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Spintronic properties of the interface between Si(111) and 3C-SiC(111) grown by the method of coordinated substitution of atoms

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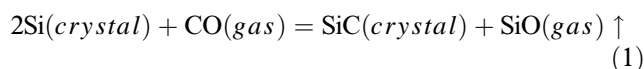
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The properties of the interface between Si(111) and 3C-SiC(111) grown by the method of coordinated substitution of atoms were studied by the density functional theory in spin-polarized approximation. The most favourable atomic configuration at the interface was found. It is shown that SiC faces Si with the carbon plane, and SiC separates 3 Si atoms out of 16 from the second layer of substrate atoms. As a result, the 3 Si atoms in the substrate each have 3 bonds instead of 4, and the 3 C atoms in the bottom layer of the SiC film also have 3 bonds. It is these atoms that have a magnetic moment due to the unpaired *p*-electrons. It was found that for the electron with spin „majority“ this interface is an ordinary semiconductor, and for the electron with spin „minority“ it is a two-dimensional ferromagnetic metal.

Keywords: silicon carbide, ferromagnetic semi-metals, terahertz radiation, density functional theory, spintronics.

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Silicon carbide (SiC) is one of the most promising wide-gap semiconductors [1–3], since its mechanical, electrical, and thermophysical parameters are close to record-high ones. Since the use of SiC in tried-and-tested silicon electronics is considered to be highly relevant [4], the methods of its epitaxial growth on silicon are of prime importance [1]. The epitaxial growth of SiC on Si via a coordinated substitution of one half of Si atoms with C atoms (method of coordinated substitution of atoms, MCSA) [5] with no lattice mismatch dislocations provides very high-quality SiC films; therefore, this method fairly promising. The substitution is „coordinated“ in the sense that the removal of a Si atom from the lattice and the incorporation of a C atom into a vacated site in reaction



are concurrent [5]. An oxygen atom acts as catalyst of the substitution reaction. The transition state of reaction (1), which corresponds to the maximum energy along the reaction path, is an almost equilateral triangle with Si, C, and O atoms at its vertices [6]. Having crossed this barrier (1.2 eV in height), a SiO molecule escapes from the system. This coordinated substitution mechanism preserves the initial cubic lattice structure of Si, thus ensuring the growth of a cubic 3C-SiC polytype [5]. Such a substitution may be performed on a Si surface of any orientation, but an especially high Si/SiC interface quality is obtained on a (111) surface. The results of numerous microscopic studies revealed that 3C-SiC(111)/Si(111) interfaces formed by MCSA do not contain lattice mismatch dislocations [5,7], since five 3C-SiC cells match almost perfectly with four Si cells. The only observed defects are various stacking

faults (specifically, twins [5]). This constitutes a fundamental distinction between MCSA and traditional growth techniques, such as chemical vapor deposition (CVD), which is characterized by the formation of multiple lattice mismatch dislocations [1].

Further experimental studies demonstrated that an MCSA 3C-SiC(111)/Si(111) interface features anomalous magnetic properties [8] that may be utilized both for absorption and for emission of electromagnetic waves in the terahertz range [8,9]. In addition, particular features of the longitudinal electrical resistance of this system were found at the same temperatures as those corresponding to thermal capacity jumps [9]. This was interpreted in [9] as phase transitions in the electron subsystem. All these experimental results need to be substantiated theoretically. With this aim in view, the MCSA 3C-SiC(111)/Si(111) interface properties are characterized in the present study using the density functional theory [10] within the spin-polarized approximation [10,11], which allows one to reveal and examine the magnetic properties of a system.

In order to characterize the properties of the 3C-SiC(111)/Si(111) interface, one first needs to determine the geometric configuration of atoms corresponding to the energy minimum (with the magnetic field contribution factored in). The energy of the system was calculated using the density functional theory with the PBE functional [12] within the spin-polarized approximation [11]. The MedeA-Vasp [13] package, which utilizes pseudopotentials and the plane wave basis, was used to determine the energy. PAW (projector augmented wave) pseudopotentials [13] were applied in all calculations; the wave cutoff energy was 400 eV. A Monkhorst–Pack *k*-point mesh in the reciprocal space

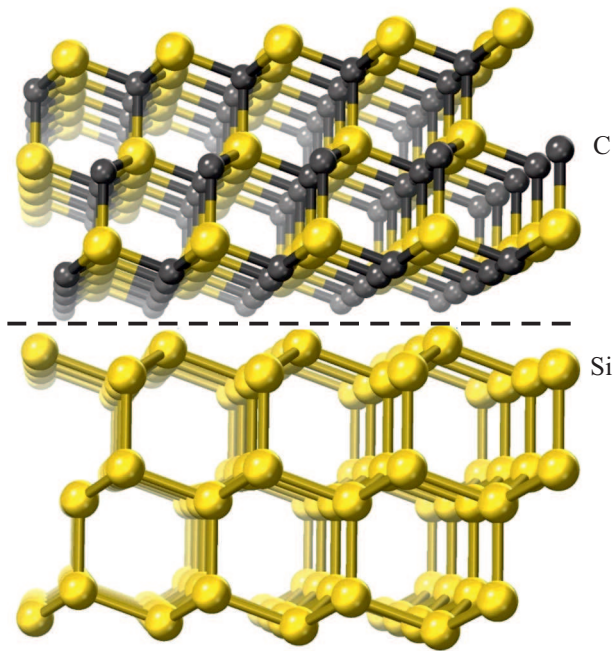


Figure 1. Initial configuration of atoms: a SiC cluster $15.39 \times 15.39 \times 7.551 \text{ \AA}$ size, which contains 75 Si atoms and 75 C atoms, is located far from a Si cluster $15.39 \times 15.39 \times 9.407 \text{ \AA}$ size, which contains 96 atoms.

with the distance between points being shorter than 0.2 \AA^{-1} was used for integration over the Brillouin zone. The band diagram and the electron state density were calculated with the MBJLDA metafunctional [14] that provides a fairly high accuracy of calculations of the band gap and characterizes the magnetic moment correctly. Searching for variants of the 3C-SiC(111)/Si(111) interface, Medea-Vasp examines numerous configurations of (111) surfaces of both Si and SiC, which are multiples of the elementary cell and are obtained via various translations and rotations, and selects those surfaces that provide the minimum mismatch. It was found that the closest lattice matching is achieved when four Si cells are aligned with five SiC cells, since the lattice parameters of Si and SiC differ exactly by 20%. The lattices may be matched in this case in eight different ways. In four configurations, the carbon plane of SiC faces Si; in the other four, its silicon plane faces Si. The following problem was solved in order to determine which one of the eight configurations is the most favourable. Energy E_0 of the initial system, where a Si cluster $15.39 \times 15.39 \times 9.407 \text{ \AA}$ size, which contains 96 atoms, is located far from a SiC cluster $15.39 \times 15.39 \times 7.551 \text{ \AA}$ size, which contains 75 Si atoms and 75 C atoms (Fig. 1), was calculated first. Si and SiC were then brought closer to each other so that the nearest atoms started interacting, and the configuration of atoms corresponding to the minimum energy $E_{\text{Si-SiC}}$ of the interacting system was identified. After that, interface energy $E_{\text{int}} = E_0 - E_{\text{Si-SiC}}$ (i.e., the energy of separation of Si(111) and 3C-SiC(111)) was calculated for all eight

variants of Si(111) and 3C-SiC(111) matching, and the most favourable configuration of atoms corresponding to the maximum interface energy E_{int} was determined. This configuration features a $P3m1$ symmetry and is presented in Fig. 2. It should be stressed that the exterior surfaces of SiC and Si along axis z were terminated with hydrogen to suppress surface effects and the interaction via boundary conditions, but hydrogen atoms are not shown in Figs. 1 and 2 for simplicity.

The calculations revealed the following. Two out of eight configurations feature a magnetic moment. SiC configurations with the carbon plane facing Si are substantially more favourable than those configurations in which the silicon plane is facing Si. The most favourable configuration has the highest magnetic moment: $5.3 \mu_B$, where μ_B is the Bohr magneton. The regions where the density of spin-up electrons differs from the density of spin-down ones by 0.05 \AA^{-3} are colored in blue in Fig. 2 (a color version of it is provided in the online version of the paper). The energy of the same interface configuration calculated without regard to the magnetic field is 0.285 eV higher; i.e., the energy of the magnetic field of the interface is 0.24 eV/nm^2 . It should be emphasized that the energy of the next-best configuration is 0.14 eV higher, and this configuration lacks a magnetic moment. Thus, it is the magnetic moment that facilitates the selection of this interface configuration. The magnetic moment emerges due to the fact that SiC attracts three Si atoms from the second layer of substrate atoms, separating them from other Si atoms (Fig. 2). These atoms, which

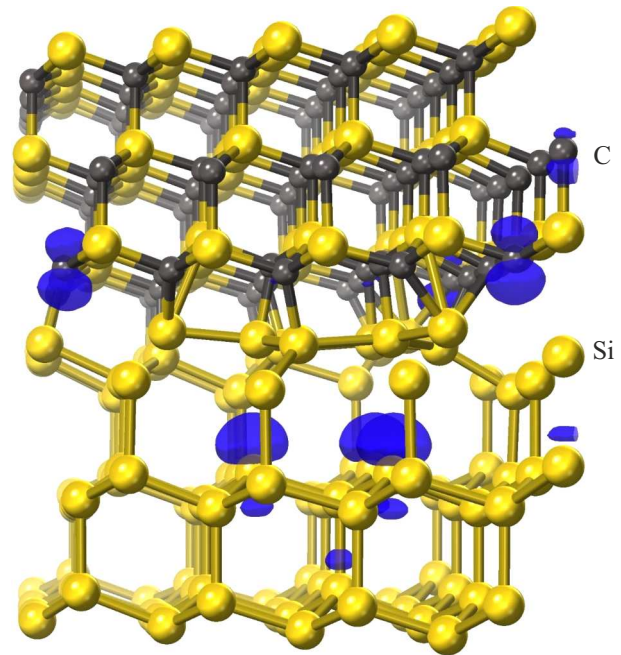


Figure 2. The most favourable configuration of atoms at the 3C-SiC(111)/Si(111) interface. The regions where the density of spin-up electrons differs from the density of spin-down ones by 0.05 \AA^{-3} are colored in blue. A color version of the figure is provided in the online version of the paper.

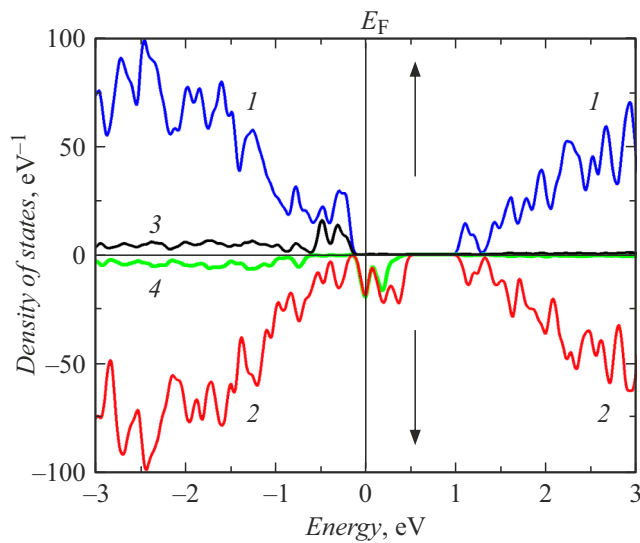


Figure 3. Density of spin-up (upper panel) and spin-down (lower panel) electron states of the 3C-SiC(111)/Si(111) interface. Curves 1 and 2 represent the total density of states, while curves 3 and 4 denote the contribution of p electrons of three C atoms in the lower SiC layer with three bonds, which have a magnetic moment. This contribution is dominant at the Fermi energy (E_F).

feature three bonds instead of four, have unpaired electrons that provide their part of the magnetic moment. The other part comes from three C atoms in the lower SiC layer. They also have just three bonds and an unpaired dumbbell-shaped p electron (Fig. 2). The results of calculations of the band diagram and the density of electron states demonstrate that this interface configuration is a magnetic semimetal. It is a common semiconductor for an electron with one spin state and a metal for an electron with the other spin state (Fig. 3). Unpaired p electrons of three C atoms with three bonds (Fig. 2) are the mobile ones, since they produce the dominant contribution to the density of electron states at the Fermi level (Fig. 3). Notably, they are mobile only in the interface plane.

Thus, the results of calculations within the density functional theory demonstrated that the most favourable configuration of the 3C-SiC(111)/Si(111) interface features a $P3m1$ symmetry and is a rather exotic two-dimensional magnetic semimetal. The magnetic moment of the interface is $4.6 \mu_B/\text{nm}^2$, and the magnetic field energy is $0.24 \text{ eV}/\text{nm}^2$. These data yield the following estimate of the Curie point in the mean field approximation: $T_C \sim 2000^\circ\text{C}$ [15]. It is conceivable that the unusual electrical, optical, and magnetic properties (the anomalous magnetic susceptibility included), which are observed in these samples specifically in the interface plane [8,9], are related to the spintronic characteristics of the 3C-SiC(111)/Si(111) interface.

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Conflict of interest

The authors declare that they have no conflict of interest.

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