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Evolution of the crystal microstructure of hybrid SiC/Si substrates grown by the method of atomic substitution

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Abstract. 3C-SiC/Si (111) hybrid structures are grown by the method of coordinated atomic substitution on the boron- and phosphorus-doped Si(111) substrates. The evolution of the microstructure is analyzed in the time range of 1–40 minutes. The results show the reconstruction of the 3C-SiC (111) film at 3–5 minutes of the growth. The difference between strain in the SiC film obtained on *p*-Si and *n*-Si is shown using XRD and Raman techniques.

Keywords: silicon carbide, elastic strain, coordinated atomic substitution, microstructure

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Материалы конференции
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Эволюция кристаллической микроструктуры гибридных подложек SiC/Si во время роста методом замещения атомов

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Аннотация. Гибридные структуры 3C-SiC/Si выращены методом согласованного замещения атомов на подложках Si(111), легированных фосфором или бором. Эволюция микроструктуры в процессе роста анализировалась для интервала времени 1–40 минут. Результаты показывают реконструкцию пленок 3C-SiC(111) на 3–5 минуте роста. Обнаружено отличие в деформации пленки SiC на подложках Si *p*- и *n*-типов проводимости.

Ключевые слова: карбид кремния, упругие деформации, согласованное замещение атомов, микроструктура

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Introduction

A series of reviews have been published describing the method of atomic substitution [1, 2]. The method enables the growth of the epitaxial SiC films on Si interface notwithstanding the high lattice mismatch (19%). The classic methods of chemical vapour deposition (CVD) do not allow for the growth of the SiC layers with the analogous crystalline quality [3]. In accord with [1, 2], the typical hybrid SiC/Si structure grown by the method of atomic substitution consists of 100 nm of the SiC film, 1–5 um of the macroporous silicon and the Si substrate.

The evolution of the Si microstructure during the substitution of the Si atoms has been studied by different methods [1–3]. In situ measurements of the reflection of 650nm laser beam show the rapid formation of the rough interface layer at the beginning of the process. This happens due to the simultaneous formation of the SiC film with the contraction pore after 14–320 seconds of the growth [1]. Then the reflectivity gradually increases with time and the SiC film becomes smoother. The interim stages of the synthesis of the hybrid SiC/Si structures are analysed by the x-ray diffraction (XRD) and total reflection methods [3]. It is shown that the evolution of the structure is influenced by the temperature, pressure in the reactor and a substrate orientation. The great change of the strain occurs in the SiC film during growth. Namely, the tensile to compressive strain replacement happens at 10-12 minutes of the process. However, the hybrid SiC/Si structures in [3] are obtained without SiH_4 in the reaction zone. It is shown in [1] that SiH4 'heals' the contraction pores, which modify the evolution of the microstructure in the growth process. Despite that, the SiC film morphology and elastic stresses are influenced by the conductivity of the Si substrate [4].

The aim of this work is to trace the evolution of the elastic strain occurring in 3C-SiC(111) film during growth by the method of atomic substitution. The hybrid 3C-SiC(111)/Si(111) structures are grown in the mixture of CO and SiH_4 gases. The Si(111) substrates with different types of conductivity are used. The structures are analyzed by XRD and Raman techniques. The optimum growth time for the formation of the 3C-SiC films on Si(111) substrate is suggested.

Materials and Methods

The growth of the SiC layer is carried out on the *p*- and *n*-type 1.5" Si(111) substrates with the resistance 50 Ω·cm and >10 Ω·cm respectively. The wafers are terminated by hydrogen in alkaline solutions with the purpose of the pre-growth passivation of the surface [5]. The synthesis of SiC is provided at a temperature of 1270 °C and a pressure of 360 Pa. The gas mixture CO/SiH_4 is used with a flow ratio of 20/1. The growth is carried out during 1, 3, 5 and 40 minutes. The samples are studied by XRD and Raman techniques. The XRD results show the presence of compressive deformations in the SiC film, which depends on the growth time.

XRD analysis

XRD spectra of the hybrid SiC/Si structures are measured using Bruker advance d8 (Fig. 1, a). The spectra show the following peaks Si(111) at $2\theta = 28.5°$, SiC(111) at $2\theta = 35.6°$, Si(222) at $2\theta = 59°$. The splitting of the Si(222) peak can be explained by the diffraction of CuKα1 and CuKα2 lines.

The SiC(220) peak is clearly seen only for 40 minutes of the growth, which confirms that the SiC film consists only of the SiC(111) layers of perfect crystalline quality (Fig. 1, *b*).

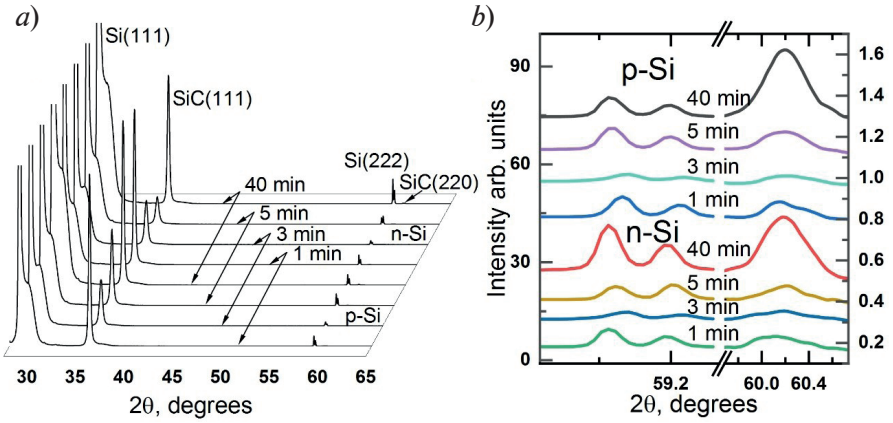

Fig. 1. XRD spectra of the 3C-SiC(111)/Si(111) substrates grown by the method of atomic substitution on *p*- and *n*-Si(111) substrates measured by Bruker advance d8 (*a*); the Si(222) and SiC(220) peaks from the spectra (*b*)

The amplitude of the SiC(220) peak is about two hundreds of times smaller than SiC(111). The elastic deformations are calculated from the positions of the 3C-SiC(111) peaks on the rocking curve ω - 2θ. The spectra are shown in the figure 2. The peaks parameters are written in the table 1. FWHM of the peaks is small for 1 and 40 minutes of the growth, which does not depend on substrate conductivity. The difference between FWHM for the interim growth time is seen, which relates to the quality of the layer. The elastic strain is less compressive for the *n*-Si substrates.

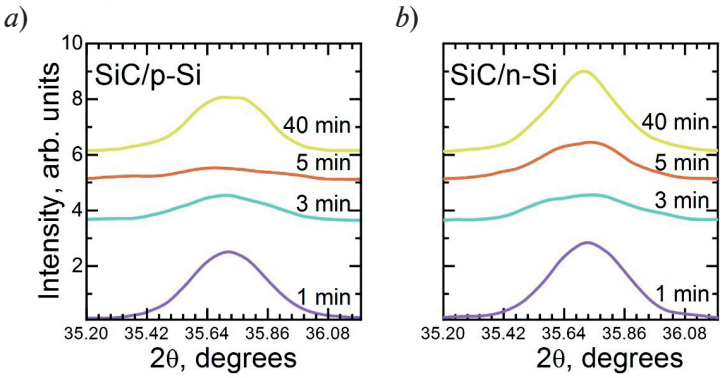

Fig. 2. XRD ω - 2θ spectra of the hybrid 3C-SiC(111)/Si (111) substrates at 3C-SiC(111) peak for the different growth times on (*a*) boron- and (*b*) phosphorus-doped silicon substrates obtained by DRON-8

Table 1

The parameters of the 3C-SiC (111) XRD peaks and related strain and stress

Time, min	2θ, degrees	FWHM, arcmin	ε
p-Si substrate			
1	35.726	16.250	-2.3×10^{-3}
3	35.721	23.491	-2.2×10^{-3}
5	35.707	18.464	-1.8×10^{-3}
40	35.710	15.156	-1.9×10^{-3}
n-Si substrate			
1	35.722	16.252	-2.2×10^{-3}
3	35.701	19.926	-1.6×10^{-3}
5	35.685	38.909	-1.2×10^{-3}
40	35.708	16.971	-1.8×10^{-3}

The theory of the method of atomic substitution declares that the SiC films are compressed at the time, when SiC and the contraction pore nucleate. This happens due to the conjugation of 5 elementary cells of 3C-SiC(111) and 4 cells of Si(111) via the formation of the intermediate structures. It was suggested that the intermediate structures emerging during the growth possess the donor-like properties [4]. Consequently, the emerging becomes harder on the *n*-type Si substrates than on *p*-Si. However, the transformation of the intermediate structures into SiC is faster for *n*-Si and the resulting film becomes less stressed. It should be noted that if SiH_4 is not used in the reaction zone, then the tense SiC film forms in the first 10 minutes of the growth [4].

In the end, the 3C-SiC(111) films obtained after 1 minute of the growth have a big intensity of the SiC(111) peaks and small FWHM for the both substrate types. Stress values in the SiC films obtained after 1 minute of growth correspond to those obtained after 40 minutes.

Raman analysis

The Raman spectra of the hybrid SiC/Si (111) structures grown by the method of atomic substitution on the Si(111) substrates are analysed. The following results are obtained. First, the SiC film consists of only cubic polytype as expected from XRD. Second, the spectra are different for the SiC film "hanging" on the contraction pore and at the SiC/Si contact (figures 3, *a* and *b*). At the pore area, the intensity of Si lines decreases (520cm^{-1}) and the intensity of the SiC line increases (figure 3, *c* and *d*). These results are explained by the multiple internal reflections of the wave inside the pore [6].

The next model is used to calculate effective strain from the positions of the TO peaks [7].

$$\varepsilon_e = \frac{\Delta a}{a} = \frac{\left(796.5 - E_c\right)}{3734}, \tag{1}$$

where $\Delta a/a$ is the elastic strain, E_c is the peak position for the SiC film.

The peak positions at the centre and the edge of the pore differ by 1 cm^{-1}. Despite that, the effective strain is smaller for the *n*-Si substrates than for *p*-Si (table 2), which is consistent with the results from the XRD measurements. The results show the change in the strain during SiC formation at the third minute of the growth.

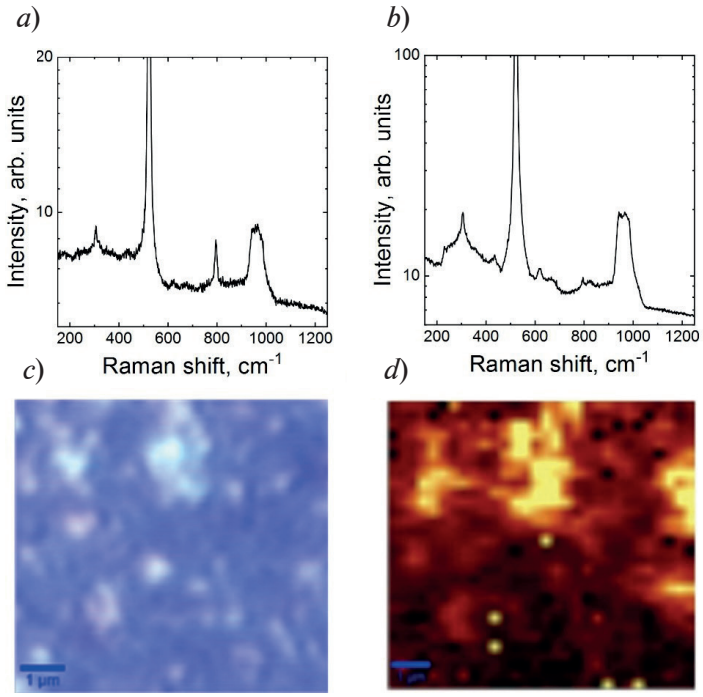

Fig. 3. The Raman spectra measured at the centre of the contraction pore area (*a*) and at the edge of the pore (*b*), micrograph of the hybrid SiC/Si (111) substrate (*c*), map of the intensity of the SiC TO-mode measured at the micrographs area (*d*); light places correspond to the high intensity of the line

Table 2

The positions of the SiC TO Raman peaks and related strain calculated in the frame of the model [7]

Time, min	Peak position, cm^{-1}	ε_e
	p-Si substrate	
1	793.1	9.2×10^{-4}
3	790.9	1.5×10^{-3}
5	793.2	8.9×10^{-4}
40	793.2	8.9×10^{-4}
	n-Si substrate	
1	794.1	6.3×10^{-4}
3	794.7	4.9×10^{-4}
5	794.2	6.1×10^{-4}
40	793.4	8.2×10^{-4}

Conclusion

The 3C-SiC/Si(111) hybrid substrates are grown by the method of atomic substitution and analyяed using XRD and Raman techniques. XRD shows that the strain in the SiC films are different for 1, 3, 5 and 40 minutes of the growth. The strain is compressive, which is the consequence of the presence of SiH_4 in the reaction zone. Raman spectra show that the strain in the SiC film is not uniformly distributed across the pore area. SiC film stretches at the region of the contact with the Si surface. The difference between the effective strain in the SiC film obtained on *n*-Si and *p*-Si substrates is demonstrated.

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