We investigate Si (001) surfaces and bulk structures of molecular beam epitaxial (MBE) grown Si/Si:C heterolayers and describe “plateau-like” surface defects with a hill shape. The diameters of these surface defects are up to few 100 nanometers and their heights lie in the range of some nanometers. Plan-view and cross-sectional TEM bulk analysis of Si/Si:C heterolayers suggest a correlation between the “plateau-like” defects on the surface and extended dislocation structures in the bulk. The nucleation of these defects seems to have a correlation with the carbon present in the Si:C alloy.

Keywords: molecular beam epitaxy, carbon doping, surface and bulk structures, dislocation, oval defect

(Received May 4, 2000; Accepted July 1, 2000)

1. Introduction

Silicon (Si) layers with a high carbon (C) concentration have been only recently achieved thanks to improvements in molecular beam epitaxy (MBE) techniques (see, e.g., IYER et al.). Lately, Si/Si:C heterolayers have gained interests due to their potential in band gap engineering (EBERL et al.) or to their influence on the mobility of dopant atoms in electronic devices (SCHOLZ et al.). The solubility of C in the Si melt lies as low as $10^{-4}$ at. % (BEAN et al.), nevertheless in the case of MBE deposition (IYER et al.) succeeded the incorporation of up to 2% C within a few nanometers thin Si layer. This large amount of C in the Si matrix causes a tetragonal distortion of the Si:C and Si layers and can initiate SiC precipitates or dislocations. These defects can locally influence the microscopic growth kinetic and thus the microscopic surface morphology during the MBE deposition. However, little information has been up to now reported concerning the microscopic surface morphologies of Si/Si:C heterolayers.

In this paper, we describe surface defects and extended dislocation structures in Si/Si:C heterolayers. We grow Si (001) layers with a relatively high C concentration of 0.8 at. % on SIMOX substrates and cover it by Si cap layers. We investigate the as-grown surface of these samples by reflection electron microscopy (REM) and atomic force microscopy (AFM). REM has a very high vertical resolution down to a height of one atomic layer and allows the observation of large surface areas. We correlate these surface investigations with plane-view and cross-sectional transmission electron microscope (TEM) bulk images.

2. Experimental

The Si and Si:C layers were grown by MBE using electron gun evaporators for Si and C, both controlled by quadrupole mass spectrometers. In-situ diffraction of reflection high
energy electrons (RHEED) imaging is helping to monitor the growth conditions. The base pressure in the deposition chamber is better than $1 \times 10^{-6}$ mbar, whereas the working pressure is about $1 \times 10^{-9}$ mbar. For deposition we used SIMOX substrates with a relative high roughness (square roughness measured by AFM $R_q = 1.9$ nm). Standard chemical cleaning procedures (RCA I and RCA II) were performed to remove organic and metallic contaminations. Before growth, a thin protective SiO$_2$ layer was removed by heating in-situ at 830°C for 20 minutes. First we have grown a thin 10 nm buffer layer to bury the possible contamination particles in keeping the substrate roughness. Further on an e.g. 100 nm Si:C layer was deposited and finally covered by a Si cap layer with a thickness from 10 to 60 nm. The C concentration of 0.8 % was measured by secondary ion mass spectrometry (SIMS) as well as by X-ray diffraction analysis. The silicon growth rate was of 0.5 Å/s, whereas the growth temperature was 450°C.

The surface morphology of the Si cap layer on top of the Si:C layer was investigated by REM. The samples were mounted into a special specimen holder and inspected in a Philips CM 20 TEM. For imaging, a higher order Bragg reflection of the surface-parallel (001) planes is used. Since the Bragg angle is of the order of a few degrees, the obtained micrographs represent a glancing view of the microtopology. In the figure presented, an additional perpendicular scale marker accounts for the corresponding foreshortening. One advantage of REM lies in its large field of view (up to 2x2 mm$^2$) without sacrificing the high lateral resolution typical for TEM. In the vertical direction, monoatomic steps can easily be resolved and even the strain fields around the emergence point of dislocations are visible, essentially due to the phase contrast (for details about REM see e.g. YAGI or TUNG HSU). For AFM imaging, a Digital Instrument Dimension 5000 was used with a standard NCH-W tip. The samples were also prepared for plane-view and cross-sectional transmission electron microscopy (TEM and XTEM respectively) in an high-voltage (1MV) electron microscope Jeol JEM 1000.

**Fig. 1**: REM micrograph of a “plateau-like” defect on the surface of a (001) Si layer covering a Si:C layer. Because of the foreshortening effect of REM, the more circular shape of the plateau appears to be elliptical. P = plateau, D = local distortion of the lattice; S = strain field.

### 3. Results and Discussion

REM and AFM investigations of the Si cap, on top of Si:C show an extremely smooth as-grown surface. The roughness of the Si(001) surface lies in the height of a few monoatomic layers. Additionally we observe a new type of defects. We may best describe the shape of the defects by a kind of plateaus with a height of up to 10 nm. Their diameters are between 50 and 300 nm. Fig. 1 shows a representative example (P). The broad, dark contrast represents the borderline of the plateau. Because of the foreshortening effect by REM the more circular shape of the plateau appears to be elliptical. A micrograph and the corresponding line scan (Fig. 2) taken by AFM demonstrate the “plateau-like” defect’s shape without foreshortening.
In Fig. 1 the bright and dark contrasts (‘D’) near the dark borderline indicate a locally distortion of the lattice (OSAKABE et al.). In an increased distance from the plateau, the contrast marked by ‘S’ indicates a weak strain field (MAREK et al.). We believe that the lattice distortion and strain field are associated with dislocations in the bulk region lying under the plateau.

Fig. 2: AFM image and the corresponding line scan of a “plateau-like” defect on the surface of a (001) Si layer covering a SiC layer. The scanned surface represents an area of 2.5x2.5 µm² and the vertical scale is three orders of magnitude expanded.

This result is in a good agreement with our cross-sectional TEM investigations. Fig. 3 shows a representative example. The dark contrast indicates a strong strain field below a plateau. The plateau is best visible, if one looks along the growth surface from the right to the left. The bright and dark lines below the surface represent dislocations. In Fig. 3 is shown an example where the dislocations nucleate at the interface between the Si buffer and the SiC layer; however we also observed the case where the dislocations begin into the SiC layer. Due to the interaction of the dislocations inside the SiC region, a complex defect structure is formed, whereas in the cap layer no additional formation and modification of the dislocation is noticed.

Fig. 4 shows an extended dislocation structure in plane-view on a TEM micrograph. The dark and bright dislocations are arranged like the “arms of an octopus”. The contrast features indicate a strong strain field. From stereomicroscopic analysis of plane-view images follows that these defects have a depth elongation which correlates to those defects seen in cross-section (Fig. 3). The density of these “octopus-like” structures (10⁶ per cm²) corresponds to that one of the “plateau-like” defects observed on the surface by REM as well as by AFM plane-view.

Fig. 3: Cross-section TEM micrograph of the Si/SiC heterostructure showing the complex dislocation structure.
The “plateau-like“ defects observed by REM, AFM as well as by cross-section TEM have the same extension on the surface, and their density is comparable to the results yielded by surface and plane-view bulk observation respectively. Therefore, we conclude that “plateau-like“ defects are localized at the top of “octopus-like“ defects.

4. Conclusion

We investigated the surface of as-grown (001) Si cap layers on top of Si:C alloys in correlation with plane-view and cross-section bulk investigations. We found “plateau-like“ defects on the surface and “octopus-like“ extend dislocation structures in the bulk of the Si/Si:C heterolayers. Our results suggest a correlation between these defects.

Due to the incorporated carbon into the Si:C layer, the Si:C/Si heterolayers are strained. This lattice strain and the substrate roughness could be the reason for the formation of complex dislocation structures. These “octopus-like“ dislocation structures cause local deformations of the growth surface and can locally influence the microscopic growth kinetic. As a result, the growth is enhanced at such defect regions and the “plateau-like“ defects can develop.

The surface and the bulk structure of the “plateau-like“ defects in correlation to the presence of doping atoms suggest an analogy to the well known oval defects [WOOD et al.] in MBE grown compound materials, such as GaAs or InGaAs. Especially in case of InGaAs, RUSSEL-HARRIOTT et al. report a significant increased In concentration in the center of the oval defects.

More work about the C concentration influence and the MBE growth parameters is carried out at the moment and will be soon published in more detail.

Acknowledgment

One of us T.M. acknowledges Prof. H.P.Strunk, Institute for Microcharacterization, University of Erlangen, for discussions about the use of reflection electron microscopy in surface analysis.

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