Dislocations at the interface between sapphire and GaN

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Abstract

GaN layers grown by metal organic vapour phase epitaxy on sapphire were imaged by synchrotron radiation X-ray topography. The threading dislocations could not be resolved in the topographs due to their high density, but a smaller density of about 10^5 cm^{-2} misfit dislocations were seen in the interface between GaN and sapphire by using large-area back-reflection topography. The misfit dislocation images in the topographs form a well-resolved cellular network, in which the average cell size is roughly 30 µm. Different cell shapes in the misfit dislocation networks are observed on different samples.

1 Introduction

GaN has been the target of concentrated research and development efforts due to its ability to emit light in the blue region of the spectrum. The *de facto* substrate for epitaxial GaN has been sapphire, however the large lattice mismatch between the two materials makes the epitaxial techniques rather difficult. The growth of GaN on sapphire has been known to produce grains in the sub-micron scale with grain boundaries having threading (TD) and misfit (MD) dislocations [1]. In this work, larger physical structures at the interface between GaN and sapphireare studied.

2 Experimental

GaN layers having a thickness between 2 to 4 µm were grown by metal organic vapour phase epitaxy (MOVPE) on 500 µm thick (00.1) sapphire substrates utilising the multistep nucleation layer technique with trimethylgallium (TMGa) and NH_3 as precursors [2]. The relatively large lattice misfit between GaN and sapphire results in an effective 30º rotation between the two lattices, and generates MDs and strain both into the epilayer and into the substrate during the MOVPE growth. Defects in the resulting heterostructure were imaged by means of synchrotron radiation X-ray topography (SR-XRT) [3] at HASYLAB-DESY in Hamburg and at ANKA in Karlsruhe. Most of the diffraction spots of GaN and sapphire in the Laue-picture do not overlap because of the differences between lattice orientation, lattice constants and crystal systems of rhombohedral sapphire and hexagonal GaN. Thus, it is possible to record images of either material individually, which can specifically be used to image the interface effects on sapphire under the relatively thick GaN layer. The imaging of the sapphire substrates instead of GaN layers is necessary because the defect densities of the GaN layers are too high for direct SR-XRT. Additionally, atomic force micrographs (AFM) of the etched GaN surfaces were recorded in order to obtain etch pit density data on GaN.

3 Results and discussion

Figure 1 shows a 1 -1 . 14 (hexagonal coordinate system) large-area back-reflection topograph recorded of sapphire substrate beneath a 2 µm thick GaN layer. The topograph shows a well-resolved irregular cellular network having a cell size of roughly 30 µm in diameter. According to the kinematical theory of diffraction the black images on the grey sapphire background indicate either a defect or a high local strain field. Because of the large size of the cells it is believed that the grains in the GaN epilayer causing the boundary defects and strain in the sapphire have the same shape as the grain images in the sapphire.

Figure 2 shows more topographs of sapphire under different GaN epilayers. Figure 2 a) shows a topograph of a sample having a GaN epilayer with a higher TD density of about 10^8 cm^{-2}. The defect network images in the topograph have noticeably smaller cell size and more signs of strain. Figure 2 b) is a topograph showing a peculiar cell structure constructed of irregular hexagons having a defect dot in the centre. The size of the cells is again about 30 µm. Figure 2 c) shows a topograph of strain and defects in sapphire caused by a macroscopic defect in the GaN epilayer. The 100-µm-thick defect is in the upper part of the topograph.

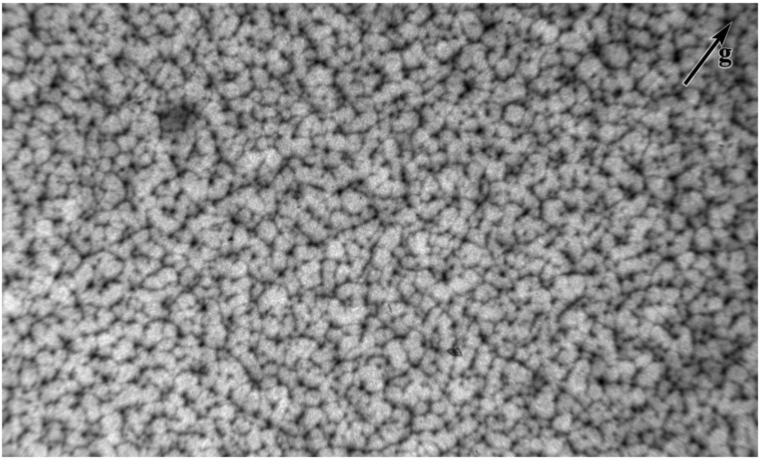

Figure 1: 1 -1 . 14 (hexagonal notation of the rhombohedral lattice) large-area back-reflection topograph of sapphire under a GaN epilayer showing strain from a MD network. Diffraction vector **g** is shown in top right corner. Image size is 1000 µm × 600 µm.

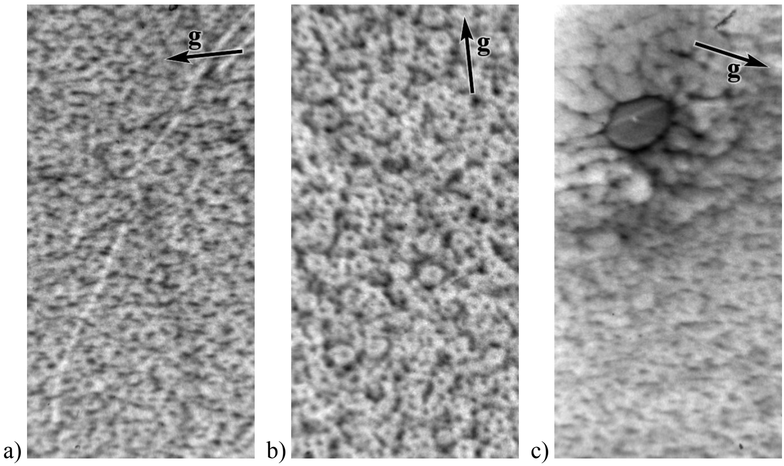

Figure 2: a) -2 2 . 14, b) 0 3 . 18, and c) 0 3 . 18 large-area back-reflection topographs of sapphire substrates under GaN layers showing strain from the MD network. GaN layer in a) has higher overall TD density of about 10^8 cm^{-2} and smaller cell size, b) shows an unusual cell pattern, and c) has a 100 µm wide macroscopic defect. Hexagonal notation of the rhombohedral lattice is used in the indices. Diffraction vectors **g** are shown in top right corners of topographs. Image size is 300 µm × 600 µm.

Overall TD dislocation densities were calculated from AFM images, examples of which are shown in Figure 3. Two distinct types of etch pits were observed. The small etch pits are circular and their density is about 10^7 cm^{-2}. The large etch pits are clearly hexagonal, and they have a density of less than 10^5 cm^{-2}. The large hexagonal etch pits are believed to be generated into the screw dislocation endpoints at the GaN surface. It was also noticed that the TD endpoints tend to form clusters and lines. It is not known whether such clustering and lining is connected to the cellular structures observed by SR-XRT.

4 Conclusions

Images of strain caused by different cellular networks of MDs at the interface between sapphire and GaN were imaged using SR-XRT. Structures having regular cellular network with cell size of roughly 30 μm were observed in the samples with the lowest overall dislocation density in the GaN layer. Samples having a GaN layer with ten times more TDs had smaller cell size and considerably more irregular cellular structure.

a) b)

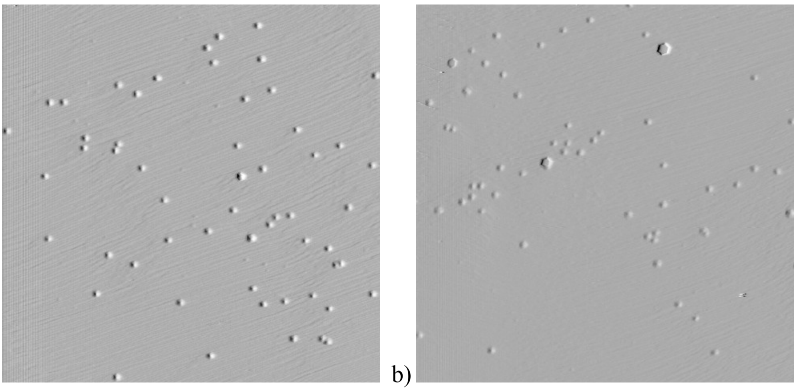

Figure 3: Deflection mode AFM-images of etched GaN surface showing a) only small circular etch pits and b) also some larger hexagonal etch pits. The hexagonal etch pits are believed to be formed at screw dislocation exit points. Image size is 10 μm × 10 μm.

References:

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