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# The Optical Properties, Energy Band Structure, and Interfacial Conductance of a 3C-SiC(111)/Si(111) Heterostructure Grown by the Method of Atomic Substitution

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**Abstract**—Epitaxial films of single-crystalline silicon carbide (3C-SiC cubic polytype) with 20- to 120-nm thickness grown on a silicon substrate by the method of atomic substitution have been studied by the spectroscopic ellipsometry technique at 0.5–9.3 eV photon energies. It is established that the dielectric permittivity of a thin intermediate layer formed at the 3C-SiC(111)/Si(111) interface is characteristic of a semimetal. This result was confirmed by quantum-chemical simulation of the properties of 3C-SiC(111)/Si(111) heterointerface, showing that the conductance of this intermediate layer is related to *p*-electrons of interfacial Si atoms that are most remote from Si atoms of the substrate.

**Keywords:** silicon carbide, heterostructures, interface, dielectric permittivity, ellipsometry, semimetals.

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In recent years, we have developed a method [1, 2] for synthesis of single-crystalline silicon carbide (SiC) in a near-surface layer of silicon substrate due to consistent substitution of Si atoms by C atoms via the chemical reaction between silicon single crystal and carbon monoxide (CO). A detailed description of processes involved in the growth of SiC by the method of atomic substitution was presented in [1, 2], where it was shown that the mechanism of consistent atomic substitution retained the structure of the initial cubic Si lattice that ensured growth of the cubic 3C-SiC polytype. This fact has also been confirmed by electron-microscopic investigations [3] indicating that lattice misfit dislocations at the SiC(111)/Si(111) interface were absent and, instead, stacking faults with hexagonal phase spacers appeared. These data showed a principal difference between the mechanism of SiC film growth via atomic substitution and their growth by other methods, e.g., chemical vapor deposition (CVD) [4].

The present work was aimed at studying optical properties of the 3C-SiC(111)/Si(111) heterostructure interface by spectroscopic ellipsometry at 0.5–9.3 eV and by means of quantum chemistry simulations.

SiC films were grown on Si(111) substrates using a technology of consistent atomic substitution as described in detail in review [1]. The as-grown 3C-SiC films had thicknesses within 20–120 nm. X-ray diffraction (XRD) patterns of 3C-SiC(111)/Si(111) heterostructures only exhibited reflections corresponding to ⟨111⟩ direction, such as Si(111), Si(222), 3C-SiC(111), and 3C-SiC(222). The absence of other reflections is an evidence of directional 3C-SiC epitaxy along ⟨111⟩ axis. The as-grown 3C-SiC(111)/Si(111) samples of various thicknesses were studied using spectroscopic ellipsometry for measuring pseudodielectric permittivity as a function of the photon energy on a J.A. Woollam VUV-WASE instrument in the range of 0.5–9.3 eV. The results of ellipsometric simulation of spectral data showed that they were poorly described by the classical ellipsometric model based on the effective medium approximation (EMA) [5], particularly in the range of photon energies below 3.3 eV. The Bruggeman medium model yields the following relation for determining effective dielectric permittivity $\varepsilon_{\text{eff}}$ of a mixture:

$$\sum_i \delta_i \frac{\varepsilon_i - \varepsilon_{\text{eff}}}{\varepsilon_i + 2\varepsilon_{\text{eff}}} = 0, \tag{1}$$

where $i$ is the number of phase in the model mixture, $\varepsilon_i$ is the permittivity of the $i$th phase, and $\delta_i$ is its volume fraction. EMA model (1) usually well describes the interfacial layers formed at the interface of two media and serves a basis for the interpretation of ellipsometric data [5]. In particular, the EMA provides excellent description of 3C-SiC(111) epilayers grown by CVD on Si(111) substrates.

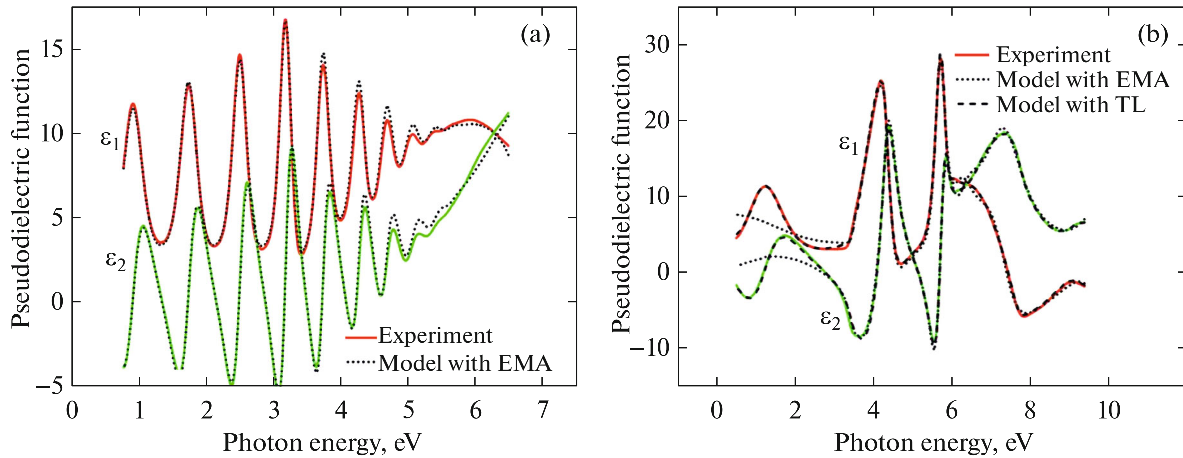


**Fig. 1.** Ellipsometric spectra of 3C-SiC(111)/Si(111) heterostructures (a) obtained by CVD by Advanced Epi Co. (with an interface containing misfit dislocations) and (b) grown in this work by method of consistent atomic substitution (with the interface free of misfit dislocations). EMA model (1) adequately describes experimental data only in the former case.

Figure 1 presents ellipsometric spectra of the 3C-SiC(111)/Si(111) heterostructures (a) obtained by the patented CVD technology of Advanced Epi Co. with a sample thickness of ~300 nm and (b) grown in this work by method of consistent atomic substitution (with a sample thickness of ~50 nm). As can be seen in the former case, a simple one-layer ellipsometric model [5] (comprising a Si substrate/interface/SiC film) using the EMA on SiC/Si boundary gives excellent results (Fig. 1a). In the latter case, the same EMA model poorly described the region of photon energies below 3.3 eV (Fig. 1b). Since the energy of 3.3 eV approximately corresponds to the first sharp peak in the real part of the dielectric permittivity of Si, it is natural to suggest that (since SiC is transparent in this spectral range) there are problems in description of dielectric function at the interface. In other words, the contribution of Si in formula (1) does not correspond to experiment. The contribution of SiC is less significant, since it is transparent almost up to 5.5 eV. To obtain an adequate description of the dependence of dielectric function at the 3C-SiC(111)/Si(111) interface on the photon energy, we used the method of spline approximation [5] and concluded that this dependence was best described with the aid of the Tauc–Lorentz (TL) approximation [6]:

$$\varepsilon_2(E) = \begin{cases} \dfrac{1}{E}\dfrac{AE_0C(E-E_g)^2}{(E^2-E_0^2)^2+C^2E^2}, & E > E_g, \\ 0, & E \le E_g. \end{cases} \quad (2)$$

Here, $E$ is the photon energy, $\varepsilon_2$ is the imaginary part of permittivity (real part is calculated using the Kramers–Kronig relation [6]), $E_g$ is the bandgap width, and $E_0$, $A$, and $C$ are the oscillator peak position, amplitude, and halfwidth, respectively. Thus, the ellipsometric spectra of 3C-SiC(111)/Si(111) heterostructures obtained by method of atomic substitution are described here using a modified single-layer model (comprising Si substrate/interface/SiC layer/roughness) in which the dielectric permittivity of interface is described using a TL oscillator (2).

Minimization of the difference between the measured and theoretical ellipsometric spectra can be used for determining the parameters of the model, including the SiC layer thickness, roughness, interfacial layer thickness, and the values of $A$, $E_0$, $C$, and $E_g$ in Eq. (2). This modified model has a 2.5- to 5-times-lower mean-square error as compared to that of the EMA model and provides better description of the experimental data (Fig. 1b). The typical value of the interfacial layer thickness in this model is 2 nm, and its dielectric function calculated for 3C-SiC(111)/Si(111) sample (Fig. 1b) is presented in Fig. 2. It should be noted that the bandgap width in all obtained 3C-SiC(111)/Si(111) samples is either zero (as in Fig. 2) or very small (<0.5 eV), which allows this interfacial layer to be treated as a semimetal. Approximation of the asymptotic behavior of $\varepsilon_2$ at large photon energies in terms of the Drude model [7] (Fig. 2) shows that the interfacial layer has a resistivity of $4 \times 10^{-7}$ Ω m and a characteristic carrier scattering time of $4 \times 10^{-16}$ s (i.e., about half as small as that in lead).

For purposes of comparison, the 3C-SiC(111)/Si(111) interface was theoretically described and its properties were calculated by methods of quantum chemistry. The energy of the 3C-SiC(111)/Si(111) system was calculated in the framework of the density functional theory and used to find the optimum atomic configuration corresponding to minimum energy. This task was performed using the Medea-VASP program package [8] with VASP for energy minimization using the PBE functional [9], pseudopotentials, and plane-wave basis set with the cutoff energy selected at 400 eV. The properties of interface were

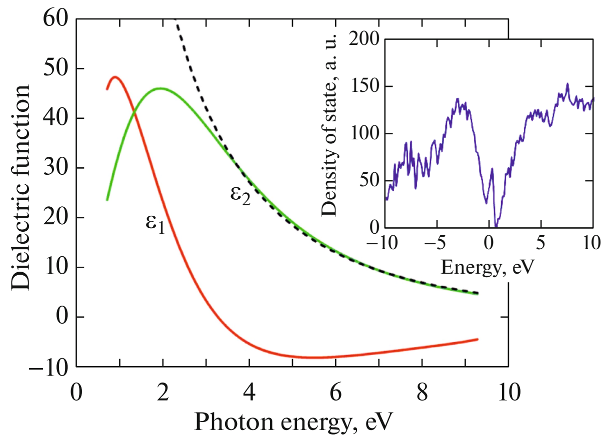


**Fig. 2.** Energy dependence of the dielectric permittivity of a dislocation-free interfacial layer between Si(111) and SiC(111). The dashed curve describes the Drude model for a medium with resistivity $4 \times 10^{-7}$ Ω m and characteristic carrier scattering time $4 \times 10^{-16}$ s. The inset shows the density of electron states in the interfacial layer as a function of the photon energy (for the Fermi energy of 0 eV).

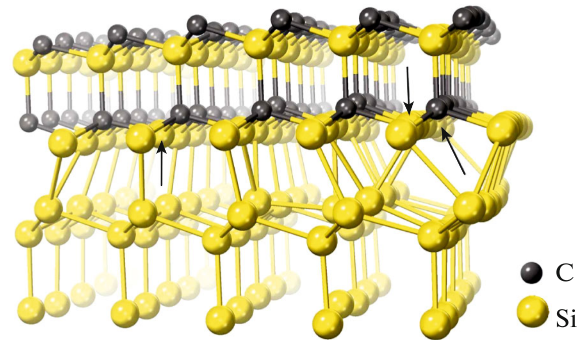


**Fig. 3.** Atomic configuration of the dislocation-free 3C-SiC(111)/Si(111) interface at minimum energy. Arrows indicate three Si atoms (of the total 25) not forming bonds with atoms of the substrate. *p*-electrons of these atoms make the determining contribution to the narrow peak of DOS observed at the Fermi energy (see the inset to Fig. 2).

analyzed taking into account the contacts of the Si(111) substrate with both Si- and C-faces of SiC(111) phase. The results of quantum-chemical simulations allowed us to establish three main properties of the system under consideration.

(i) A Si(111) substrate produces almost no deformation of SiC, and the latter attracts 1 of 16 Si atoms occurring in the lower of the two layers of Si(111) bilayer, thus modifying the near-surface Si layer (Fig. 3). That is, the Si atom passes from the lower to upper layer of the Si(111) bilayer and forms a bond with the attracting Si layer of SiC (Fig. 3).

(ii) The interfacial atomic configuration corresponds to $P_3m_1$ symmetry.

(iii) The bandgap width in the interface decreases to almost zero. The energy band structure of this system as depicted in Fig. 3 was calculated using SCAM functional [10]. These calculations showed that the conduction band penetrated by several $10^{-2}$ eV into the valence band. In other words, the interface behaves as a semimetal between two semiconductors.

The inset to Fig. 2 shows a plot of the electron density of states versus energy (for a Fermi energy of 0 eV). As can be seen, there is a sharp DOS peak near the Fermi energy that accounts for the unusual electrical and optical properties of this system. Analysis shows that this DOS peak is related to three *p*-Si atoms (12% of the total 25) in the SiC at the boundary with the Si substrate (indicated by arrows in Fig. 3) are furthest from (and do not form chemical bonds with) the Si atoms of the substrate. Each of these 12% of Si atoms at the interface has one unsaturated bond, which leads eventually to semimetallic properties of the 3C-SiC(111)/Si(111) interface.

Thus, it has been established that the interface of 3C-SiC(111)/Si(111) heterostructure grown by the method of consistent atomic substitution exhibits unusual electrical and optical properties characteristic of a semimetal (Fig. 2) rather than a semiconductor. The interfacial layer medium has a resistivity estimated at $4 \times 10^{-7}$ Ω m and the characteristic carrier scattering time estimated at $4 \times 10^{-16}$ s.

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## CONFLICT OF INTEREST

The authors declare that they have no conflict of interest.

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