DISLOCATION CORE IN GaN

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Light emitting diodes and blue laser diodes[1] grown on GaN have been demonstrated despite six orders of magnitude higher dislocation density than that for III-V arsenide and phosphide diodes. Understanding and determination of dislocation cores in GaN is crucial since both theoretical[2,3] and experimental work[4-5] are somewhat contradictory. Earlier work suggested that dislocations are not radiative recombination centers.[2,4] However, recent work has shown that screw dislocations can be electrically active[6] and suggested that the core structure of screw dislocations can be influenced by growth conditions.

Transmission Electron Microscopy (TEM) has been applied to study the layers grown by hydride vapor-phase epitaxy (HVPE) and molecular beam epitaxy (MBE) (under Ga rich conditions) in plan-view and cross-section samples. Only plan-view samples were used for the structure determination of dislocation cores. In cross-section samples grown by HVPE under **g.b**=0 diffraction conditions, for which screw dislocations are out of contrast, small voids along dislocation line were observed (Fig. 1a,b). These voids were not observed for edge dislocations in the same material and not at all in the MBE grown samples (Figs. 1c,d). In plan-view configuration the voids had a hexagonal shape (Fig. 1e). No displacement vector can be observed around screw dislocations in plan-view configuration (Fig.1e,f).

In order to obtain information about dislocation core structures, high-resolution focal series (20 images) were taken using the NCEM OÅM (a modified 300keV field emission Phillips electron microscope). A numerical reconstruction procedure[7,8] was used to reconstitute the electron wave at the specimen exit surface by using 20 images obtained with constant focus step. Earlier studies showed that application of this procedure leads to experimental reconstruction of the phase of the electron exit wave (and the crystal structure information it carries) to sub-Ångstrom resolution. The OÅM is capable of resolving the dumbbell structure of carbon columns separated by 0.89Å in diamond[9]. By operating at an "α-null" value of underfocus, Si atomic columns viewed in the [112] orientation separated by only 0.78Å have been successfully resolved.[10]

For screw dislocations accompanied by voids in HVPE samples, such reconstructions were obtained for [0001] projection where atomic columns separated by 1.84Å can be clearly seen (Figs. 1g-i). In the dislocation core, one atomic column is very weak (Fig. 1h-area A) and another column very bright (Fig. 1h-area B). Our calculations show that weaker or stronger intensity of such column cannot be obtained simply by sample tilt, therefore such a difference in their intensity can be assigned only to the stoichiometry of the particular column. Higher intensity of the atomic column (area B) must be related to a dislocation core that might have more Ga atoms.

It is also noticeable that the surrounding of the atomic column (Fig. 1h-area A) with the weaker contrast is different in comparison to other areas. We conclude that light elements must be present there and segregate to the tip of the void. This conclusion would be consistent with our earlier observation[11], and theoretical calculations[2] showing the possibility of V_{Ga}-$(O_N)_3$ pair formation along particular crystallographic planes. When such complexes are formed, the GaN does not grow on these planes, leading to void formation.

This study would suggest that despite the fact that voids are formed along the dislocation line, the dislocations have closed cores. Similar results of closed core are obtained for the screw dislocation in the MBE material, confirming earlier studies[5] and details of these studies will be presented.

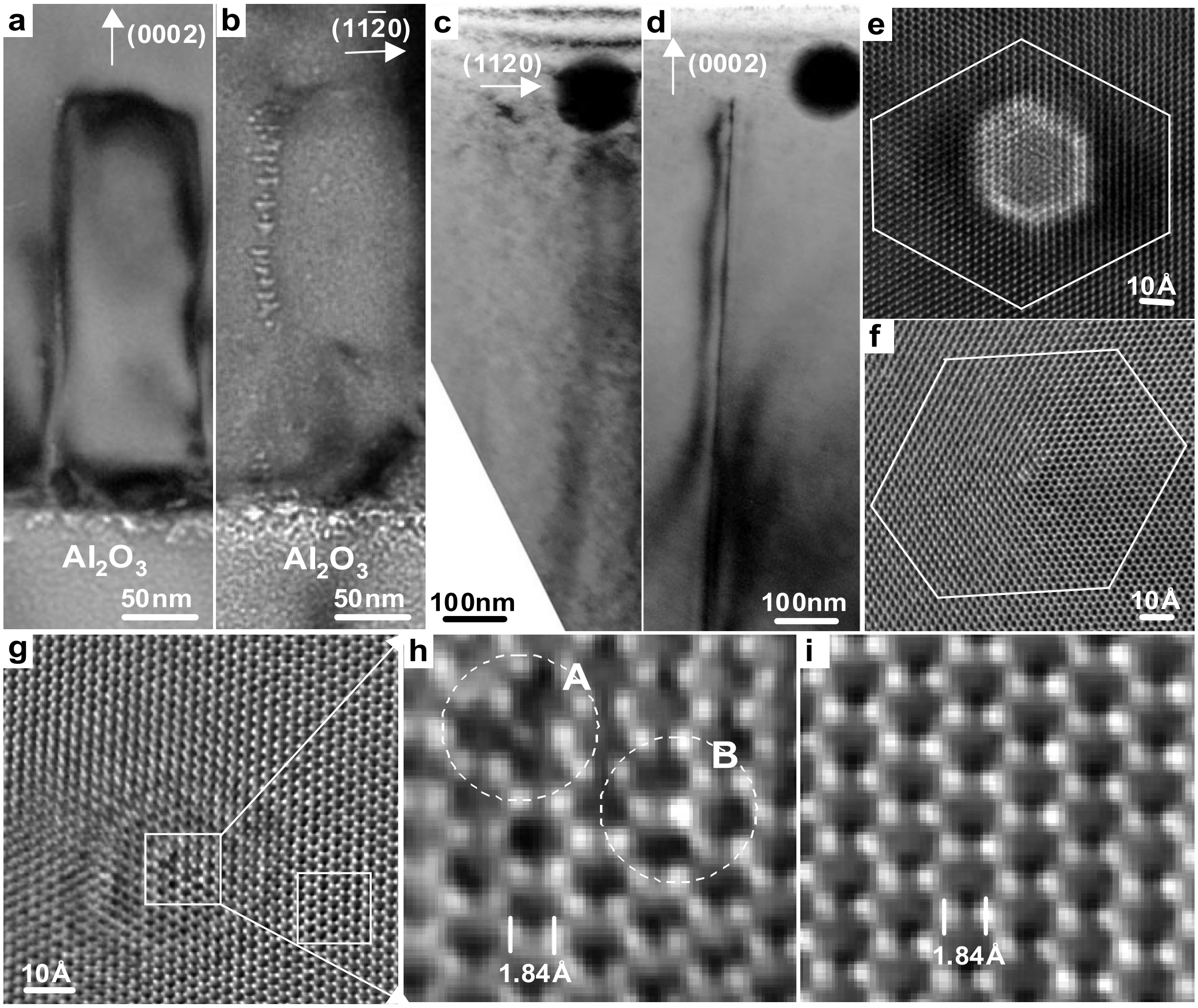

Fig. 1. (a) Screw dislocations in HVPE GaN for g = (0002); (b) when g = (11$\underline{2}$0), voids are visible along a dislocation line; (c, d) Screw dislocations in MBE GaN for g = (0002) and g =(11$\underline{2}$0); (e,f) Burgers circuits around screw dislocation from the HVPE and MBE material in plan view configuration; (g,h,i) phase of the electron wave reconstruction from a screw dislocation surrounded by a void; (h) dislocation core structure – around the tip of the void (circle A) and around the dislocation core (circle B); (i) the perfect area (outlined by the box in the lower right of (g)).

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