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1999 J. Phys.: Condens. Matter 11 10019

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Step-bunching in 6H-SiC growth by sublimation epitaxy

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Received 13 May 1999

Abstract. Thick 6H-SiC epitaxial layers grown by sublimation epitaxy have been investigated concerning step-bunching. The macrostep appearances on the surfaces were studied for both (0001) Si and $(000\overline{1})$ C faces. The surface structure on the Si face is less regular compared with the C face. Data on the steps have been collected and the step height shows a linear relation with the step width.

1. Introduction

Silicon carbide (SiC) has excellent potential in high-power and high-frequency applications. At present, chemical vapour deposition (CVD) is an established method for epitaxial growth of device quality SiC. For high-voltage power device applications, substantial layer thicknesses are required and the CVD method is inconveniently slow due to the low growth rate $(<5 \,\mu m h^{-1})$. Recently, we have shown that sublimation epitaxy is suitable for growth of thick high-quality layers with a high growth rate [1]. The surface morphology of epitaxial layers is critical for device processing. Large disturbances like triangular shaped defects may appear in SiC epitaxial layers and these defects affect device performance [2]. However, once these defects can be avoided, one has to pay more attention to the surface step structure. The structure is especially important when step-bunching occurs. This effect generates an increasing step size due to coalescence of several microscopic steps thus forming macrosteps. Step-bunching is not desirable since it gives a less smooth surface and makes the impurity distribution in the layers non-uniform. To date, only a limited number of papers have reported on the stepstructure of SiC epitaxial layers grown on off-oriented substrates [3–5]. However, no studies have been performed on thick epitaxial layers of SiC. In this study, the as-grown surfaces of thick (50–120 μ m) 6H-SiC layers grown by sublimation epitaxy have been investigated with respect to the step-bunching.

2. Experiment

The layers were grown on both Si and C faces of 6H-SiC substrates by sublimation epitaxy with growth rates ranging from 50 to 120 μ m h⁻¹. The substrates were off-oriented 3.5° from the basal plane in the [1120] direction. The configuration of the method consists of a SiC source plate and a SiC substrate. The general principle of the growth technique is illustrated in

0953-8984/99/4910019+06\$30.00 © 1999 IOP Publishing Ltd

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Figure 1. Schematic view of the growth process used for sublimation epitaxy.

figure 1. By applying a temperature gradient, with a higher temperature at the source compared with the substrate, Si- and C-containing species are sublimated from the source and transported to the substrate where SiC is nucleated. The mass transport to the growing epilayer occurs via the vapour phase due to the shift of the solid–vapour equilibrium along the temperature gradient. With sublimation epitaxy, the growth rate can be varied between 20 μ m h⁻¹ to 2 mm h⁻¹. For a detailed description of the growth process see [1]. The as-grown surfaces were studied with optical microscopy using Nomarski interference contrast and atomic force microscopy (AFM).

3. Results and discussion

The morphology of the specular surfaces was smooth and it was difficult or impossible to observe growth steps with optical microscopy. It is reasonable to expect the appearance of macrosteps on thick epitaxial layers grown on off-oriented substrate surfaces due to the phenomenon of step-bunching. There exist several models for the step-bunching mechanism. The shape of a crystal growth surface is often determined by a decrease in the total surface free energy and this has been suggested to appear in step-flow growth [3, 5]. Based on this surface equilibrium process, a model has been proposed for step-bunching in SiC epitaxial growth [5]. The model is illustrated in figure 2. Due to the structure of the SiC crystal lattice, there exists three types of terrace on 6H-SiC{0001}, figure 2(a). Growth on off-oriented substrates makes the epilayer replicate the substrate polytype. The growth is determined by lateral growth of the terraces. On the terraces different energies are required for nucleation. In the model suggested in [5], deposition on 6H2 terraces is energetically most favourable and that on the 6H1 terrace most costly [5]. The step velocity on the 6H2 terrace is then higher due to a higher probability of nucleation at the steps. Two bilayer height steps are formed by the 6H2 terraces which overtake the 6H1 terraces, figure 2(b). This two bilayer step will proceed slower than the single bilayer step on the 6H3 terrace since the step velocity is inversely proportional to the step height. In a similar way the faster advancing steps on 6H3 terraces will subsequently overtake the two bilayer step and finally form a three bilayer height step, figure 2(c). This will mean that three Si-C bilayer steps (one bilayer 0.25 nm) are preferred for 6H-SiC and this has been shown to be the case [3, 5].

A clear difference of the surface morphology of thick epitaxial layers grown by sublimation epitaxy on the Si and C-face is observed using AFM. On the C face the macrosteps are very



Figure 2. Model for step-bunching in SiC: (a) initial; (b) intermediate; (c) final stage. See text for details.

regular and straight (figure 3(a)). On the Si-face (figure 3(b)) the steps are not as regular and the appearance of the steps is more roundish. The terrace widths vary. The results in the present study can be compared with AFM investigations on epitaxial layers grown by CVD [3] where the average terrace width of macrosteps on the Si face of 6H-SiC layers grown on substrates off-oriented 5° was 280 nm, whereas no steps could be observed on the C face using AFM. It is worth noting that the CVD layer thicknesses were only 5–10 μ m. The height profile of a 6H-SiC layer grown by sublimation epitaxy is shown in figure 4. The surface resembles a hill and valley structure [3, 6]. This appears often for layers grown on surfaces off-oriented from a low-index plane. The step-bunching is probably formed by a rearrangement of the surface which lowers the total surface free energy even though this causes an increasing surface area [3,6]. The difference in layer surfaces grown on the Si and C face might be related to the difference in the surface free energy on the two faces. The surface free energy is lower on the C face than on the Si face for 6H-SiC [7]. Since the surface free energy on the Si face surface is high, the total surface free energy on the Si face is reduced by formation of the hill and valley structure. The off-oriented surface rearranges to minimize the total surface free energy. On the $(000\bar{1})$ C face the surface free energy is low enough for maintaining a stable growth. In this case, the hill and valley structure does not appear and macrosteps are not formed. TEM investigations on CVD grown epilayers show that step heights of three Si-C bilayers appear



Figure 3. AFM images of off-oriented 6H-SiC (0001) epitaxial layer surfaces: (a) C face and (b) Si face; layer thickness \sim 120 μ m.



Figure 4. Height profile of 3.5° off-oriented 6H-SiC (0001) Si-face epitaxial layers; layer thickness ${\sim}50~\mu m.$

with the highest probability for 6H-SiC (0001) Si-face surfaces [5]. On the $(000\overline{1})$ C-face, single bilayer height steps dominate.

A step is made up of a terrace and a riser, figure 4. It seems that step height, terrace width and riser width are proportional to step width, figure 5. A similar relation was observed for steps on the C face. The step widths ranged from 30 to 60 nm. However, the step heights were similar as observed on the Si face which is in contradiction to what was observed for CVD grown epilayers [3]. It was reported that step-bunching also appears in CVD growth on the C face when the C/Si ratio increases [5]. An almost linear relationship of step height to step width has also been observed in CVD grown epilayer surfaces grown on the Si face [8].



Figure 5. Data taken from AFM image of 3.5° off-oriented 6H-SiC (0001) Si-face epitaxial layer surface. Step width against terrace width, riser width and step height; layer thickness \sim 50 μ m.

4. Conclusion

The surface morphology in thick epitaxial layers grown by sublimation epitaxy is good considering that the growth rate is high. Step-bunching does appear for both Si and C faces where the morphology is smoother than the one on the Si face. The step width varies within one epilayer but the cause of this needs further studies.

Acknowledgments

The authors would like to acknowledge E A M Johansson and J Benesch, Linköping University for AFM images, T Kimoto for valuable discussions, and SSF Program SiCEP as well as Okmetic AB for support.

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