

# Heteroepitaxial growth and characterization of 3C-SiC films on on-axis Si (1 1 0) substrates by LPCVD

Haiwu Zheng<sup>a,b</sup>, Jianfeng Su<sup>a</sup>, Zhuxi Fu<sup>a</sup>, Guang Li<sup>a</sup>, Xiaoguang Li<sup>a,\*</sup>

<sup>a</sup> *Department of Physics, Hefei National Laboratory for Physical Sciences at Microscale,  
University of Science and Technology of China, Hefei 230026, China*

<sup>b</sup> *Institute for Physics of Microsystem, School of Physics and Electronics, Henan University, Kaifeng 475004, China*

Received 10 June 2006; received in revised form 1 January 2007; accepted 2 February 2007

Available online 19 March 2007

## Abstract

Cubic SiC (3C-SiC) film has been deposited on Si (1 1 0) substrate by the low pressure chemical vapor deposition (LPCVD) with gas sources of SiH<sub>4</sub>, C<sub>3</sub>H<sub>8</sub> and carrier gas of H<sub>2</sub>. The 3C-SiC crystalline film can be confirmed through the observations using reflection high-energy electron diffraction (RHEED) images. The X-ray diffraction (XRD) pattern and the rocking curve indicate that the (1 1 1) plane of SiC film is parallel to the surface of the Si (1 1 0) substrate and the film is of high crystallinity. The results of the field emission scanning electron microscope (FESEM) images show that the film has smooth surface morphology. Transmitted electron diffraction (TED) pattern and high resolution transmission electron microscope (HRTEM) image further confirm the high quality of the film.

© 2007 Elsevier Ltd and Techna Group S.r.l. All rights reserved.

**Keywords:** Si (1 1 0); 3C-SiC film; Surface morphology; LPCVD

## 1. Introduction

Cubic silicon carbide (3C-SiC) is an attractive wide band gap semiconductor material utilized under severe conditions due to its superior physical and chemical properties [1,2]. 3C-SiC film can be grown epitaxially on Si substrate by chemical vapor deposition (CVD) technique [3], showing a significant advantage in the low-cost fabrication of large diameter wafers. However, defects generation due to the mismatch of lattice constant between SiC and Si is one of the most serious problems in the heteroepitaxial growth of 3C-SiC. In order to reduce the mismatch, Si (1 1 0) substrates [4] have been adopted instead of Si (1 1 1) or (1 0 0) substrates, which are focused by most of researchers [5,6] by atmospheric pressure chemical vapor deposition (APCVD) technique. However, the surface morphology of 3C-SiC films grown on on-axis Si (1 1 0) substrate is rough [4]. Compared to APCVD, low pressure chemical vapor deposition (LPCVD) has lower deposition rate but provides smoother surface morphology

[7] of the film. In this work, high crystalline quality 3C-SiC films with smooth surface morphology were deposited on Si (1 1 0) substrate by the LPCVD. The crystalline quality, surface morphology and microstructure of the films were investigated.

## 2. Experimental

3C-SiC film was deposited on an on-axis one-polished Si (1 1 0) substrate at a pressure of  $1.3 \times 10^3$  Pa. Prior to the growth, oxidized layer on the surface of the substrate was removed by hydrogen (H<sub>2</sub>) etching at 1200 °C for 5 min. After that, conventional carbonization process was carried out with propane (C<sub>3</sub>H<sub>8</sub>) flow rate of 5 standard cubic centimeter per minute (sccm) and substrate temperature of 1100 °C for 10 min. The growth of 3C-SiC film with silane (SiH<sub>4</sub>) flow rate of 5 sccm and C<sub>3</sub>H<sub>8</sub> flow rate of 10 sccm was carried out at 1300 °C. H<sub>2</sub> gas flow rate was kept at  $1.5 \times 10^3$  sccm during the etching, carbonization and the growth process.

Reflection high-energy electron diffraction (RHEED) images were used to determine the polytype kind of the film. The crystalline quality of the film was evaluated by X-ray diffraction (XRD) and the rocking curve. Raman spectrum was performed by an Ar-ion laser with the wavelength of 514.5 nm.

\* Corresponding author. Tel.: +86 551 3603408; fax: +86 551 3603408.

E-mail address: [lixg@ustc.edu.cn](mailto:lixg@ustc.edu.cn) (X. Li).

The plan views and the microstructure of the films were characterized by field emission scanning electron microscope (FESEM) and high resolution transmission electron microscopy (HRTEM), respectively. For the necessary of testing, the film was separated from the substrate by the mixed acid solution ( $\text{HF} + \text{HNO}_3 + \text{H}_2\text{O}$ ).

### 3. Results and discussion

RHEED is a powerful tool to determine the polytype of SiC epilayers [8]. Fig. 1(a) and (b) show the typical RHEED patterns of the surface of the SiC film along  $[1\ 1\ \bar{2}]$  and  $[0\ 1\ \bar{1}]$  azimuth, respectively. The spotty diffraction patterns indicate that high crystalline quality 3C-SiC film has been deposited on the Si (1 1 0) substrate. No additional diffraction spots of defects such as twins or stacking faults can be observed.

Fig. 2 shows the XRD pattern of the SiC film. The peaks at  $2\theta = 35.6^\circ$  and  $75.4^\circ$  correspond to cubic SiC (1 1 1) and SiC (2 2 2), respectively, which is consistent with the literature (JCPDS 74-2307). The Si (2 2 0) peak appeared at  $2\theta = 47.2^\circ$  comes from Si (1 1 0) substrate. No other diffraction peaks appear except for those from the Si substrate, indicating that the (1 1 1) plane of SiC film is parallel to the surface of Si substrate and the film at least has a strong preferred orientation. The rocking curve is used to assess the crystallinity of the SiC film. From the rocking curve of the SiC (1 1 1) peak in the inset of Fig. 2, the value of full-width at half-maximum (FWHM) is  $0.7^\circ$ , demonstrating that the film is of high crystallinity.

The XRD pattern reveals that the strong preferred orientation SiC (1 1 1) film has been successfully deposited on the Si (1 1 0) substrate. However, the crystallographic orientations of 3C-SiC films grown on Si (1 1 1) or (1 0 0) substrates have been reported to be identical with those of the Si substrates. In the case of 3C-SiC (1 1 1) film on Si (1 1 0) substrate, the density of aligned atoms per unit is 4 times higher than that in the case of 3C-SiC (1 1 0) film on Si (1 1 0) substrate, therefore the growth of 3C-SiC (1 1 1) film on Si (1 1 0) substrate is more stable than that of 3C-SiC (1 1 0) on Si (1 1 0) substrate [9]. It has been reported that the reaction between  $\text{C}_3\text{H}_8$  and Si (1 1 0) substrates was more reactive than that between  $\text{C}_3\text{H}_8$  and Si (1 0 0) or (1 1 1) substrates during the carbonization process, then a decreased  $\text{C}_3\text{H}_8$  flow rate was

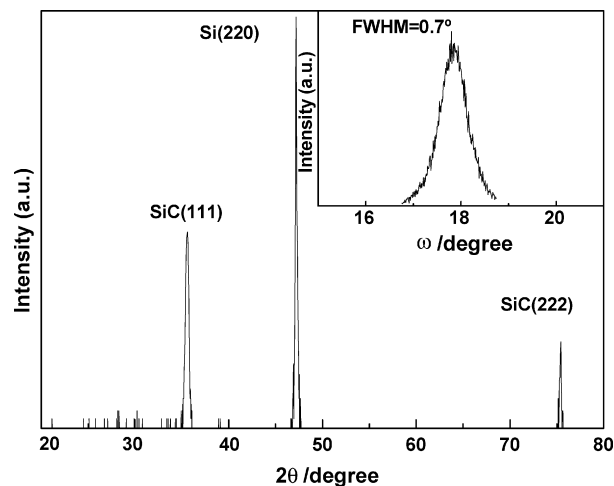


Fig. 2. XRD pattern of the 3C-SiC film. Inset in the figure is the rocking curve of SiC (1 1 1).

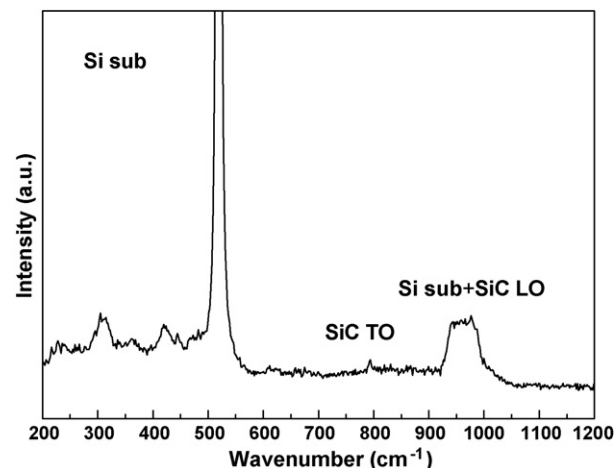


Fig. 3. A typical Raman spectrum of the SiC film. The strongest peak located at about  $520\text{ cm}^{-1}$  is ascribed to the silicon substrate phonon mode. TO and LO indicate the peaks attributed to transverse optical phonon mode and longitudinal optical phonon mode of SiC, respectively.

employed in order to obtain single crystalline 3C-SiC at atmospheric pressure [4]. For the current case, 3C-SiC film with high crystallinity has been deposited on Si (1 1 0) substrate at a higher  $\text{C}_3\text{H}_8$  flow rate. The reason may be that the gas

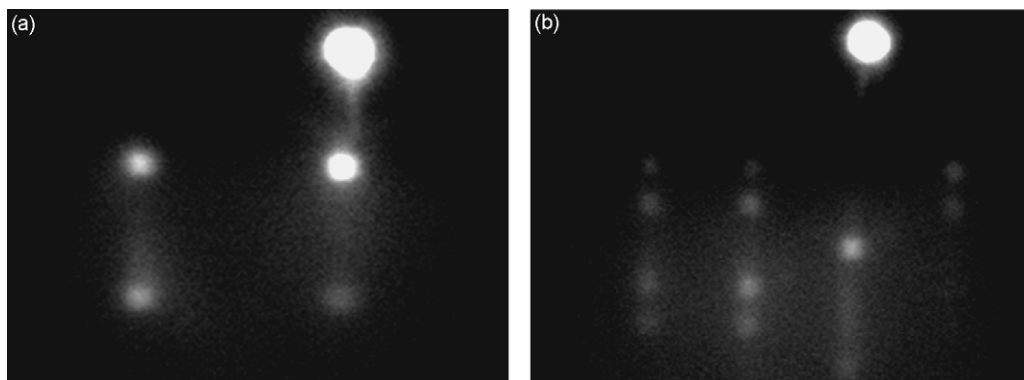


Fig. 1. (a) and (b) show the typical RHEED patterns of the 3C-SiC film along  $[1\ 1\ \bar{2}]$  and  $[0\ 1\ \bar{1}]$  azimuth, respectively.

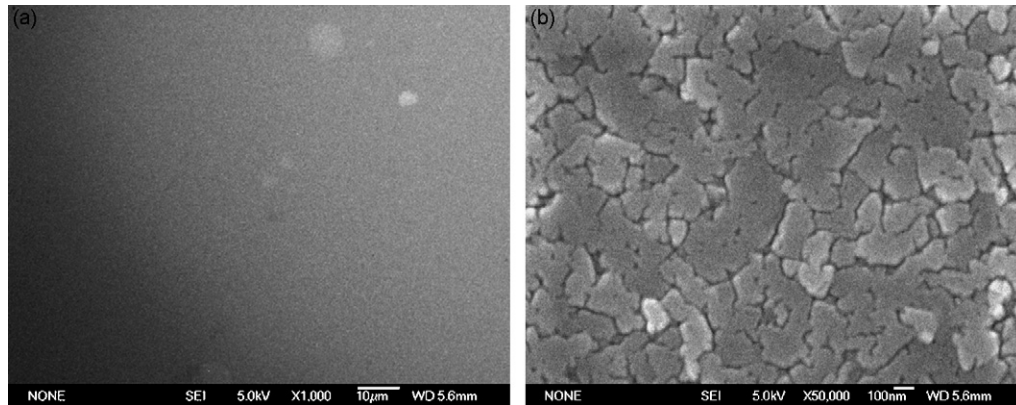


Fig. 4. Plan views ((a) 1000 $\times$  and (b) 50,000 $\times$ ) of the SiC film with FESEM.

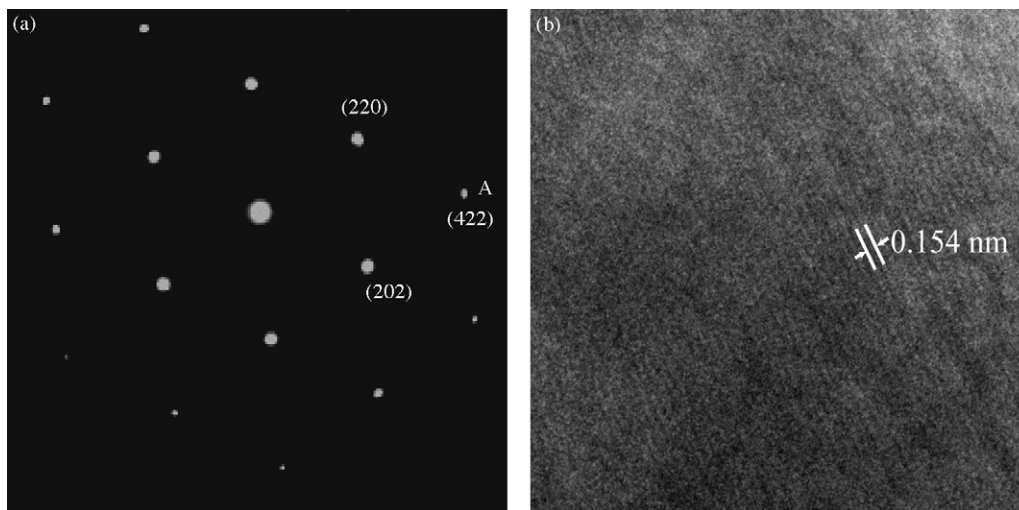


Fig. 5. TED pattern (a) and HRTEM image (b) of the SiC film. The transmitted electron beam are incident along  $[1\ 1\ 1]$  direction of 3C-SiC film.

utilization efficiency of  $C_3H_8$  at low pressure is lower than that of  $C_3H_8$  at atmospheric pressure.

A typical Raman spectrum for a 3C-SiC  $(1\ 1\ 1)$  film was shown in Fig. 3. The strongest peak located at about  $520\text{ cm}^{-1}$  is ascribed to the silicon substrate phonon mode. Besides this, the relatively weak peak located at around  $200\text{--}500\text{ cm}^{-1}$  come from amorphous silicon and the Si substrate [10]. The residua of  $SiH_4$  decomposition may be responsible for creating the amorphous silicon [11,12]. The weak intensity of SiC characteristic peaks indicates that the film used in the testing is thin. 3C-SiC TO phonon mode is clearly observable at about  $794\text{ cm}^{-1}$  but the LO mode is overlapped with the second-order Raman spectrum of silicon situated between  $940$  and  $980\text{ cm}^{-1}$ . The stress value, calculated from Raman data by employing Oleo and Cardona's method [13], is 0.65 GPa with tensile formation. The origin of tensile formation comes from the difference between the thermal expansion coefficient of 3C-SiC ( $\delta = 6.85 \times 10^{-6}\text{ K}^{-1}$ ) and Si ( $\delta = 6.95 \times 10^{-6}\text{ K}^{-1}$ ). It is also found that the stress in the film deposited on Si  $(1\ 1\ 0)$  substrate is less than that in the film deposited on Si  $(1\ 0\ 0)$  substrate with the same growth conditions. The reason is that the lattice mismatch between Si  $(1\ 1\ 0)$  and 3C-SiC  $(1\ 1\ 1)$  is lower than that between Si  $(1\ 0\ 0)$  and 3C-SiC  $(1\ 0\ 0)$  [9].

The plan views of the SiC film at magnification of 1000 and 50,000 were carried out using field emission scanning electron microscope (FESEM) techniques, as shown in Fig. 4(a) and (b), respectively. As indicated by Fig. 4(a), the film shows a smooth surface morphology. The surface morphology of the film is smoother than that of the film at almost the same magnification observed in the literature [4], in which the 3C-SiC  $(1\ 1\ 1)$  film on on-axis Si  $(1\ 1\ 0)$  substrate contained a high density DPBs (domain position boundary). Fig. 4 (b) shows the film consists of rectangular-like SiC crystals, which are also seen in the literature by Boo et al. [14].

The transmitted electron diffraction (TED) pattern and the HRTEM image of the film are shown in Fig. 5. One can see that the measurements of interplanar spacings and interplanar angles in the pattern are consistent with the  $[1\ 1\ 1]$  diffraction pattern of cubic SiC. The six intense dots close to the transmitted beam in six-fold symmetry correspond to diffraction spots of  $\{2\ 2\ 0\}$  planes of cubic SiC. Following the parallelogram law, spot marked with letter A can be expressed as  $(4\ 2\ 2)$ . The high crystallinity of the film can also be affirmed by the TED pattern. The smaller dots of  $1/3\{2\ 4\ 2\}$  reflections cannot be seen, which is different from the result of the 3C-SiC film on Si  $(1\ 1\ 1)$  substrate [12]. Moreover, the value of FWHM

of rocking curve of the film on Si (1 1 0) substrate is less than that of the film on Si (1 1 1) substrate [12]. Therefore it can be concluded that the density of defects such as stacking faults or twins in the film are less than that in the film on Si (1 1 1) substrate. Fig. 5(b) shows the corresponding HRTEM image of the SiC film. The lattice spacing is 0.154 nm, corresponding to the lattice spacing of {2 2 0} planes of the cubic SiC.

#### 4. Conclusions

In summary, high crystalline quality 3C-SiC film has been successfully deposited on Si (1 1 0) substrate by the LPCVD. The XRD pattern and the rocking curve indicate that the SiC film is of high crystallinity and the (1 1 1) plane of the film is parallel to the surface of the Si (1 1 0) substrate. The results of the surface morphology and microstructure further confirm that the film is of high quality.

#### Acknowledgements

Financial support from the National Natural Science Foundation of China under the grant nos. 50132040, 50472009 and 10474091 is gratefully acknowledged.

#### References

- [1] F.L. Via, G. Galvagno, F. Roccaforte, A. Ruggiero, L. Calcagno, *Appl. Phys. Lett.* 87 (2005) 142105–142107.
- [2] K. Biswas, G. Rixecker, F. Aldinger, *Ceram. Int.* 31 (2005) 703–711.
- [3] N. Kubo, T. Kawase, S. Asahina, N. Kanayama, H. Tsuda, A. Moritani, K. Kitahara, *Jpn. J. Appl. Phys.* 43 (2004) 7654–7660.
- [4] T. Nishiguchi, M. Nakamura, K. Nishio, T. Isshiki, S. Ohshima, S. Nishino, *Mater. Sci. Forum* 483 (2005) 193–196.
- [5] A. Gupta, D. Paramanik, S. Varma, C. Jacob, *Bull. Mater. Sci.* 27 (2004) 445–451.
- [6] K.C. Kim, C.I.I. Park, J.I.I. Roh, K.S. Nahm, Y.H. Seo, *J. Vac. Sci. Tech. A* 19 (2001) 2636–2641.
- [7] J.D. Hwang, Y.K. Fang, Y.J. Song, D.N. Yaung, *Jpn. J. Appl. Phys.* 34 (1995) 1447–1450.
- [8] R.S. Kern, K. Järrendahl, S. Tanaka, R.F. Davis, *Phys. Stat. Sol. (b)* 202 (1997) 379–404.
- [9] T. Nishiguchi, M. Nakamura, K. Nishio, T. Isshiki, S. Nishino, *Appl. Phys. Lett.* 84 (2004) 3082–3084.
- [10] Z.X. Ma, X.B. Liao, G.L. Kong, *Sci. China (Series A)* 30 (2000) 169.
- [11] A. Masuda, R. Iiduka, A. Heya, C. Niikura, H. Matsumura, *J. Non-cryst. Solids* 227–230 (1998) 987.
- [12] H.W. Zheng, J.J. Zhu, Z.X. Fu, B.X. Lin, X.G. Li, *J. Mater. Sci. Tech.* 21 (2005) 536–540.
- [13] D. Olego, M. Cardona, *Phys. Rev. B* 25 (1982) 3878–3888.
- [14] J.H. Boo, S.B. Lee, K.S. Yu, M.M. Sung, Y. Kim, *Surf. Coat. Tech.* 131 (2000) 147–152.