Dependence of Chemical Composition and Bonding of Amorphous SiC on Deposition Temperature and the Choice of Substrate

Li Wang*

*Queensland Microtechnology Facility, Queensland Micro- and Nanotechnology Center,
Griffith University, Nathan, Queensland, 4111, Australia*

Keywords: Amorphous SiC; Chemical vapour deposition; X-ray photoelectron spectroscopy; Stoichiometry.

Abstract

Amorphous SiC has superior mechanical, chemical, electrical, and optical properties which are process dependent. In this study, the impact of deposition temperature and substrate choice on the chemical composition and bonding of deposited amorphous SiC is investigated, both 6 in. single-crystalline Si and oxide covered Si wafers were used as substrates. The deposition was performed in a standard low-pressure chemical vapour deposition reactor, methylsilane was used as the single precursor, and deposition temperature was set at 600 and 650 °C. XPS analyses were employed to investigate the chemical composition, Si/C ratio, and chemical bonding of deposited amorphous SiC. The results demonstrate that these properties varied with deposition temperature, and the impact of substrate on them became minor when deposition temperature was raised up from 600 °C to 650 °C. Nearly stoichiometric amorphous SiC with higher impurity

concentration was deposited on crystalline Si substrate at 600 °C. Slightly carbon rich amorphous SiC films with much lower impurity concentration were prepared at 650 °C on both kinds of substrates. Tetrahedral Si–C bonds were found to be the dominant bonds in all deposited amorphous SiC. No contribution from Si–H/Si–Si but from sp^2 and sp^3 C–C/C–H bonds was identified.

*Author to whom correspondence should be addressed. Electronic mail: l.wang@griffith.edu.au.

Phone:+61-7-37358006. Fax:+61-7-37358021.

1. Introduction

Crystalline SiC is a wide energy-gap semiconductor that exhibits superior mechanical properties, thermal stability, resistance to oxidation, and very high thermal conductivity compared to crystalline Si. As its counterpart, amorphous SiC (a-SiC) would have similar superior properties if a large majority of chemical bonds are tetrahedral Si–C bonds with a very small fraction of other types of bonds. In recent years, amorphous SiC has been widely used as wear-resistant coating layer [1], passivation layer [2], diffusion barrier against both metal and dopant diffusion [3], and window layer in SiC/Si heterojunction solar cell [4]. The chemical composition and bonding, thermal stability and conductivity, optical and electrical properties of a-SiC are strongly influenced by deposition parameters [5,6], and optical and electrical properties have a strong correlation with chemical composition and bonding [7–9]. There are some evidence showing that the choice of substrate influences the microstructure [10] and deposition rate of deposited SiC [11], while to date detailed scientific research performed on the variation of chemical composition and bonding of a-SiC with the choice of substrate is scarce, it is usually taken for granted that the a-SiC films deposited on different substrates should have the same optical and chemical properties [9,12,13].

The commonly employed precursor sources for the deposition of a-SiC are the gas mixtures of $\text{SiH}_4 + \text{CH}_4$ [1,7] and $\text{H}_2 + \text{SiH}_4 + \text{C}_2\text{H}_4$ [4], as well as single precursor methylsilane [14–16] (H_3SiCH_3 , MS). Comparatively, single source precursor MS, containing directly bonded Si and C atoms, has the advantage of a simpler and the possibility of a more efficient chemical vapour deposition process. The incorporation of

H₂ during the deposition can either widen or narrow the optical energy gap of deposited SiC films [17–19]. The composition and chemical bonds of a-SiC prepared from MS had been reported [15,16], however, the employed deposition method was plasma enhanced chemical vapour deposition (PECVD) rather than standard low-pressure chemical vapour deposition (LPCVD). In this paper, the deposition of a-SiC is performed using MS as a single precursor (without dilution gas) in a standard LPCVD reactor at medium deposition temperatures, and the aim is to investigate the dependence of chemical composition and bonding of a-SiC on deposition temperature and the choice of substrate.

2. Experimental procedures

SiC films were deposited on single-crystalline Si(100) wafers (*p* type, with a resistivity of 5–15 Ω cm, 6 in. in diameter) and 5 μ m SiO₂ (thermal growth) covered single-crystalline Si(100) wafers (*p* type, with a resistivity of 1–20 Ω cm, 6 in. in diameter). Deposition of SiC was performed using MS (purity > 99.98 %) as the single precursor in a standard horizontal hot-wall LPCVD reactor (the details of the reactor can be found in ref. [20]). Prior to being loaded into the reactor, the Si wafers were cleaned following the standard Radio Corporation of America (RCA) cleaning procedures. No wet-cleaning process was performed to oxide covered Si wafers, and they were loaded into the reactor (operated in cleaning room) as received. After loading the wafers into the LPCVD reactor, the reactor temperature was ramped up from 600 °C to the desired deposition temperature in vacuum with a ramp up rate of 5 °C/min. The deposition of SiC was performed at both 600 and 650 °C with an MS pressure of 0.06

mbar¹. The flow rate of MS was maintained at 9.5 standard cubic centimetres per minute (sccm) for all deposition processes, and the duration of each deposition process was set to be 10 h. In the sample label, “OX” indicates that the substrate is oxide covered Si wafer. More information on sample label is detailed in Table 1. Microstructure analyses were performed elsewhere by x-ray diffraction (XRD) and high-resolution transmission electron microscopy (HRTEM), indicating that the SiC films deposited on Si substrate under these conditions are amorphous [21,22]. The SiC films deposited on oxide covered substrates are also amorphous in microstructure according to XRD and HRTEM analyses (figures not shown here). Film thickness was measured with a Nanospec AFT 200 made by the company Nanometric, assuming a refractive index of 2.65 for a-SiC.

X-ray photoelectron spectroscopy (XPS) analyses were performed using a nonmonochromatic Mg $K\alpha$ x-ray source (1253.6 eV) with a Perkin-Elmer PHI model 560 XPS surface analysis system incorporating a hemispherical electron analyzer. The electron take-off-angle from the normal of sample surface was set at 0°. Ar sputtering was used to slowly remove the top surface layer (etch rate about 1.0 nm/min). After 10 minutes of etching, a rough scan in a wide binding energy range was performed first, and then multiple high resolution scannings were performed in the binding energy

¹ Based on our previous experimental results (published in Ref. [21]), at a given MS pressure of 0.06 mbar, the microstructure of SiC would transform from amorphous to crystalline states when deposition temperature was set at equal or above 700 °C. An temperature increment of 50 °C was employed. For the temperature of 550 °C, a very slow deposition rate (less than 2.0 nm/h) was observed; it is hard to yield a desirable thickness for various characterization methods.

ranges of interest for each element, with a pass energy of 25 eV. The core level spectra of Si 2*p*, C 1*s*, O 1*s*, and N 1*s* were recorded. The concentrations of these four elements were calculated by taking into account their sensitivity factors and the area below the measured curves. The sensitivity factors for Si 2*p*, C 1*s*, O 1*s*, and N 1*s* were 0.328, 0.278, 0.780, and 0.477, respectively. In order to distinguish the chemical bonding, the original XPS spectra were deconvolved by fitting the spectra according to Gaussian distribution function and by fixing the chemical bond positions and making the Si–C bond number equal to C–Si bond number in the form of tetrahedral SiC. All spectra were charge compensated to C–Si bond at 283.4 eV to account for surface charging. The detection limit of an element by XPS is around 0.1 at. %.

3. Results

3.1 Chemical composition analyses conducted by XPS

The relative atomic concentrations of Si, C, N, and O, as well as Si/C ratios in samples T600_Si, T650_Si, T600_OX, and T650_OX given by XPS analyses are shown in Table 2. Sample T600_Si was nearly stoichiometric with a Si/C ratio of 0.99 and other a-SiC films were carbon rich with a Si/C ratio in a range of 0.88–0.91. Oxygen atomic concentration decreased significantly with increasing deposition temperature, from 19.6 at. % in sample T600_Si to 3.9 at. % in sample T650_Si and from 13.5 at. % in sample T600_OX to 3.4 at. % in sample T650_OX. Nitrogen atomic concentration was in the range of 1.6–2.5 at. % in all deposited a-SiC films, also decreased with the increase in deposition temperature. The quantitative accuracy of the

atomic percent values for SiC material by XPS measurements ranges from 80 to 95 %, and it applies to the data shown in Table 2.

3.2 Chemical bonding analyses conducted by XPS for a-SiC deposited on single-crystalline Si substrate

High resolution Si 2*p*, C 1*s*, N 1*s*, and O 1*s* XPS spectra of sample T600_Si are shown in Figs. 1–3. The Si 2*p* spectrum [shown in Fig. 1(a)] can be deconvolved into four components, labeled as Si-1, Si-2, Si-3, and Si-4, respectively. Four components are fitted to the C 1*s* spectrum [shown in Fig. 1(b)], labeled as C-1, C-2, C-3, and C-4, respectively. High resolution N 1*s* spectrum is shown in Fig. 2 and can be deconvolved into two components, labeled as N-1 and N-2 respectively. High resolution O 1*s* spectrum is shown in Fig. 3 and can be deconvolved into three components, labeled as O-1, O-2, and O-3, respectively. The detailed deconvolution data of Si 2*p*, C 1*s*, N 1*s*, and O 1*s* XPS spectra of sample T600_Si are summarized in Table 3. The accuracy of the deconvolution data shown in Tables 3–6 is around 95 %.

The Si/C ratio is nearly 1 in sample T600_Si, and the percentage of Si atoms incorporated into Si-1 is nearly equal to that of C atoms incorporated into C-1 at around 64 %, and the binding energy difference between the two states is 182.9 eV, similar to what is found in references for that of tetrahedral Si–C bond [23,24], therefore, the Si-1 (FWHM= 1.5 eV) with a binding energy of 100.5 eV is assigned to Si–C bond in tetrahedral SiC and the C-1 component located at 283.4 eV is assigned to C–Si bond (FWHM= 1.3 eV) in tetrahedral SiC. The carbon peaks located at 284.4–285.6 eV are usually assigned to sp^2 and sp^3 C–C/C–H bonds [24–27]. The carbon peak located at

285.6 eV might also originate from C–O–Si/O–Si–C bonds in oxycarbide [28]. According to the results reported by Jackson and Nuzzo, the binding energy difference between sp^2 and sp^3 C–C bonds is 1.0 eV [29], therefore, the C-2 located at 284.6 eV is assigned to sp^2 hybridized C–C/C–H (FWHM= 1.5 eV) bonds, some of them might bond to Si atoms, while others might not; the C-3 is assigned to both sp^3 hybridized C–C/C–H bonds and C–O–Si/O–Si–C bonds present in oxycarbide, located at 285.6 eV with a FWHM of 1.2 eV. Correspondingly, the Si-2 (FWHM= 1.8 eV) with a binding energy of 101.0 eV is assigned to Si–C–C/Si–C–H bonds in which Si atoms bond to sp^2 C–C/C–H bonds; the Si-3, located at 102.0 eV having a FWHM of 1.6 eV, is assigned to three different bonds, including Si–O–C/O–Si–C bonds present in oxycarbide [28,29], N–Si–O bond present in oxynitride [30,31], and Si–C–C/Si–C–H bonds in which Si atoms bond to sp^3 C–C/C–H bonds. The N-1 component located at 397.9 eV (FWHM= 1.6 eV) is assigned to N–Si–O bond present in oxynitride [31,32], and the O-1 component located at 531.9 eV is assigned to O–Si–N bond present in oxynitride [33], having a FWHM of 1.0 eV; the O-2 located at 532.6 eV is assigned to Si–O–C/O–Si–C bonds present in oxycarbide [28], and it has a FWHM of 1.7 eV. The binding energy difference for stoichiometric silicon dioxide between oxidized Si 2*p* and O 1*s* levels is reported to be 429.6 eV [34], as a result, the Si-4 is assigned to Si–O bond in stoichiometric silicon dioxide, with a binding energy of 103.2 eV (FWHM= 1.4 eV); and the O-3 located at 533.0 eV is assigned to O–Si bond in stoichiometric silicon dioxide, with an FWHM of 1.8 eV. Now, there are only two tiny components left without assignment, they are N-2 and C-4. Based on the current experimental results and due to their low concentrations, it is difficult to achieve absolute assignment for these two components. If the N-2 located at 399.2 eV is assigned to sp^3 N–C bond in β -

C_3N_4 (FWHM= 1.4 eV), then the C peak from sp^3 C–N bond should occur at 287.9 eV [35,36]. The satellite sp^2 C–C peak shifts from the main sp^2 C–C peak by 2.0 eV [29], which should occur at 286.6 eV, so the presence of C-4 (FWHM= 1.6 eV) might result from the overlap of satellite sp^2 C–C and sp^3 C–N bonds. The binding energy of Si–H bond is the same as Si–Si bond located at 99.7 eV [28], and no contribution from Si–H/Si–Si bonds was identified.

Following the same deconvolution procedure used in sample T600_Si, the deconvolution of Si 2*p*, C 1*s*, N 1*s*, and O 1*s* XPS spectra (shown in Figs. 4–6) of sample T650_Si was performed and the detailed deconvolution data are listed in Table 4. The Si/C ratio in this sample was 0.88, and to make Si–C bond number equal to C–Si bond number, the percentages of Si atoms and C atoms incorporated into tetrahedral SiC were found to be 76.6 % and 67.5 % respectively.

3.3 Chemical bonding analyses conducted by XPS for a-SiC deposited on oxide covered single-crystalline Si substrate

Following the same deconvolution procedure used in sample T600_Si, the deconvolution of Si 2*p*, C 1*s*, N 1*s*, and O 1*s* XPS spectra (shown in Figs. 7–9) of sample T600_OX was performed and the detailed data are summarized in Table 5. The binding energy difference for substoichiometric silicon oxide between oxidized Si 2*p* and O 1*s* levels was reported to be 430.6 eV [34], as a result, the component Si-4 in Fig. 7(a) is assigned to Si–O bond in substoichiometric silicon oxide, with a binding energy of 103.4 eV (FWHM= 2.0 eV), and correspondingly, the O-3 located at 533.8 eV in Fig. 9 is assigned to O–Si bond in substoichiometric silicon oxide, with an FWHM of 1.6 eV.

Similarly, deconvolved high resolution Si 2*p*, C 1*s*, N 1*s*, and O 1*s* XPS spectra of sample T650_OX are shown in Figs. 10–12 and the detailed deconvolution data are summarized in Table 6.

4. Discussion

4.1 Dependence of chemical composition on deposition temperature and the choice of substrate

Comparing samples T600_Si with T650_Si, it can be seen that Si/C ratio decreased with increasing deposition temperature, and the same trend is also seen in samples T600_OX and T650_OX, indicating that Si to C ratio deviates further away from perfect stoichiometry with increasing deposition temperature regardless of the choice of substrate. The Si to C ratio in samples T600_Si and T600_OX was 0.99 and 0.91 respectively; indicating better stoichiometry was obtained for a-SiC deposited on Si substrate at a given deposition temperature of 600 °C. However, the Si to C ratios in samples T650_Si and T650_OX were very close at around 0.88. All the films are carbon rich, in contrary to what was reported by other groups [15,16], demonstrating that film composition is process dependent, though the same precursor MS was used. The oxygen atomic concentration in a-SiC deposited on Si substrate was higher than that deposited on oxide covered Si substrate at constant deposition conditions and the difference was minimized with increasing deposition temperature. The reason why such high level of oxygen contamination occurred at a deposition temperature of 600 °C is not clear yet, but raising deposition temperature did help greatly to reduce oxygen atomic concentration. The nitrogen atomic concentrations were quite close in all

samples, and slightly decreased with increasing deposition temperature and were slightly higher in a-SiC deposited on oxide covered Si substrate than those on Si substrate. Based on these results, it can be seen that the Si/C ratio and chemical composition of a-SiC depend on both deposition temperature and substrate choice, and the dependence on the latter is quite strong at a relatively lower deposition temperature of 600 °C and become negligible at a deposition temperature of 650 °C.

4.2 Dependence of chemical bonding on deposition temperature and the choice of substrate

The results from Fourier transform infrared spectra demonstrated that Si–C bonds were the dominant bonds in the deposited a-SiC films [21], with an absorption peak located at around 750 cm^{-1} , close to that of single-crystalline SiC (798 cm^{-1}). The shift was caused by the alteration in chemical bonding environment in a-SiC. XPS results were in strong agreement, showing tetrahedral Si–C bonds are the major bonds, and the fraction of Si and C atoms incorporated into tetrahedral SiC increased with increasing temperature from 64.4 and 64.1 % in sample T600_Si to 76.6 and 67.5 % in sample T650_Si, respectively, indicating higher temperature supports the formation of tetrahedral Si–C bonds. The same trend was also found in samples T600_OX and T650_OX. The fraction of carbon atoms incorporated into sp^2 C–C/C–H bond was quite similar in these four samples: it was in the range of 19.5–23.4 %, their presence indicates the network of these a-SiC does not completely follow the tetrahedral structure. Si–O bonds contributed by stoichiometric silicon dioxide were only detected in sample T600_Si rather than in sample T650_Si, demonstrating that chemical bonding changes with deposition temperature and Si–O bonds in stoichiometric silicon dioxide vanish

when oxygen atomic concentration is lower than a certain level. Comparing sample T600_OX with sample T650_OX, it can be seen that Si–O bonds in substoichiometric silicon oxide were only detected in sample T600_OX, not in sample T650_OX, again demonstrating that chemical bonding changes with deposition temperature and Si–O bonds in substoichiometric silicon oxide also vanish when oxygen atomic concentration is lower than a certain level. The general trend is that Si–O bonds gradually transformed from stoichiometric to substoichiometric silicon oxide until finally it disappears when oxygen concentration is below a certain limit. Oxynitride and oxycarbide bonds were detected in all of them.

Si–O bonds in stoichiometric silicon dioxide in sample T600_Si transform into Si–O bonds in substoichiometric silicon oxide in sample T600_OX due to the difference in oxygen atomic concentration which was believed to be caused by the difference in substrate choice. For samples T650_Si and T650_OX, no significant difference in chemical bonding was observed. These results indicate that the chemical bonding of a-SiC deposited at 600 °C depends greatly on the substrate choice, but this dependence becomes negligible when deposition temperature was raised up to 650 °C.

5. Conclusion

Amorphous SiC was deposited on both 6 in. crystalline Si and oxide covered Si substrates using MS as the single precursor in a standard LPCVD reactor at 600 and 650 °C. Based on the results from XPS analyses, strong dependence of chemical composition, Si/C ratio, and chemical bonding of deposited a-SiC on deposition temperature was found, while their dependence on the choice of substrate is very strong

at a deposition temperature of 600 °C and becomes negligible at a deposition temperature of 650 °C. Both oxygen and nitrogen atomic concentrations decreased at an elevated deposition temperature. Oxygen relative atomic concentration of a-SiC deposited on Si substrate was higher than that on oxide covered substrate and the difference minimized at an elevated deposition temperature. Nitrogen atomic concentration was slightly higher in a-SiC deposited on oxide covered substrate than that on single-crystalline Si substrate at a given deposition temperature. Stoichiometric a-SiC was deposited on crystalline Si substrate at 600 °C and other a-SiC films were slightly carbon rich in composition. The Si/C ratio deviated further away from perfect stoichiometry with increasing deposition temperature regardless of the choice of substrate. Tetrahedral Si–C bonds were found to be the dominant bonds in the deposited a-SiC films. Si–O bonds in stoichiometric silicon dioxide only occurred in a-SiC with an oxygen atomic concentration of 19.6 at. % and they transformed into Si–O bonds in substoichiometric silicon oxide with an oxygen atomic concentration of 13.5 at. %, and finally Si–O bonds from silicon oxide disappeared when oxygen atomic concentration was lower than 4.0 at. %. The fraction of Si and C atoms incorporated into tetrahedral SiC ranged from 63.8 to 77.7 %, increasing at higher deposition temperature. The presence of sp^2 C–C/C–H bond indicates the network of a-SiC does not completely follow the tetrahedral structure.

Acknowledgments

The author thanks Dr. Barry Wood, Dr. Philip Tanner, and Prof. Sima Dimitrijevic for their help in performing XPS measurements and valuable suggestions on XPS spectra deconvolution.

References

- [1] T. Blum, B. Dresler, St. Kaßner, M. Hoffman, *Surf. Coat. Technol.* 116–119 (1999) 1024.
- [2] I. Martín, M. Vetter, A. Orpella, J. Puigdollers, A. Cuevas, R. Alcubilla, *Appl. Phys. Lett.* 79 (2001) 2199.
- [3] Z. Chen, K. Prasad, C.Y. Li, P.W. Lu, S.S. Su, L.J. Tang, D. Gui, S. Balakumar, R. Shu, R. Kumar, *Appl. Phys. Lett.* 84 (2004) 2442.
- [4] S.Y. Myong, K.S. Lim, J.M. Pearce, *Appl. Phys. Lett.* 87 (2005) 193509.
- [5] W. Halverson, G.D. Vakerlis, *J. Vac. Sci. Technol. A* 10 (1992) 439.
- [6] J. Meneve, E. Dekempeneer, R. Jacobs, L. Eersels, V. Van Den Bergh, J. Smeets, *Diamond Relat. Mater.* 1 (1992) 553.
- [7] A.L. Baia Neto, S.S. Camargo Jr, R. Carius, F. Finger, W. Beyer, *Surf. Coat. Technol.* 120–121 (1999) 395.
- [8] K. Mui, D.K. Basa, F.W. Smith, R. Corderman, *Phys. Rev. B* 35 (1987) 8089.
- [9] D.K. Basa, *Phys. Stat. Solidi A* 195 (2003) 87.
- [10] B. Goldstein, C.R. Dickson, I.H. Campbell, *Appl. Phys. Lett.* 53 (1988) 2672.
- [11] Y. Oshita, *J. Cryst. Growth* 147 (1995) 111.
- [12] A. Kumbhar, S.B. Patil, S. Kumar, R. Lal, R.O. Dusane, *Thin Solid Films* 395 (2001) 244.

- [13] I.A. Yunaz, K. Hashizume, S. Miyajima, A. Yamada, M. Konagai, Sol. Energ. Mat. Sol. C. 93 (2009) 1056.
- [14] M. Lee, S.F. Bent, J. Phys. Chem. B 101 (1997) 9195.
- [15] M.J. Loboda, J.A. Seifferly, F.C. Dall, J. Vac. Sci. Technol. A 12 (1994) 90.
- [16] M.P. Delplancke, J.M. Powers, G.J. Vandesep, M. Salmeron, G.A. Somorjai, J. Vac. Sci. Technol. A 9 (1991) 450.
- [17] Z. Yu, I. Pereyra, M.N.P. Carreño, Sol. Energ. Mat. Sol. C. 66 (2001) 155.
- [18] D. Girginoudi, A. Thanailakis, J. Appl. Phys. 69 (1991) 1490.
- [19] J. Fölsch, H. Rübel, H. Schade, Appl. Phys. Lett. 61 (1992) 3029.
- [20] A.V. Iacopi, A Chemical Vapour Deposition System and Process, Australia Patent, Publication Number WO/2010/091473.
- [21] L. Wang, S. Dimitrijević, J. Han, F. Iacopi, J. Zou, J. Cryst. Growth 311 (2009) 4442.
- [22] L. Wang, S. Dimitrijević, P. Tanner, J. Zou, Appl. Phys. Lett. 94 (2009) 181909.
- [23] T. Maruyama, S. Mitani, J. Non-Cryst. Solids 319 (2003) 219.
- [24] A. Santoni, R. Frycek, P. Castrucci, M. Scarselli, M. De Cresenzi, Surf. Sci. 582 (2005) 125.
- [25] A. Avila, I. Montero, L. Galan, J.M. Ripalda, R. Levy, J. Appl. Phys. 89 (2001) 212.
- [26] S. Trusso, F. Barreca, F. Neri, J. Appl. Phys. 92 (2002) 2485.
- [27] P.W. Wang, S. Bader, L.P. Zhang, M. Ascherl, J.H. Craig Jr, Appl. Surf. Sci. 90 (1995) 413.
- [28] A.M. Wróbel, A. Walkiewicz-Pietrzykowaska, J.E. Klemberg-Sapieha, Y. Nakanishi, T. Aoki, Y. Hatanaka, Chem. Mater. 15 (2003) 1749.
- [29] S.T. Jackson, R.G. Nuzzo, Appl. Surf. Sci. 90 (1995) 195.

- [30] R.K. Brow, C.G. Pantano, J. Am. Ceram. Soc. 69 (1986) 314.
- [31] P. Hoffmann, D. Schmeißer, G. Roters, Z. Nenyai, Thin Solid Films 428 (2003) 216.
- [32] J.R. Shallenberger, D.A. Cole, S.W. Novak, J. Vac. Sci. Technol. A 17 (1999) 1086.
- [33] J. Finster, E.D. Klinkenberg, J. Heeg, W. Braun, Vac. 41 (1990) 1586.
- [34] A. Cros, R. Saoudi, G. Hollinger, C.A. Hewett, S.S. Law, J. Appl. Phys. 67 (1990) 1826.
- [35] E. D'Anna, M.L. De Giorgi, A. Luches, M. Martino, A. Perrone, A. Zocco, Thin Solid Films, 347 (1999) 72.
- [36] S. Kumar, K.S.A. Butcher, T.L. Tansley, J. Vac. Sci. Technol. A 14 (1996) 2687.

Captions for Tables

Table 1 Detailed information on sample labels for SiC films deposited on different substrates.

Table 2 The relative atomic concentrations of Si, C, N, and O, as well as Si/C ratios in samples T600_Si, T650_Si, T600_OX, and T650_OX.

Table 3 The deconvolution data of Si 2*p*, C 1*s*, N 1*s*, and O 1*s* XPS spectra of sample T600_Si.

Table 4 The deconvolution data of Si 2*p*, C 1*s*, N 1*s*, and O 1*s* XPS spectra of sample T650_Si.

Table 5 The deconvolution data of Si 2*p*, C 1*s*, N 1*s*, and O 1*s* XPS spectra of sample T600_OX.

Table 6 The deconvolution data of Si 2*p*, C 1*s*, N 1*s*, and O 1*s* XPS spectra of sample T650_OX.

Captions for Figures

Fig. 1 High resolution Si 2*p* and C 1*s* XPS spectra of sample T600_Si, detailed information on the particular Si 2*p* and C 1*s* component bands is shown in Table 3.

Fig. 2 High resolution N 1*s* XPS spectrum of sample T600_Si, detailed information on the particular N 1*s* component bands is shown in Table 3.

Fig. 3 High resolution O 1*s* XPS spectrum of sample T600_Si, detailed information on the particular O 1*s* component bands is shown in Table 3.

Fig. 4 High resolution Si 2*p* and C 1*s* XPS spectra of sample T650_Si, detailed information on the particular Si 2*p* and C 1*s* component bands is shown in Table 4.

Fig. 5 High resolution N 1*s* XPS spectrum of sample T650_Si, detailed information on the particular N 1*s* component bands is shown in Table 4.

Fig. 6 High resolution O 1*s* XPS spectrum of sample T650_Si, detailed information on the particular O 1*s* component bands is shown in Table 4.

Fig. 7 High resolution Si 2*p* and C 1*s* XPS spectra of sample T600_OX, detailed information on the particular Si 2*p* and C 1*s* component bands is shown in Table 5.

Fig. 8 High resolution N 1*s* XPS spectrum of sample T600_OX, detailed information on the particular N 1*s* component bands is shown in Table 5.

Fig. 9 High resolution O 1*s* XPS spectrum of sample T600_OX, detailed information on the particular O 1*s* component bands is shown in Table 5.

Fig. 10 High resolution Si 2*p* and C 1*s* XPS spectra of sample T650_OX, detailed information on the particular Si 2*p* and C 1*s* component bands is shown in Table 6.

Fig. 11 High resolution N 1*s* XPS spectrum of sample T650_OX, detailed information on the particular N 1*s* component bands is shown in Table 6.

Fig. 12 High resolution O 1*s* XPS spectrum of sample T650_OX, detailed information on the particular O 1*s* component bands is shown in Table 6.

Tables

Table 1 Detailed information on sample labels for SiC films deposited on different substrates.

Sample label	Deposition temperature (°C)	Deposition rate (nm/h)	Substrate	Thickness (nm)
T600_Si	600	5.0	Single-crystalline Si	50±2
T600_OX	600	5.0	Oxide covered Si	50±2
T650_Si	650	21.0	Single-crystalline Si	210±2
T650_OX	650	21.0	Oxide covered Si	210±2

Table 2 The relative atomic concentrations of Si, C, N, and O, as well as Si/C ratios in samples T600_Si, T650_Si, T600_OX, and T650_OX.

Sample label	Si (at. %)	C (at. %)	N (at. %)	O (at. %)	Si/C ratio
T600_Si	39.1	39.3	2.0	19.6	0.99
T650_Si	44.3	50.3	1.6	3.9	0.88
T600_OX	40.0	44.0	2.5	13.5	0.91
T650_OX	44.6	50.3	2.0	3.4	0.89

Table 3 The deconvolution data of Si 2*p*, C 1*s*, N 1*s*, and O 1*s* XPS spectra of sample T600_Si.

Sample label	Chemical bonding	Binding Energy (eV)	Symbols occurring in Figs. 1–3	FWHM (eV)	Percentage (%)
T600_Si	Si–C bond in tetrahedral SiC	100.5	Si-1	1.5	64.4
	Si bond to sp^2 C–C/C–H	101.0	Si-2	1.8	10.8
	Si–O–C/O–Si–C bonds in oxycarbide	102.0	Si-3	1.6	16.4
	Si bond to sp^3 C–C/C–H				
	O–Si–N bond in oxynitride				
	Si–O bond in stoichiometric silicon dioxide	103.2	Si-4	1.4	8.4
	C–Si bond in tetrahedral SiC	283.4	C-1	1.3	64.1
	sp^2 C–C/C–H bonds	284.6	C-2	1.5	20.3
	C–O–Si/C–Si–O bonds in oxycarbide	285.6	C-3	1.2	12.8
	sp^3 C–C/C–H bonds				
	sp^3 C–N bond in β -C ₃ N ₄	287.0	C-4	1.6	2.8
	sp^2 C–C/C–H bonds satellite				
	N–Si–O bond in oxynitride	397.9	N-1	1.6	70.7
	sp^3 N–C bond in β -C ₃ N ₄	399.2	N-2	1.4	29.3
	O–Si–N bond in oxynitride	531.9	O-1	1.0	29.4
	C–O–Si/O–Si–C bonds in oxycarbide	532.6	O-2	1.7	37.4
	O–Si bond in stoichiometric silicon dioxide	533.0	O-3	1.8	33.2

Table 4 The deconvolution data of Si 2*p*, C 1*s*, N 1*s*, and O 1*s* XPS spectra of sample T650_Si.

Sample label	Chemical bonding	Binding Energy (eV)	Symbols occurring in Figs. 4–6	FWHM (eV)	Percentage (%)
T650_Si	Si–C bond in tetrahedral SiC	100.4	Si-1	1.3	76.6
	Si bond to sp^2 C–C/C–H	101.0	Si-2	1.3	16.0
	Si–O–C/O–Si–C bonds in oxycarbide	102.0	Si-3	1.2	7.4
	Si bond to sp^3 C–C/C–H				
	O–Si–N bond in oxynitride				
	C–Si bond in tetrahedral SiC	283.4	C-1	1.3	67.5
	sp^2 C–C/C–H bonds	284.6	C-2	1.5	21.9
	C–O–Si/C–Si–O bonds in oxycarbide	285.6	C-3	1.2	8.6
	sp^3 C–C/C–H bonds				
	sp^3 C–N bond in β -C ₃ N ₄	287.0	C-4	1.3	2.0
	sp^2 C–C/C–H bonds satellite				
	N–Si–O bond in oxynitride	397.9	N-1	1.3	76.3
	sp^3 N–C bond in β -C ₃ N ₄	399.2	N-2	0.8	23.7
	O–Si–N bond in oxynitride	531.9	O-1	1.1	30.9
	C–O–Si/O–Si–C bonds in oxycarbide	532.6	O-2	1.6	69.1

Table 5 The deconvolution data of Si 2*p*, C 1*s*, N 1*s*, and O 1*s* XPS spectra of sample T600_OX.

Sample label	Chemical bonding	Binding Energy (eV)	Symbols occurring in Figs. 7–9	FWHM (eV)	Percentage (%)
T600_OX	Si–C bond in tetrahedral SiC	100.4	Si-1	1.4	70.2
	Si bond to sp^2 C–C/C–H	101.0	Si-2	1.4	9.2
	Si–O–C/O–Si–C bonds in oxycarbide	102.0	Si-3	1.9	16.6
	Si bond to sp^3 C–C/C–H				
	O–Si–N bond in oxynitride	103.4	Si-4	2.0	4.0
	Si–O bond in substoichiometric silicon oxide				
	C–Si bond in tetrahedral SiC	283.4	C-1	1.3	63.8
	sp^2 C–C/C–H bonds	284.6	C-2	1.6	19.5
	C–O–Si/C–Si–O bonds in oxycarbide	285.6	C-3	1.3	13.1
	sp^3 C–C/C–H bonds				
	sp^3 C–N bond in β -C ₃ N ₄	287.0	C-4	1.5	3.6
	sp^2 C–C/C–H bonds satellite				
	N–Si–O bond in oxynitride	397.9	N-1	1.3	72.7
	sp^3 N–C bond in β -C ₃ N ₄	399.2	N-2	1.3	27.3
	O–Si–N bond in oxynitride	531.9	O-1	1.3	55.3
	C–O–Si/O–Si–C bonds in oxycarbide	532.6	O-2	1.3	35.8
	O–Si bond in substoichiometric silicon oxide	533.8	O-3	1.6	8.9

Table 6 The deconvolution data of Si 2*p*, C 1*s*, N 1*s*, and O 1*s* XPS spectra of sample T650_OX.

Sample label	Chemical bonding	Binding Energy (eV)	Symbols occurring in Figs. 10–12	FWHM (eV)	Percentage (%)
T650_OX	Si–C bond in tetrahedral SiC	100.4	Si-1	1.2	77.7
	Si bond to sp^2 C–C/C–H	101.0	Si-2	1.1	20.5
	Si–O–C/O–Si–C bonds in oxycarbide	102.0	Si-3	1.0	1.8
	Si bond to sp^3 C–C/C–H				
	O–Si–N bond in oxynitride	283.4	C-1	1.3	68.7
	C–Si bond in tetrahedral SiC				
	sp^2 C–C/C–H bonds	284.6	C-2	1.6	23.4
	C–O–Si/C–Si–O bonds in oxycarbide	285.6	C-3	1.0	6.9
	sp^3 C–C/C–H bonds				
	sp^3 C–N bond in β -C ₃ N ₄	287.0	C-4	1.2	1.0
	sp^2 C–C/C–H bonds satellite				
	N–Si–O bond in oxynitride	397.9	N-1	1.7	69.1
	sp^3 N–C bond in β -C ₃ N ₄	399.4	N-2	1.6	30.9
	O–Si–N bond in oxynitride	531.9	O-1	1.1	37.3
	C–O–Si/O–Si–C bonds in oxycarbide	532.8	O-2	1.8	62.7