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An atomic force microscopy and optical microscopy study of various shaped void formation and reduction in 3C-SiC films grown on Si using chemical vapor deposition

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Abstract

The formation of various uncommon shaped voids along with regular triangular and square voids in the epitaxial 3C-SiC films on Si has been investigated by optical microscopy and atomic force microscopy. Heteroepitaxial growth of 3C-SiC films on Si (001) and (111) substrates has been performed using hexamethyldisilane in a resistance-heated chemical vapor deposition reactor. The influence of the orientation of the Si substrate in determining the shape of the voids has clearly been observed. In addition, the growth period and the growth-temperature have been considered as the major parameters to control the size, density and shape of the voids. Generally, voids are faceted along {111} planes, but depending upon growth conditions, other facets with higher surface energy have also been observed. Finally the size and density of the voids are remarkably reduced, by suitable growth technique.

Keywords: 3C-SiC; CVD; HMDS; Void; AFM

1. Introduction

3C-SiC is an excellent semiconducting material for high temperature, high power and high frequency electronic devices due to its wide bandgap (~2.23 eV), high electron mobility, high saturated electron drift velocity and high thermal stability, etc. [1]. In addition, amorphous and polycrystalline SiC are often used as a coating material for structural applications and for micro-electro-mechanical systems applications due to their excellent mechanical properties and chemical inertness. Chemical vapor deposition (CVD) is most commonly utilized for the epitaxial growth of 3C-SiC on Si. Since 1983, the heteroepitaxial growth of 3C-SiC on Si substrates has become very attractive, but due to the large mismatch of the lattice constant (20%) and of the thermal expansion coefficient (8%) between 3C-SiC and Si, a high density of defects such as dislocations, stacking faults, microtwins etc. is found at the interface, which drastically influences the grown films [2]. These defects can be reduced by using 2°–4° tilted Si substrates and preparing a buffer layer on the Si substrate by carbonization at high temperature before the growth [3]. During this carbonization process, voids are generated at the SiC/Si interface. Voids, which are the common interfacial defect associated with heteroepitaxial growth of 3C-SiC on Si, are created by the coalescence of Si vacancies, which result from Si out-diffusion from the Si substrate. Growth of voids is most rapid before and during the coalescence of SiC nuclei. For the most part, voids seem to remain as empty sites during their expansion, with the grown SiC layer bridging the voids. However, there are also reports of SiC material protruding from SiC layer bottom surfaces [4,5] or of voids partly filled with SiC [6–8] indicating a certain ingrowth of SiC into voids or the substrate, respectively. The formation of voids generates microstructural defects and roughness at the interface. As a result, it poses a problem in SiC/Si device applications, such as p–n junction diodes, metal oxide semiconductor field effect transistor (MOS-FET) and heterojunction bipolar transistor. The key issue for obtaining a power-switching MOS-FET using 3C-SiC is to reduce the leakage-current of the p–n junction by

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eliminating planar defects like stacking faults [9]. Reduction of planar defects in 3C-SiC through heteroepitaxial growth using Si (001) substrate has been reported by Nagasawa et al. [10]. However, void formation or reduction has not been discussed in these reports.

Li and Steckl [5] demonstrated that at the earliest stages of growth, Si diffused out from the substrate non-uniformly, particularly at the periphery of the nuclei. If the nucleation density is low, this results in the formation of irregular trenches, which are then transformed into faceted voids as the growth proceeds. The shape of these voids in a Si (111) substrate is always triangular and in a Si (001) substrate, a square is formed by {111} facets [11,12].

In this paper, we discuss the formation and microstructure of various uncommon shaped voids such as hexagonal, octagonal, etc. along with regular triangular and square voids as observed by optical and atomic force microscopy (AFM) studies in case of 3C-SiC thin film growth on Si by CVD on Si substrates. Truncated voids have been formed in Si (111) and (001) substrates with primary facets on {111} planes. In addition, facets are observed by AFM on the higher energy planes such as {113}, {117}, {112} etc. to form equilibrium void shape. Finally, the reduction of the void density and size has also been investigated by using a two-step growth mechanism.

2. Experimental details

Atmospheric pressure chemical vapor deposition of 3C-SiC was carried out on Si (111) and (001) substrates in a hot-wall CVD reactor using a resistance-heated furnace (ELECTRO-HEAT EN345T). Single crystalline Si (111) or Si (001) wafers (p-type) were used as substrates. Before introducing the substrate into the reaction chamber, the native oxide was removed from the substrate surface by dipping in HF solution (5%) for 5 min and then washing in de-ionized (DI) water. After that it was dipped into acetone to eliminate organic contamination, and finally cleaned by DI water. Hydrogen, at a flow rate of 3 slm, was used as the carrier gas and argon, at a flow rate of 3 slm, was used for purging. Propane at a flow rate of 10 to 20 sccm was used for preliminary carbonization just before growth. For actual growth, an organo-metallic single source, hexamethyldisilane (HMDS), at a flow rate of 50 sccm was used. Growth temperature was varied from 1100 °C to 1250 °C. Due to the use of a resistance-heated hot-wall furnace, maximum deposition takes place on the hot wall of the reactor resulting in very low growth rate on the substrates. To grow thicker films, a series of runs was contributed on the same sample sometimes. For this, after each growth, the system was cooled down to room temperature and the reactor was removed from the furnace. The reactor was cleaned and re-growth was carried out on the same sample under the same conditions. The samples were in contact with air during the cleaning process in between two runs in the repeated growth process. The thickness of the film for 2 h growth at 1250 °C is ~0.5 μm.

After growth, the films were characterized using optical microscopy with Nomarski differential interference contrast (LEICA DM LM), XRD (Philips PW1729 X-ray diffractometer using Cu-Kα radiation and θ–2θ geometry) and AFM (Nanonics SPM-100 operated in intermittent contact mode using Nanonics AFM glass probe having force constant 40 N/m and resonant frequency 134.56 KHz) to study the microscopic structure, crystalline nature and defects.

3. Results and discussion

3.1. X-ray diffraction of SiC films

X-ray diffraction analysis was used in the present work to characterize the crystallinity of the films. Fig. 1a corresponds to diffraction from a film grown on a Si (111) substrate for 2 h at 1250 °C. Similarly, Fig. 1b corresponds to diffraction from the same sample after repeated (two times) growth, which was adopted for growing thicker films at the same temperature. The peak at 28.68° arises from the Si (111) planes due to the CuK_α radiation. In both cases, i.e. Fig. 1a and b, the presence of a peak at ~35.75° indicates that the films are 3C-SiC (111). In case of repeated growth on the same sample, Fig. 1b, peaks at 60.2° and 75.8° appear due to the diffraction from (220) and (222) planes of the grown 3C-SiC film, respectively. In single growth on Si (111) i.e. Fig. 1a, only the presence of 3C-SiC (111) peak proves that the grown film is probably epitaxial. But the appearance of other SiC peaks after repeated growth indicates the polycrystallinity of the film. Therefore it can be concluded that after repeated growth on the same sample, the films become polycrystalline for Si (111). The reason could be that after one run, the sample surface was modified by cooling (stress relief) and exposure to air.

The XRD patterns from the film grown on a Si (001) substrate after first time (2 h at 1250 °C) and after repeated (two times) growth are shown in Fig. 2a and b respectively. The peaks at 69.15° and 41.7° arise due to the diffraction from Si (400) and 3C-SiC (200) planes, respectively. In case of repeated growth, (Fig. 2b), peaks at ~90° appear due to the diffraction from the SiC (400) planes. In Fig. 2a, only the presence of 3C-

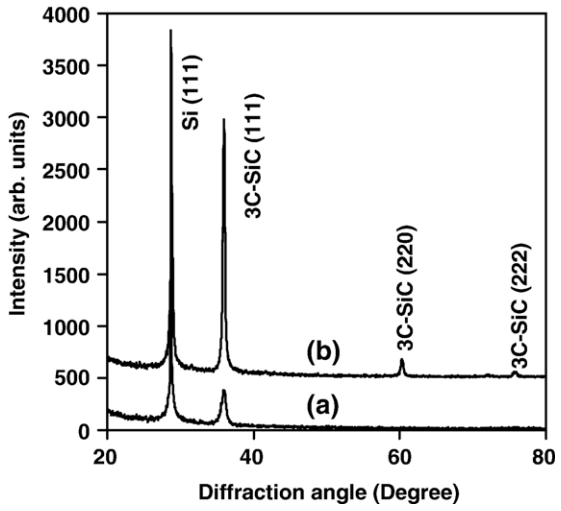

Fig. 1. X-ray diffraction spectra of 3C-SiC films grown on Si (111) substrate (a) for 2 h at 1250 °C and (b) for 4 h at 1250 °C in case of repeated growth.