential formation of states in the band-gap, which can act as non-radiative recombination centres. However, very little is known about the core structure of dislocations in AlGaN.

AlGaN and InGaN epilayers were grown by metal-organic vapour phase epitaxy (MOVPE) in a Thomas Swan 6x2 inch close-coupled showerhead reactor. The epilayers were grown on a c-plane sapphire substrate. Further details are given in ref 10. Dislocations in the AlGaN epilayer were imaged using aberration-corrected high-angle dark field scanning transmission electron microscopy (HAADF-STEM) using FEI Titan G2 Chemi STEM and FEI Titan G3 PICO microscopes operating at 300kV and a detector semi-angle of 69 mrad. The sample was prepared using mechanical polishing and Ar^+ ion milling. The dislocations were viewed end-on, along the [0001] zone axis. Eshelby twist was observed for all dislocations with a screw component. The composition around the dislocations was studied using energy dispersive X-ray spectroscopy (EDX). For further details see ref 11. 100% of the edge dislocations have 5/7 atom ring cores. Some mixed dislocations were undissociated and some dissociated. The core structures in AlGaN are similar to those in InGaN.

EDX mapping of the dislocations was performed inside the TEM, and geometric phase analysis of the HAADF-STEM images was performed for edge and mixed dislocations in both AlGaN and InGaN. This shows that the dislocation core is bounded on either side by a region of compressive strain and a region of tensile strain. EDX shows that there are compositional fluctuations around the dislocation, for AlGaN there is higher Ga content on the side of the dislocation under tensile strain, and higher Al content on the side under compressive strain. This is consistent with the Al-N bond being shorter than the Ga-N bond (valence force field simulations predict being 2% shorter), which leads to a reduction of the elastic strain around the dislocations.

A key question is whether the segregation of Al and Ga around the dislocations in AlGaN affects the optical properties of the dislocations. We have therefore studied the same region of an AlGaN sample using AFM and CL [11] and compared the results with InGaN. Figures 1(a) and 2(a) show the dislocations at the surface of an AlGaN and InGaN sample respectively. There is a one-to-one correspondence between the dislocations imaged by AFM and the dark spots on the CL intensity maps from AlGaN (figure 1b), consistent with the dislocations being non-radiative recombination centres. However, for InGaN the dislocations in the CL intensity image appear as bright spots surrounded by a dark ring (figure 2b). This bright spot has previously been linked to carrier localisation due to the segregation of In atoms at the dislocations [12]. This is consistent with carrier localization induced by In atoms to be much stronger than carrier localization by Al or Ga atoms. This may provide an explanation for the relative insensitivity of InGaN-based visible LEDs to dislocations compared with AlGaN-based UV LEDs. It also suggests that adding some In to AlGaN-based LEDs may be advantageous and decrease the sensitivity of such UV-LEDs to dislocations [13].

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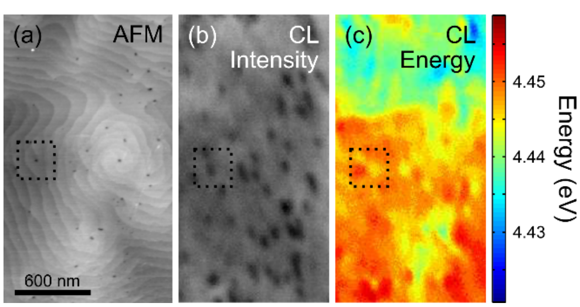

Figure 1. (a) AFM, (b) CL integrated intensity, and (c) CL peak emission energy of the same region in AlGaN sample.

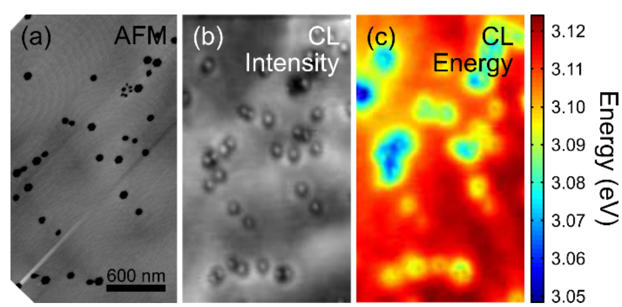

Figure 2. (a) AFM, (b) CL integrated intensity, and (c) CL peak emission energy of the the same region in the InGaN sample.