

A cause determining the crystalline orientation of hexagonal GaN grown on AlAs/GaAs(001)

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GaN has the hexagonal structure as its stable structure and hexagonal GaN (h-GaN) grown on sapphire (0001) substrates is in practical applications. On the other hand, GaAs substrates as well attain an increasing interest due to higher conductivity and cleavability. Basically, h-GaN is grown on GaAs(111) and c-GaN is grown on GaAs(001). In contrast with this, we have recently found that h-GaN can be grown on GaAs(001) by using thin AlAs intermediate layers [1]. In this report, the crystallographic relation involved in GaN/AlAs/GaAs(001) is experimentally revealed and a cause determining the in-plane crystalline orientation of h-GaN is investigated by means of simulation using a simplified model.

GaN was grown by atmospheric-pressure metalorganic vapor phase epitaxy (MOVPE) using triethylgallium and dimethylhydrazine as source precursors on GaAs(001) substrates. AlAs thin layers (20nm) were inserted between the epitaxial layers and the substrates. Although GaN directly grown on GaAs(001) substrates was in the cubic phase, that grown with the AlAs intermediate layer was in the hexagonal phase, as shown below.

The crystallographic relation involved in GaN/AlAs/GaAs(001) was investigated experimentally by X-ray diffraction measurements and atomic force microscopy (AFM). By the X-ray pole figure measurements, six-fold h-GaN{10-11} diffractions and four-fold GaAs{115} diffractions were detected, from which the crystallographic relation between them was extracted as schematically shown in Fig. 1. C-oriented h-GaN was grown on AlAs(001) with the in-plane relation of h-GaN(10-10)//AlAs (1-10). On the other hand, Fig. 2 shows the AFM image of the h-GaN surface. There are several hexagonal islands, whose direction agrees with that of the h-GaN lattice revealed by the X-ray pole figure measurements. This suggests that the h-GaN growth is in the island growth mode with hexagonal islands.

In order to find a cause for the observed in-plane crystallographic relation of h-GaN(10-10)//AlAs (1-10), we performed computer simulation in following way. The model used for the simulation is explained using Fig. 3, where the closed circles represent the h-GaN lattice points and the open circles the absorption sites determined by the AlAs lattice points. It was assumed that one of the h-GaN lattice points completely agreed with an absorption site (point A in Fig. 3). Based on the AFM observation (Fig. 2), the GaN island shape was simulated by simple hexagon. Therefore, the smallest island consists of point A and its nearest neighbors, as shown in Fig. 3. First, this smallest h-GaN island was rotated around point A, that is, on its c-axis at 0.25° interval. At each rotated position, the distances between the h-GaN lattice points and the most neighboring AlAs absorption sites were calculated for each lattice point. When average distance is minimum, the distortion is also considered minimum. Then, the same procedure was applied for larger h-GaN islands by considering up to the 2nd, 3rd, 4th,... nearest neighbors of point A.

The results are shown in Fig. 4. In Fig. 4, θ refers to the angle between the AlAs[1-10] direction and a h-GaN $\langle 10-10 \rangle$ direction (cf. Fig. 3), and r denotes that the hexagonal island is formed by up to the r -th nearest neighbors of point A. Taking the symmetry of h-GaN and GaAs into account, the results between $\theta = 0^\circ$ and 30°

are shown. For the islands with $r = 1$ and $r = 2$, average distance becomes minimum when $\theta = 0^\circ$ (h-GaN[10-10]//AlAs[1-10]). This orientation relation agrees with that appeared in Fig. 1. For the islands larger than $r = 3$, on the other hand, the minimum of the average distance does not always appear at $\theta = 0^\circ$. Comparing the simulation with the experiments, we consider that the crystalline orientation of h-GaN on AlAs/GaAs(001) is determined at the very early stages of the growth so as to minimize the average distance. In other words, the distortion between the h-GaN epitaxial layers and the AlAs is considered to cause the crystallographic relation between them.

It has been reported that [111]-oriented CdTe can grow on GaAs(001) with the in-plane crystallographic relation of CdTe(-211)//GaAs(110). This relation could also be accounted by the same manner presented here. Therefore it is reasonable to consider that the distortion generally plays an important role in determining the crystallographic relation between an epitaxial layer and a substrate. The model employed here is rather simple, though may provide a guiding principle for predicting in-plane crystalline orientation.

[1] M. Funato, T. Ishido, A. Hamaguchi, Sz. Fujita and Sg. Fujita, to be presented at ICMOVPE-X, Th-A3

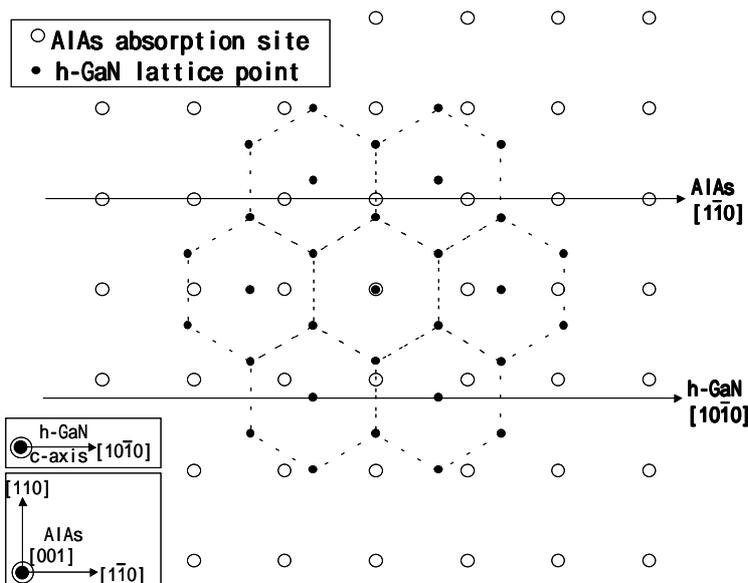


Fig. 1. Crystallographic relation revealed by the X-ray pole figure measurements.

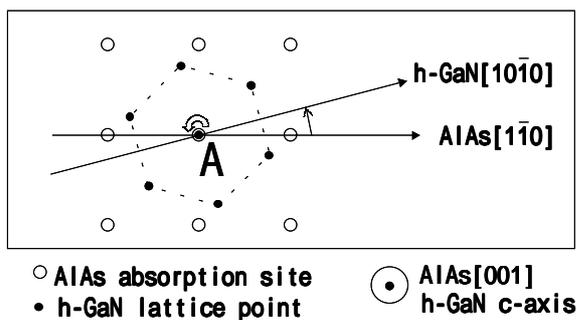


Fig. 3. The model used for the simulation.

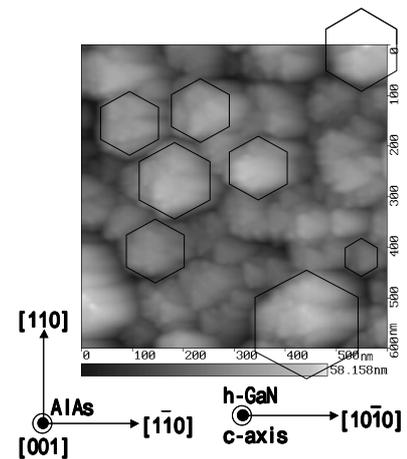


Fig. 2. AFM image of the h-GaN surface.

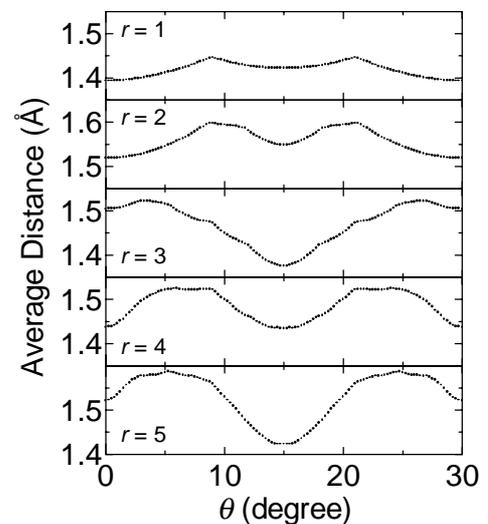


Fig. 4. The result of the simulation