Elastic properties of porous silicon layer of hybrid SiC/Si substrates

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Abstract. Elastic properties of porous silicon layer of hybrid SiC/Si substrates grown by the atomic substitution method are investigated. The feature of the growth method is the formation of the macroporous silicon layer at the SiC/Si interface during growth. The elastic properties of the layer are studied using the finite element method. The biaxial modulus of the porous silicon is obtained as a function of porosity considering the different shape of the pores and presence of thin SiC boundary layer. The presence of the pores in the silicon layer adjacent to SiC results in the decrease of the elastic moduli by about 35%. However, this leads to a negligibly small change of the substrate curvature.

1. Introduction

Epitaxial silicon carbide thin films synthesized on silicon substrates by the atomic substitution method enable the growth of crack-free thick AlN, GaN and AlGaN layers using HVPE technique [1]. Mentioned wide gap semiconductors are widely used for optoelectronic devices, HEMT transistors, GaN power electronics, etc. Defect formation and the growth mechanism of AlGaN films are influenced by the residual mechanical stress in the hybrid SiC/Si substrate. The latter contains a porous silicon layer that emerged during SiC growth by the method of atomic substitution. There have been relatively few works regarding the stress relaxation mechanisms in the SiC/Si-porous/Si substrates. Telyatnik et al. [2] estimated the residual mechanical strain in the SiC layer (about 1.7×10⁻³ that corresponds to the stress about 1 GPa) using the dependence of the substrate curvature on temperature. Also, different mechanisms of stress relaxation in AlN/SiC/Si were investigated in [2]. However, the real structure of porous silicon was not considered.

Osipov [3] analyzed the SiC/Si interface using UV ellipsometry. It is found that the structure of the hybrid SiC/Si(111) substrate obtained at 1250°C after 15 min of annealing of Si(111) in the CO atmosphere contains a Si-porous layer having ~20% of porosity and ~100 nm of 3C-SiC(111) film. The cubic polytype of SiC is predominantly formed under this condition. The porosity is determined in the frame of Bruggeman’s effective medium approximation. The thickness of the porous layer is clearly seen from the SEM micrographs and equals about 2-4μm having the structure of dendritic cavities with a thin SiC boundary layer [4]. Consequently, the model geometry of the structure contains Si(111) wafer (400μm), porous-Si layer (4μm), 3C-SiC film (100nm). Elastic constants of Si wafer and SiC film are known both in cases of monocrystal and polycrystal [5, 6]. The elastic constants of the porous silicon layer were estimated as a function of porosity using the model of spherical pores in [7]. This report continues the investigation of the porous silicon layer considering the octahedral form of the pores and the presence of a thin SiC layer on the surface of pores. Also, the stress relaxation mechanism in the SiC layer is suggested.
2. Dependence of biaxial modulus on porosity

The calculation of elastic tensor of porous Si is performed by the finite element method (FEM) using Comsol Multiphysics software (Cell Periodicity node) [7]. The method is based on the prescribed deformation of the opposite faces of representative volume element (RVE), three normal and three shear traction components. The six strains are set on the opposite boundaries of RVE successively accounting the periodic displacement boundary condition (PDBC).

\[ u_1(r_1) = u_2(r_2) + \varepsilon_0(r_1 - r_2) \]  

(1)

where \( u_1(r_1) \) and \( u_2(r_2) \) are the displacements of the opposite faces of RVE, \( H = r_1 - r_2 \) is the characteristic size of RVE geometry, \( \varepsilon_0 \) is the prescribed deformation tensor. Combination of principal of virtual work with PDBC enables calculation of the displacement field over the RVE [8].

The elastic tensor \( \mathbf{C} \) of the heterogeneous material is obtained from the Hook’s law using homogenization approach.

\[ \mathbf{\sigma} = \mathbf{C} \times \mathbf{\varepsilon} \]  

(2)

where \( \mathbf{\sigma} = \{\sigma_{11}; \sigma_{22}; \sigma_{33}; \sigma_{12}; \sigma_{23}; \sigma_{13}\} \) and \( \mathbf{\varepsilon} \) are the stress and deformation tensors correspondingly obtained by averaging over the volume of RVE. The method enables the independent calculation of components of the elastic tensor.

RVE of the porous silicon is represented in the form of a cube with pores added to the structure (see figure 1). In this work, the octahedral pores having boundaries in (111) plane and spherical pores are considered. The pores have fixed characteristic size \( R \), which is the height of the half of the regular octahedron and the radius of the pores for the spherical ones. The spherical pores have a thin SiC boundary layer. The positions of the pores are randomly chosen and generated at least 10 times to minimize statistical fluctuations.

![Figure 1](image.png)

Figure 1. The geometries of the model for the form of the pores of regular octahedron (a) and of the spheres with SiC/R=0.04 (b).

The three types of errors are minimized during computation: the finite size effect, discretization error, and statistical fluctuations. The characteristic size of the system should be large enough to describe the properties of homogeneous material. The optimization via H/R parameter for the fixed R=0.25 \( \mu \text{m} \) is carried out using calculation of elastic constants. The procedure shows less than 2% deviation from the converged value for H/R greater than 6 in the case of spherical pores and greater than 4 in the case of octahedral pores. The second source of errors is analyzed via decreasing the size of the maximum partitioning element \( \Delta \) having constant relation to the minimum element equals to 5.56. It was shown that the variation of \( \Delta/H \) in the range from 0.05 to 0.45 leads to less than 2% deviation from the average value within the range. The partitioning elements for the discretization are tetrahedra. The remaining parameters for the discretization in Comsol are the resolution of narrow
regions (0.5), the curvature factor (0.6) and the maximum element growth rate (1.5). The statistical fluctuations for every calculated elastic constant lead to less than 3% of standard deviation.

The calculation shows three independent constants of the elastic tensor \((C_{11}, C_{12}, C_{44})\) for the porous silicon. The dependence of biaxial modulus in the \([111]\) direction \(M_{\{111\}}\) on the porosity of porous silicon layer is shown in figure 2. \(M_{\{111\}}\) obtained for the model with octahedral pores is slightly lower than that of the spherical form (filled circles and daggers respectively [7]). Solid lines show the linear approximation of the results, namely \(M_{\{111\}}=229.7-282.6\times\varphi\) in the case of octahedra. The value of \(M_{\{111\}}\) increases with the thickness of SiC layer \(t_{\text{SiC}}\). The results calculated with \(t_{\text{SiC}}/R=0.04\) and 0.12 are shown by the circles. It is seen from SEM that the \(t_{\text{SiC}}/R\) is less than 0.04 for the most part of the porous silicon layer, which allows us to omit the influence of SiC boundary layer [4]. The calculated value of Young modulus of porous silicon with octahedral form of the pores for 30% of porosity \(E_{\{111\}}=119\ \text{GPa}\) is consistent with the experimental data \(E_{\{111\}}=110\ \text{GPa}\) [9].

Figure 2 shows \(M_{\{111\}}\) to be close to silicon value in the case of \(t_{\text{SiC}}/R=0.12\). Ellipsometry and Auger electron spectroscopy show the layer to be adjusted to SiC film at the SiC/Si interface for the different polytypes of SiC [3,10]. The dependence of elastic constants on the porosity for each geometry is shown in table 1. Monocrystalline and polycrystalline elastic constants are considered for the thin SiC layer.

Table 1. The dependence of the elastic constants of the porous silicon on the porosity \(\varphi\).

|                | C11              | C12              | C44              |
|----------------|------------------|------------------|------------------|
| Octahedra      | 166-195.4×\varphi| 64.6-85×\varphi  | 79.5-96×\varphi  |
| \(t_{\text{SiC}}/R\) | \(0.04\)         | \(0.12\)         | \(0.28\)         |
| Monocrystalline 3C-SiC: \(C11=395\ \text{GPa}, C12=132\ \text{GPa}, C44=236\ \text{GPa}\) [6] |
| \(t_{\text{SiC}}/R\) | \(0.04\)         | \(0.12\)         | \(0.28\)         |
| Polycrystalline SiC: \(C11=500\ \text{GPa}, C33=535\ \text{GPa}, C44=165\ \text{GPa}, C66=210\ \text{GPa}, C13=50\ \text{GPa}\) [6] |
| \(t_{\text{SiC}}/R\) | \(0.04\)         | \(0.12\)         | \(0.28\)         |

Figure 2. \(M_{\{111\}}\) Dependence on the porosity of porous silicon. Filled circles depict the case of the octahedra. Dashed lines show the linear extrapolation of \(M_{\{111\}}\) to 30% of porosity for \(t_{\text{SiC}}/R=0.04\) and 0.12 in the case of monocrystalline SiC. The data obtained in the case of spherical pores is shown by daggers [7].
3. Stress relaxation in the SiC film
Using density functional method, Kukushkin et al. [11] have shown that the 3C-SiC/Si(111) interface is the conjugation of 5 elementary cells of 3C-SiC(111) and 4 cells of Si(111). Such configuration corresponds to the minimum energy of the system. This feature of the structure grown by the atomic substitution method greatly decreases the lattice mismatch leading to a compressive strain of SiC film to $|\varepsilon_m|=0.34\%$.

The influence of the porous layer has been analyzed using FEM. The lateral component of the stress tensor in the SiC film is investigated. The following relaxation mechanisms are considered: the reduction of the elastic moduli of the porous silicon layer; the folding of the 3C-SiC(111) film; the bending of the substrate. The geometry of the model to be analyzed: 400um of the Si substrate, 4um of the Si-porous layer and 100 nm of the SiC film. The stress in the SiC film for $|\varepsilon_m|=0.34\%$ equals to 1.97 GPa. The reduction of the elastic moduli of the porous silicon layer leads to less than 1% of relaxation of the stress. Moreover, the contact surface decrease shows about 1% of the relaxation. The latter has been studied via adding the ring-shaped cavities under the surface of 3C-SiC(111) film. The curvature influence is considered during FEM calculation.

4. Conclusion
The dependence of elastic constants of the porous silicon on the porosity is analyzed using FEM. It was found that the porosity reduces the elastic moduli of the porous silicon by about 35%. However, the presence of the porous layer at the SiC/Si interface decreases the stress in the SiC film by less than 1%. The obtained value of the Young modulus of porous layer is consistent with experimental data.

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