Materials Science Forum Vols. 600-603 (2009) pp 223-226
online at http://www.scientific.net

Influence of growth parameters on the residual strain in 3C-SiC epitaxial layers on (001) silicon

G. Wagner, J. Schwarzkopf, M. Schmidbauer and R. Fornari

Institute for Crystal Growth, Max-Born-Str. 2, 12489 Berlin

wagner@ikz-berlin.de

Keywords: 3C-SiC/Si, heteroepitaxy, hot-wall-CVD, strain, wafer bow

Abstract. 3C-SiC epitaxial layers were grown on on-axis Si (001) substrates by low-pressure hot-wall chemical vapour deposition. Depending on the growth parameters, the residual strain in the 3C-SiC layer was seen to be tensile or compressive. In this work, the influence of parameters, such as growth temperature and C/Si ratio in the vapour phase, on residual strain and macroscopic layer bow is investigated. We found that the wafer bow changes from convex, at a deposition temperature of 1270° C, to concave at 1370° C. High resolution x-ray diffraction data indicate that the crystalline perfection of the layers is lower for decreasing deposition temperature and increasing compressive strain. No remarkable influence of the C/Si ratio in the gaseous atmosphere on the FWHM of the rocking curve was observed.

Introduction

The difference in lattice parameters (20 %) and thermal expansion coefficients (8%) between 3C-SiC and Si is responsible for the generation of a large number of planar defects, e.g. stacking faults and twins, in epitaxially grown SiC layers. This is caused by the high residual strain at room temperature [1]. Due to the large difference of lattice parameter, the 3C-SiC layers exhibit a tridimensional nucleation and growth so that the layers consist of coalesced individual crystallites. A large number of defects are located at the crystallite boundaries, and these defects lead to poor electrical characteristics of the layers. This, consequently, limits the application of 3C-SiC layers for electronic devices [2]. The size of the crystallites depends on the growth technique and the layer thickness. The final macroscopic layer bow at room temperature is the result of two different stress fields with opposite signs: the thermoelastic strain and the mismatch strain. Depending on the growth parameters, the residual strain in the 3C-SiC layer can be tensile or compressive [3, 4]. As a result the layer surface may be concave, undulated or convex.

Experiment

The heteroepitaxial growth of 3C-SiC layers on on-axis 2-inch (001) Si substrates (thickness 275µm) was carried out in a low-pressure hot-wall CVD reactor. A detailed description of the CVD-system was already published elsewhere [5]. The reaction gases, SiH_4 and C_3H_8 diluted in hydrogen, are carried by palladium-purified H_2. The (001) Si substrates were cleaned by using the standard RCA procedure followed by immersion in a HF solution in order to remove the surface oxide before loading them into the reactor. The carbonisation of the Si surface before layer deposition was identified as a most critical step, independently of the deposition temperature. The carbonisation of the Si surface started with introduction of C_3H_8 at 800° C for 2 minutes followed by a heating ramp up to the growth temperature. A small amount of SiH_4 (C/Si ratio: 30) was added to the input gas mixture to prevent evaporation of Si from the substrate and to avoid the formation of voids at the interface between substrate and layer when the substrate reached a temperature of about 1000° C. This carbonisation process produced a nucleation layer consisting of 3C-SiC crystallites of about 20 nm in size. The subsequent 3C-SiC layer deposition took place at temperatures between 1370° C and 1270° C under a reactor backpressure of 150 mbar. The deposition rate was fixed at

1.7 µm/h. The silane flux was kept constant and the propane flux was varied in order to vary the C/Si ratio between 2 and 3.5 in the different deposition experiments. The homogeneity of the layer thickness is known to depend on the carrier gas flow therefore it is necessary to tune the growth parameters in order to obtain identical concentrations of all components in the reaction gas during the different growth experiments. In particular, since the viscosity of the hydrogen carrier gas decreases for decreasing growth temperatures, it was necessary to modify the hydrogen flow and the flows of the Si– and C–sources as a function of the deposition temperature. The hydrogen flow was varied between 50 slm and 28 slm. The final thickness of the 3C-SiC layers was about 5 µm.
The macroscopic bow and the surface morphology of the epitaxial layers were measured by a contact less surface profiler and an atomic force microscope. The crystalline quality of the layers was assessed by full width at half maximum (FWHM) of the (002) and (004) SiC rocking curves from high-resolution x-ray diffraction (HRXRD) measurements.

Results

The carbon deposited during the carbonisation reacts with Si atoms from the substrate and forms a 3C-SiC seed layer with a thickness of approximately 20 nm. Owing to the large differences of lattice parameters and structure of the seed layer, tri-dimensional growth mode (3D islands) takes place in the layer. From TEM images (not shown here) we know that close to the substrate/layer interface many defects such as stacking faults, twins and dislocations are present in high density. However, the defect density remarkably decreases and individual islands coalescence to larger 3C-SiC crystallites with increasing layer thickness (d > 1 µm).
After optimisation of the carbonisation of the Si surface, flat epitaxial layers without macro-defects and a mirror like surface could be grown at temperatures between 1270° C and 1370° C (Fig. 1). The layer roughness was found to increase with increasing layer thickness and with the growth temperature.

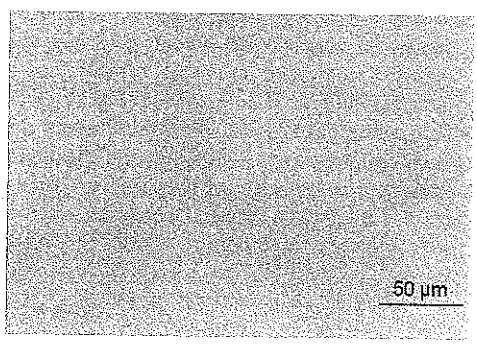

Fig.1: Normarski differential interference contrast (NDIC) micrograph of the surface of 5 µm thick epitaxial 3C-SiC on(001) Si, grown at 1310° C.

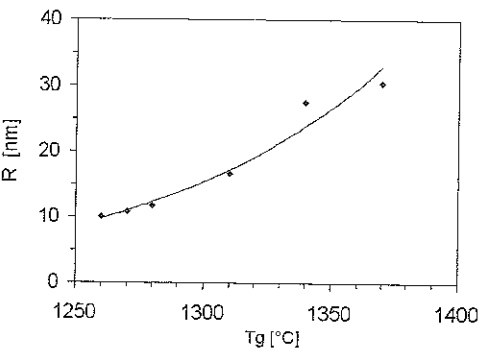

Fig.2: Temperature dependence of the average surface roughness R_a of 3C-SiC epitaxial layers on (001) Si, thickness 5 µm.

The deposition temperature indeed influenced the island size and the layer roughness. The average surface roughness R_a decreases from 30 nm at 1370 °C to 10 nm at 1270 °C, in layers with constant thickness of about 5 µm (Fig. 2). In this temperature interval all layers exhibited a flat and smooth surface. However, outside of this temperature range the surface morphology was seen to degrade, probably in connection with the surface kinetic mechanisms. At temperatures below 1270° C the layer growth was strongly disturbed and a high density of holes and a rough surface were observed. In this case the layer growth probably takes place below the critical kinetic conditions, when the surface diffusion of the adsorbed atoms is still too low. On the other hand, since the surface diffu-

sion of atoms and molecules increases with increasing deposition temperature, the island size increases. The growth in [111] direction is faster than in [001] direction, which is responsible for the larger size of the islands. The growth rate has the minimal value on the border between different islands. As a result an increase in the island size and an increasing difference of the thickness in the centre of the islands and on the border between individual islands was observed.

We have detected a distinct influence of the deposition temperature on the wafer bow. As shown in Fig. 3 the layer bow changes from a concave shape to a convex shape with decreasing temperature, in dependence of the strain conditions. At a deposition temperature of 1370°C we measured a concave bow of 60 µm while at a temperature of 1270 °C the bow was convex, again with a maximum deviation from planarity of about 60 µm. Correspondingly the residual strain changes from tensile to compressive.

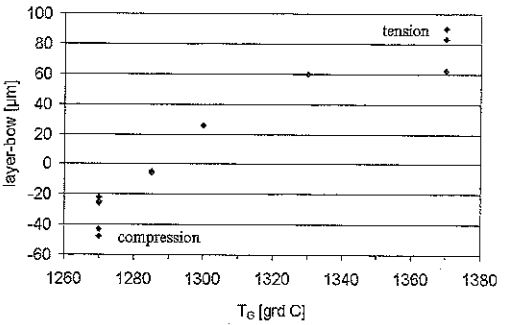

Fig.3: Layer bowing of 5 µm thick 3C-SiC layers, resulting from the combined tensile and compressive strain, in dependence on the deposition temperature

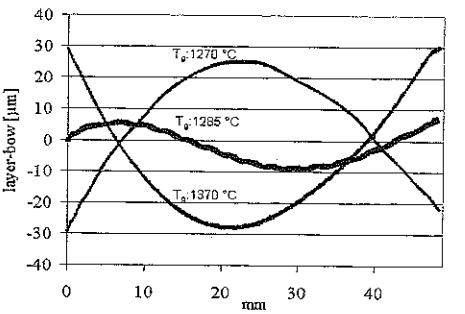

Fig.4: Surface profiles of three different 5 µm thick 3C-SiC layers grown on 2 inch (001) Si, 275 µm thick, at different temperatures

At 1285 °C the layer exhibits a slightly undulated shape with a waviness of ± 8 µm (see Fig. 4). The transition from tensile to compressive strain with decreasing deposition temperature also influences the crystalline perfection of the grown layer. The HRXRD rocking curves of the samples deposited at different temperatures are shown in Fig. 5. The FWHM increases from 470 arcsec at 1370° C to 670 arcsec at 1270° C. This indicates that the crystalline perfection of the layers decreases with decreasing deposition temperature and increasing compressive strain.

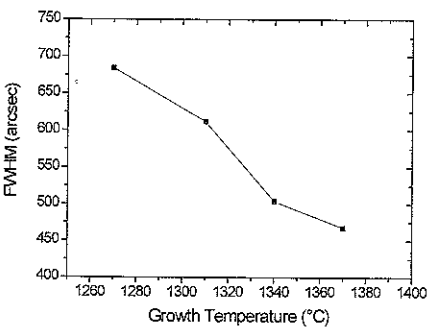

Fig.5: FWHM of XRD SiC (002) rocking curves as a function of temperature, C/Si ratio: 2

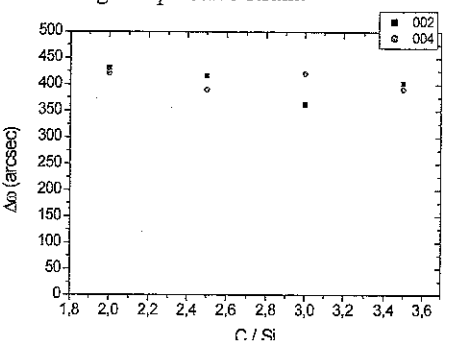

Fig.6: FWHM of XRD SiC (002 and 004) rocking curves as a function of C/Si ratio, T_g: 1370 °C

This observation is supported by an AFM study of the layer morphology (see Fig.7). At 1270° C a higher density of small-coalesced 3C-SiC islands characterises the layer. This implies a higher density of grain boundaries and therefore the presence of more dislocations and planar nucleation defects. With increasing deposition temperature the surface diffusion of absorbed species is higher and the size of the crystallites increases considerably. As shown in Fig.7 (a) crystallites with sizes up to 10 µm can be observed at 1370 °C. The decreasing number of grain boundaries results in lower density of dislocations and planar defects and thus in narrower FWHM of XRD rocking curves. The influence of the C/Si ratio in the nutrient gas phase on the FWHM of the rocking curve is reported in Fig. 6. Using C/Si ratios between 2 and 3.5 and a constant deposition temperature of 1370° C, we did not observe any remarkable change in the FWHM: the FWHM remains about 400 arcsec, independently of the C/Si ratio in the gas mixture. This observation is in contradiction to Ref. 3, which reported on a strong dependence of the bow on C/Si ratio.

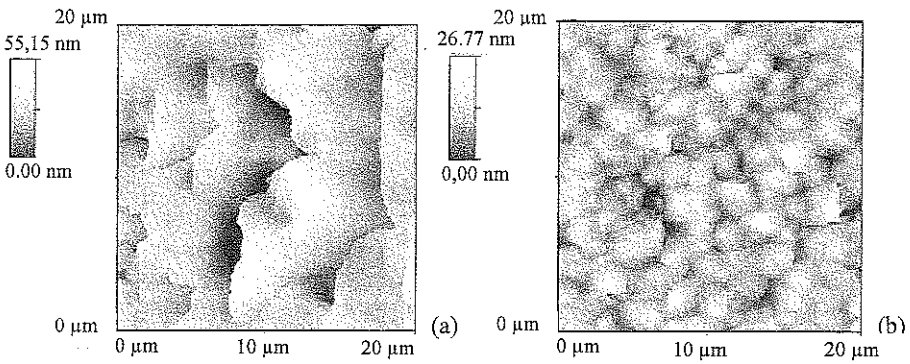

Fig. 7: (a) Atomic force micrographs of 3C-SiC islands with sizes of about 10 µm at T_g: 1370 °C and (b) about 3 µm at T_G: 1270 °C, layer thickness: 4.9 µm.

Summary

3C-SiC epitaxial layers were grown on 2" diameter 275 µm thick (001) Si substrates by low-pressure hot-wall chemical vapour deposition. The influence of the deposition temperature and of the C/Si ration in the gaseous phase on the residual strain and the final layer bow was investigated. We have detected a distinct influence of the deposition temperature on the wafer bow. The wafer bow changes from concave to convex when the deposition temperature decreases from 1370° C to 1270° C. Correspondingly, the residual strain in the layers changes from tensile to compressive. Investigation of the layers by HRXRD showed that the FWHM of the rocking curves increases with decreasing growth temperature. This indicates that the crystalline perfection of the layers decreases when using lower deposition temperature (increasing compressive strain). We did not observe any clear dependence of the FWHM on the C/Si ratio in the gaseous phase.

References

[1] J. Yun, T. Takahashi, Y. Ishida, H. Okumura: J. Crystal Growth 291 (2206) 140

[2] H. Nagasawa, K. Yagi, T. Kawahara: J. Crystal Growth 237-239 (2002) 1244

[3] M. Zielinski, S. Ndiaye, T. Chassange, S. Juillaguet, R. Lewandowska, M. Portail, A. Leycuras, J. Camassel : phys. stat. sol. (a) 204 (2007) 981

[4] E. Bustarret, D. Vobornik, A. Roulot, T. Chassagne, G. Ferro, Y. Monteil, E. Martinez-Guerrero, H. Mariette, B. Daudin, L. Si Dang: phys. stat. sol. (a) 195 (2003) 18

[5] G. Wagner, D. Schulz, D. Siche: Progress of Crystal Growth and Characterization of Materials 47 (2005) 139