

Investigation of Si/SiC Ceramic Composite Properties

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Abstract: Intensive investigations are presently being carried out to study various aspects of material processing and characterization of SiC (Silicon Carbide) film structure. Although, some preliminary investigations have been undertaken to study the properties of SiC ceramics with substrate and film bulk structures, no report exists as yet on detailed thermal conduction mechanisms with considering the interface layer. The aim of the present investigation is to study the role of interface layer components on the density of ceramic, silicon and SiC/ Si (silicon carbide and silicon) interface.

Key words: Thin film • Silicon Carbide • Surface and Interface

INTRODUCTION

SiC is the only chemical compound of carbon and silicon. It was originally produced by a high temperature electro-chemical reaction of sand and carbon. It has been produced and made into grinding wheels and other abrasive products for over one hundred years. Today the material has been developed into a high quality technical grade ceramic with very good mechanical properties. It is composed of tetrahedra of carbon and silicon atoms with strong bonds in the crystal lattice [1-5]. This produces a very hard and strong material.

Moreover, the studies of electrical properties of SiC ceramics and composites have tremendous scientific significance and have been proved to be of practical interests as well. In addition, SiC is a wide band gap semiconductor characterized by high breakdown voltage, electron mobility, thermal conductivity, chemical inertness and good hardness. Its typical characteristics also include low density, high strength, good high temperature strength (Reaction bonded), oxidation resistance (Reaction bonded), excellent thermal shock resistance, high hardness and wear resistance, excellent chemical resistance, low thermal expansion and high thermal conductivity, fixed and moving turbine components, seals, bearings, pump vanes, ball valve parts, wear plates, kiln furniture, heat exchangers and semiconductor wafer processing equipment [3-6].

These unique properties of SiC have attracted great interest for the technological applications that require the production of devices able to work in extreme conditions.

Though few SiC-based devices are available today, the main problems of the SiC technology are the large cost for wafer production and the poor quality for electronic applications. In the last decade several routes [1-6] have been explored to obtain high quality 3C-SiC (cubic silicon carbide) films on silicon substrates in terms of good SiC/Si interface, low density of voids and lattice defects. All these limitations are mainly connected with the high growth temperatures (1300-1600 K), the different thermal expansion coefficient, the large lattice mismatch between SiC and Si and the large Si out diffusion from the substrate. In order to bridge the lattice mismatch and prevent silicon out diffusion, an appropriate interfacial layer, has been used for taking into account carbon atoms and the silicon surface. Indeed, they are responsible of two competitive silicon supply mechanisms, namely Si out diffusion from the substrate and Si diffusion from uncovered surface areas. Therefore, temperature and C amount are important parameters describing the ceramic nano structure with silicon voids inside the Si substrate and stoichiometric SiC formation.

THEORY AND DISCUSSION

As mentioned above, there are some key parameters which can affect the properties of silicon carbide film. We have thus studied analytically the effect of temperature on this film.

It is assumed in this study that the interaction between Si and C atoms is stoichiometric without changing the silicon carbide dimensions due to

hibrydation. Furthermore, there are no outcoming carbon and silicon atoms during ceramization. These assumptions lead us to consider an ideal dense SiC/ Si ceramic composites, so that the ceramic density is:

$$\rho_{ceramic} = \sum_i \rho_i v_i \quad (1)$$

Where ρ_i and v_i show the density and fractional volume of ceramic elements, respectively. If we suppose there are silicon carbide, silicon bulk, film surface and SiC/ Si interface, equation (1) can be given as;

$$\rho_{ceramic} = \rho_{SiC} v_{SiC} + \rho_{Si} v_{Si} + \rho_{Surface} v_{Surface} + \rho_{Interface} v_{Interface} \quad (2)$$

But the surface has two dimensional (2D) structure, meaning $v_{surface} \ll 1$, where the surface area is also small.

By noting this point, we can rewrite equation (2) as follow:

$$\rho_{ceramic} = \rho_{SiC} v_{SiC} + \rho_{Si} v_{Si} + \rho_{Interface} v_{Interface} \quad (3)$$

Now, we focus to SiC/ Si interface by considering the four layer model as shown in Fig. 1 and the bonds between silicon atoms and incoming carbon atoms.

As shown in Fig. 1 the spectrum contains four distinguished silicon components labeled based on different chemical bonding configurations and assigned them formally to Si^{+1} , Si^{+2} , Si^{+3} and Si^{+4} . We have indicated

Si^{+3}
Si^{+4}
$Si^{+1} + Si^{+2}$
Si^0

Fig. 1: Four-region model for the evolving C on Si. The near interface consists of a few atomic layers containing Si atoms in intermediate carbonization states, i.e., Si^{+1} , Si^{+2} and Si^{+3}

their peak positions in Fig. 2, but we note that positions and intensities of peaks depend on coverage, signal-to-noise ratio and deconvolution procedure. Hence Si^{+3} and Si^{+4} denote the Si atom bonded to three carbon atoms and one Si atom and the Si atom bonded to four carbon atoms, respectively. For example, the Si atom bonded to carbon atom is assumed to have a higher probability of bonding to the carbon atom than to the Si atom that is not bonded with the carbon atom. Hence, the near interface consists of a few atomic layers containing Si atoms in intermediate carbon states, i.e., Si^{+1} , Si^{+2} and Si^{+3} . The unaffected Si atoms are assigned Si^0 .

As one can see in Fig. 1 for ultrathin carbide film the interface layer consists of Si^{+1} and Si^{+2} in where from Fig. 2 and our recently works [11-12], the thickness of interface layer is so small (less than 2-3 Å). We can

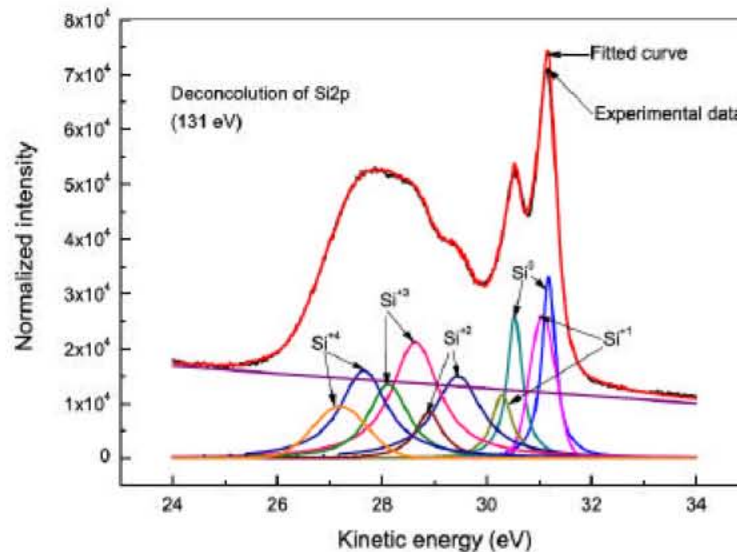


Fig. 2: Decomposition of Si 2p photoelectron spectra of Si(100) exposed to oxygen for 70 min at 500°C and to nitrogen for 10 min at 500°C [7-14].

thus neglect $v_{\text{interface}}$ in equation (2) just for ultra thin film which grown in ultra high vacuum conditions. In high vacuum conditions, we can assume that C atoms make bonds with silicon atoms wherever they meet each other. It yields a film without any pores and dimensional change during ceramization. For ideally dense duplex Si/SiC ceramic composites, the ceramic density can be given as:

$$\rho_{\text{ceramic}} = \rho_{\text{SiC}} V_{\text{SiC}} + \rho_{\text{Si}} V_{\text{Si}} = \rho_{\text{Si}} + 1.038 \rho_{\text{ceramic}} (\rho_{\text{SiC}} - \rho_{\text{Si}}) \quad (4)$$

where $V_{\text{SiC}} = (\rho_{\text{Ceramic}} M_{\text{SiC}}) / (\rho_{\text{SiC}} M_{\text{C}}) = 1.038 \rho_{\text{Ceramic}} / \rho_{\text{Ceramic}}$ and M_{C} being the density of carbon preform and molecular weight of carbon (12 g/ mole), ρ_{SiC} and M_{SiC} the density and molecular weight of SiC (40 g/ mole) respectively and ρ_{Si} the density of Si. For an average carbon density of 0.47 gm/cc, equation (4) gives a ceramic density of 2.759 gm/cc. Ignoring the presence of pores and other phases in the duplex Si/SiC ceramics, the volume % of Si and SiC-phases may be computed from the experimental density value as 67 and 33%, respectively.

It demonstrates that the role of charge transport in SiC is of important. The variation of velocity of carriers versus time. According to Mott's method [1], we can write;

$$\rho = \rho_0 T e^{\left(\frac{T_0}{T}\right)^{\gamma}} \quad (5)$$

Where the exponent γ is related to the dimensionality (d) of the system by $\gamma = (d+1)^{-1}$ relation; ρ_0 and T_0 are constants which, within the framework of Mott's model, are given by:

$$\rho_0 = (e^2 R^2 N(E_F))^{-1} \quad (6)$$

$$T_0^{-1} = N(E_F) r^3 \quad (7)$$

Where r , the radius of the polaron is a constant, $N(E_F)$ is the density of states at the Fermi level and R is the average hopping distance. The activation (EA) [15] and the hopping energies (W) are given by

$$E_A = K_B \left[\frac{d \ln\left(\frac{\rho}{T}\right)}{d\left(\frac{1}{T}\right)} \right] T^{1-\gamma} \quad (8)$$

It is clear that the Mott model is normally found applicable in-structurally or electronically-disordered systems. In Si/SiC composites, prepared through conventional route, small polaron hopping conduction describes the resistivity patterns.

CONCLUSION

The four model layer indicates that we should not neglect the interface layer for getting an accurate model in particularly, for ultrathin film. We thus suggest a new approach to correct the above equations by considering interface layer.

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