Void shapes in the Si (111) substrate at the heteroepitaxial thin film / Si interface

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Abstract: Transmission electron microscopy (TEM) images of 3C-SiC thin films on Si (111) grown by solid-source molecular beam epitaxy (MBE) often reveal interfacial voids just underneath the film because of the Si outdiffusion from the substrate into the layer. The same phenomenon can be seen in the 2H-AlN thin film / Si (111) heterosystem grown by plasma-assisted MBE. We demonstrate in both cases the influence of growth parameters on the created voids. In the SiC/Si system we show an important influence of the growth temperature. At 850°C a well-known triangular void is formed, whereas at 1050°C we found an unusual hexagonal void shape. In this case not only low surface energy {111} facets form the void shape, but also facets with higher surface energy. We discuss this new appearance as a void shape which is near the equilibrium void shape in a cubic crystal. In the AlN/Si heterosystem the initial covering of the substrate has an influence on the amount of the Si outdiffusion and therefore on the size of the voids. In samples with an initial nitrogen cover the Si content in the AlN layer is higher (~10^{21} cm^{-3}) and the voids are more larger compared to samples with an initial Al cover (Si content ~10^{18} cm^{-3}).

1.Introduction

Silicon carbide (SiC) is a leading wide-band-gap semiconducting material with unique thermal, electronical and physical properties which make it suitably for high power, high temperature and high frequency devices [1]. Aluminium nitride (AlN) is a wide-band-gap III-V compound with desirable thermal conductivity, chemical and thermal stability, electrical resistivity, and acoustical properties. Therefore it can be a promising material for applications in microelectronic and optoelectronic devices such as passivation and dielectric layers in integrated circuits, short wavelength emitters, high frequency surface acoustic wave (SAW) devices [2], and also as a template substrate for epitaxial group III nitride layers [3]. The heteroepitaxial growth of cubic (3C) SiC thin films on Si and the growth of hexagonal (2H) AlN thin films on Si is a challenging task due to the large mismatches in lattice constants (~20%) and thermal expansion coefficients but the deposition allows to integrate the SiC and the nitride technology into the mature Si technology.

In the heteroepitaxy of these two materials on Si one of the problems is the Si outdiffusion from the substrate into the layer during the film growth process. That can lead to a formation of voids at the film/substrate interface just beneath the film [4,5,6]. This poses a great problem in device applications requiring an excellent interface such as the wide-band-gap emitter SiC/Si heterobipolar transistor (HBT) [7]. First the void creation has to be understood before it can be avoided.

In SiC/Si(111) it is known [8] that the interfacial voids are formed by coalescence of Si vacancies which result from the Si outdiffusion into the growing SiC film. The void shape in a Si(111) substrate is always described as reverse truncated trigonal pyramid [9], mainly facetted by {111}. We found an unusual hexagonal shape of the voids [10] which have not been reported so far.

In the AlN/Si(111) heterosystem an outdiffusion of the Si also takes place from the film/substrate interface into the layer and leads under special conditions to a void creation [5,6]. There should be the same void creation process as described in the SiC/Si case because the Si outdiffusion as the reason is similar. To the best of our knowledge we found no description about the interfacial voids in the AlN/Si(111) case in the literature.
In this work we show by transmission electron microscopy (TEM) studies that the appearance of the interfacial voids is influenced in both cases by special film growth parameters . In the 3C-SiC/Si heterosystem, deposited by solid-source MBE, we compare the influence of the substrate temperature (850°C (for more details see [11]) and 1050°C (for more details see [12]) on the resulting void shape. We discuss the appearance of void facets with higher surface energy than Si{111}. In the 2H-AlN/Si heterosystem, deposited by plasma-assisted MBE [13], we compare the influence of the initial process (Al cover or nitridation) on the Si substrate during the film growth. We discuss how the initial process has an influence on the Si content in the grown AlN film and therefore on the size of the created interfacial voids.

2. Results

2.1. SiC/Si(111) heteroepitaxial system

2.1.1 Triangular void shape at 850°C substrate temperature

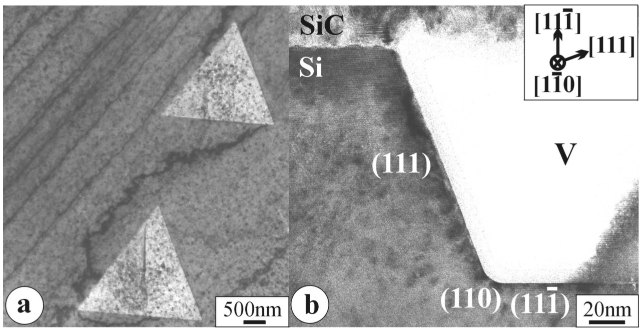

Figure 1 (a) Plan-view brigth-field TEM image, obtained in the [111] zone of Si, and **(b)** high-resolution cross-sectional bright-field TEM image, viewing along the [1-10] zone axis of Si, showimg the shape of an interfacial triangular

Figure 1 shows TEM images of an interfacial void in a SiC thin film specimen grown at 850°C substrate temperature on Si (111). In the plan-view TEM image (Fig. 1a) the exact void shape as a triangular is seen. This is formed by the energetically favourable {111} planes in the Si substrate showing the typical angle of 70.53° between them. The cross-sectional HRTEM image in the [1-10] zone (Fig. 1b) shows a {110} facet between the {111} planes. Although they have a higher surface energy [14], their occurrence reduces the surface area and the entire surface energy of the void [10].

2.1.2 Hexagonal void shape at 1050°C substrate temperature

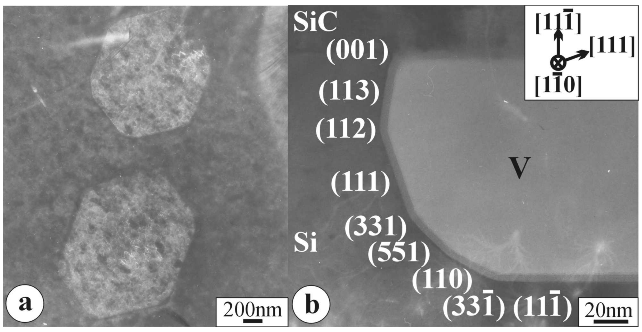

Figure 2 (a) Plan-view brigth-field TEM image, obtained in the [111] zone of Si, and **(b)** high-resolution cross-sectional bright-field TEM image (zone axis close to the [1-10] of Si) showing the shape of an interfacial hexagonal void

Figure 2 shows an unusual void shape in a SiC specimen grown at 1050°C substrate temperature on Si (111). The modification to the hexagonal void is possible to see in the plan-view TEM image (Fig. 2a). There are truncations of the corners compared to the regular shape of a hexagon. All facets of the hexagonal void are indexed in the cross-sectional HRTEM image (Fig. 2b). In addition to facets of a triangular void ({111}, {110}), other facets (see indexes in Fig. 2b) with higher surface energies [14] are formed. Their appearance can be explained due to the higher substrate temperature during the growth [10].

2.2 AlN/Si(111) heteroepitaxial system

2.2.1 Voids in specimens with initial nitridation

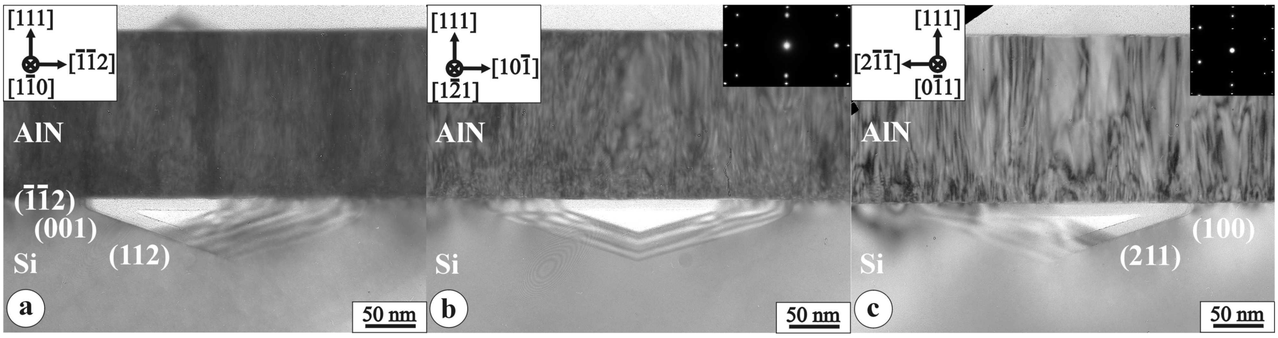

Figure 3 Cross-sectional bright-field TEM images of the same void in different zone axes of Si (tilted perpendicular to the [111] Si axis), **(a)** and **(c)** show two <110> zones ([1-10] and [0-11], tilt of 60°) and **(b)** shows the [1-21] zone which is exactly between them (30°)

The cross-sectional TEM images in Figure 3 show the same void in [1-10] (a), in [1-21] (b), and in [0-11] respectively zone axis orientation at the interface in a AlN/Si(111) system. The layer was grown under initial nitridation of the Si substrate. The void is relatively elongated along the interface underneath the layer. The main facets are the Si {112} planes which could be indexed in the different Si <110> zone axes (see Fig. 3a,c). A small truncation at {100} planes is seen.

2.2.2 Voids in specimens with an initial aluminium cover

Figure 4 Cross-sectional TEM images of the same void in different zone axes of Si (tilted perpendicular to the [111] Si axis), **(a)** at [1-10] zone and **(b)** at [1-21] zone axis orientation (tilt of 30° between them), **(c)** showing the void edge (arrowed in (a)). Note the bright contrast along the AlN/Si interface starting at a defect (arrowed) and ending at the void edge (right-hand side)

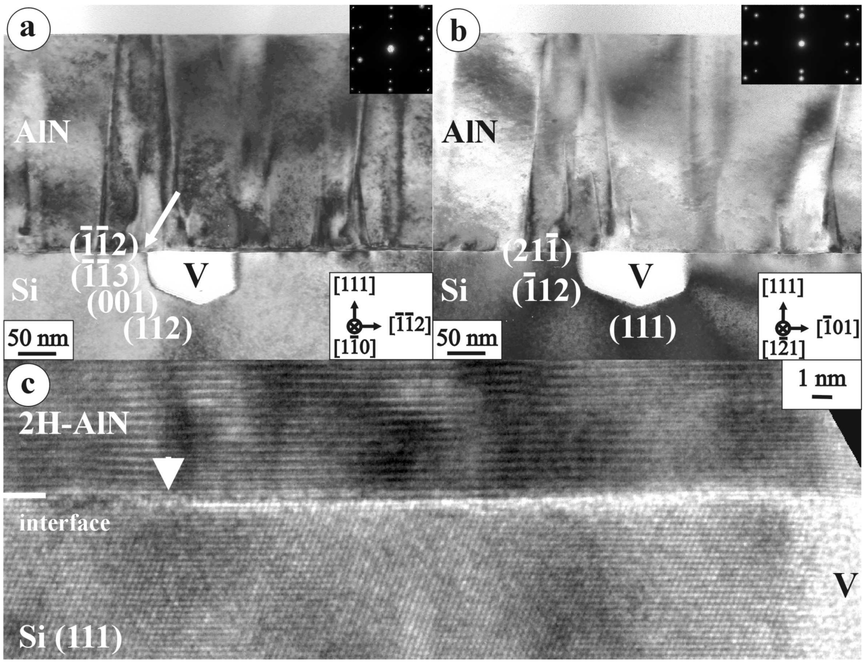

Figure 4a,b shows in cross-sectional view the void shape in a specimen with an initial Al cover on the Si(111) substrate. These micrographs are taken at the same magnification and at the same zone axes orientation as shown in Fig. 3a,b. Here also the Si {112} facets are important but this void is dominantly truncated by facets ({111}, {100}, and {113}) (compared with Fig. 3). The result is a smaller expansion of the voids along the interface underneath the AlN film. As the depth of the voids in both cases is very similar, the voids volume is smaller in case of an initial Al cover. SIMS measurements have proved that the Si content in the sample with the initial Al cover is much lower (~10^{18} cm^{-3}) than in the specimen with initial nitridation (~10^{21} cm^{-3}). Figure 4c shows a arrowed part of Fig. 4a at higher magnification. A stripe of bright contrast along the AlN/Si interface is obviously seen starting at a surface defect of the Si substrate (arrowed) and ending at the void (right-hand side). Because of the lighter contrast, there should be less amount of material, which can be explained by Si diffusion from the defect as an energetically favourable place along the interface to the already created void.

3. Conclusions

Interfacial voids formed in the Si (111) substrate underneath the film were investigated by TEM in the 3C-SiC/Si(111) and in the 2H-AlN/Si(111) heteroepitaxial systems. We demonstrated the influence of special growth parameters on the shape of the created voids.

In the SiC/Si case we found an influence of the growth temperature on the void shape. At 850°C a well-known triangular void with its primary {111} facets was founded and indexed. At 1050°C an unusual hexagonal void shape was created. In the latter case not only low surface energy facets ({111}Si) were observed, but also facets with higher surface energy [14]. Their appearence can be understood due to the higher mobility of the Si adatoms on these facets. Therefore a void shape approaching the equilibrium shape in Si (tetrakaidecahedron [14]) could be reached.

In the AlN/Si heterosystem we found an influence of the initial covering of the Si. The volume of the interfacial voids and the Si content in specimens with an initial nitridation are larger than in samples with an initial Al cover. For these reasons we assume that an initial nitridation process not absolutely leads to a thin silicon nitride layer which prevents the Si outdiffusion. This seems to be in agreement with [15] where is reported based that a considerable amount of N species migrates into the subsurface layers of the substrate.

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