

Mechanisms of Semiconductor Interface Formation and its Electronic Properties based on Quantum Theory

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In the fiscal year of 2019, on the basis of the total-energy electronic-structure calculations and molecular dynamics simulations within the density-functional theory, we have studied atom-scale behavior during the epitaxial growth of power semiconductors, silicon carbide (SiC) and gallium nitride (GaN). The main computational tools are our RSDFT (Real Space Density Functional Theory) code and RS-CPMD (Car-Parrinello Molecular Dynamics) code. We have clarified 1) the structures and energetics, and then the morphology of SiC surface steps [1,2], 2) the liquid-like behavior of the topmost Ga atoms [3] and 3) the mechanism of oxygen incorporation during the epitaxial growth of GaN [4,5]. The group identification codes for the achievements above are k0042 and m0001. Below, I explain the issues 1) and 2).

1. Step structures and morphology of Si-face SiC Polar Surface

SiC is now emerging as a promising material for power electronics. This is due to its physical properties superior to Si, a current premier material, such as the wider band gap and the higher electric break-down voltage. The thin-film growth of SiC in the step-flow mode is essential

in the fabrication of electronic devices. Understanding of bond configurations near the step on the atomistic level is necessary in order to identify the reactivity at the step edges. Furthermore, epitaxial graphene can be prepared on SiC surfaces, and the surface steps of SiC also play an important role. Hence, it is certainly important and inevitable from both science and technology viewpoints to identify the atomic steps on SiC and clarify their energetics, that has not been achieved yet. Our previous calculations [6] show that the single-bilayer height steps are

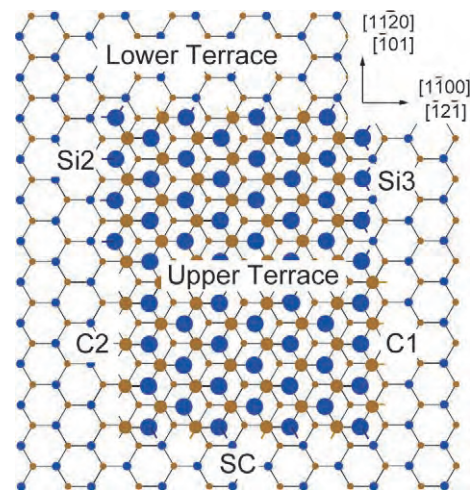


Fig.1: Schematic view of the five distinct mono-bilayer steps on SiC (0001) surface. Si and C atoms are represented by the larger (blue) and smaller (brown) balls, respectively. The Si2, Si3, C1 and C2 steps along the $\langle 11-20 \rangle$ direction and the SC step along the $\langle 1-100 \rangle$ direction are shown all together.

energetically favorable compared with higher steps on SiC(0001) or (111) surface.

Figure 1 shows schematic view of 5 distinct single-bilayer height steps. There are two different classes of steps: One is [11-20] oriented and the other is the [1-100] oriented; further in the latter, four different step edges exist which are labelled by the atomic species at the edge and the number of the dangling bonds before the structural relaxation as Si2, Si3, C1 and C2.

We have performed detailed structural optimization for all the possible atomic steps and determined their structures. Near step edges we have found prominent rebonding between the upper-terrace and the lower terrace Si atoms in Si2 and SC steps and also a peculiar resonant-like rebonds for Si3 steps, as well as the C dimerization for the C2 step.

Figure 2 shows calculated formation energies

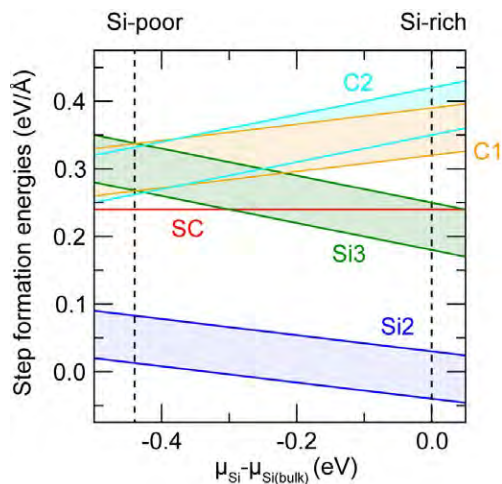


Fig. 2: Calculated formation energies of the mono-bilayer atomic steps on SiC(0001) surface as a function of the Si chemical potential μ_{Si} , measured from that in crystalline Si, $\mu_{\text{Si(bulk)}}$. Shaded areas surrounded by each pair of solid lines represent the uncertainty in the calculated formation energy.

for 5 distinct steps as a function of Si chemical potential (Near step edges, the numbers of Si and C atoms are different so that we need the chemical potential). We have found that Si2 step toward [1-100] is the most stable and Si3 step follows. The SC step toward [11-20] is comparable with the Si3 step.

The energetics obtained above predicts some interesting morphology of atomic steps on SiC(0001). Experimentally, the (0001) surface is slightly inclined along either [1-100] or [11-20] direction. When it is inclined along the [1-100], the surface consists of the [0001] terrace and several steps among Si2, Si3, C1 and C2, whereas it consists of the terrace and SC steps when inclined along [11-20]. In the former, the Si2 or Si3 steps are energetically favorable (Fig. 2). However, in the latter, the SC step is energetically unfavorable compared with Si2 and also Si3 in some range of the Si chemical potential. Hence we expect that the steps toward [11-20] show zig-zag shape consisting of, for instance, Si2 and Si3. We have indeed found that such zigzag-shaped step-edge pairs of Si2 + Si3 is lower in the formation energy than the straight-shape SC step on the [0001] surface inclined along [11-20] direction.

2. Two-Dimensional Ga liquid on growing GaN surface

GaN, a fundamental material worldwide used for high performing opto-electronic devices, is rapidly becoming another candidate to unseat Si in power electronics. Yet, their practical

realization asks for the realization of thin epitaxial films of higher quality with respect to what is done nowadays for optoelectronic applications. It is thus highly demanded to clarify the nature of the growing GaN surface at atomistic level.

It is known that under typical conditions of the epitaxial growth of GaN, the surface is Ga-rich. Hence we prepare Ga-rich surface and raise the temperature by CPMD simulations from room temperature. We have found that, when the temperature reaches the typical growth temperature, i.e., 1300 K, the topmost Ga atom suddenly moves from their original position. The calculated Ga-Ga pair correlation function is shown in Fig. 3. At room temperature, the top-layer Ga atoms vibrate around their original positions. The pair correlation function shows a peak determined by the Ga coverage. Then with increasing temperature, the pair correlation function shows the peak at the same position with increasing peak width, showing the enhanced thermal vibration. However, at the growth

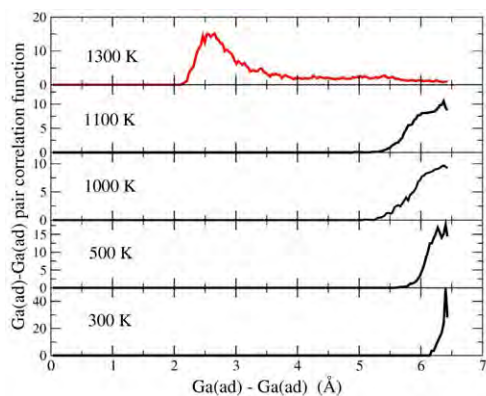


Fig. 3: Evolution of the Ga-Ga pair correlation function in the top-layer of GaN during the heating process. The initial distance of 6.4 Å corresponds to the relaxed system from which dynamical simulations were started.

temperature, the top-layer Ga atoms get together and exhibit the peak at much shorter distance, indicating some condensed phase of Ga.

By using Kubo-formula (velocity-velocity correlation function), we have computed the diffusion coefficient of the top-layer Ga atom. We have found that the diffusion coefficient jumps at 1300 K from its value of $0.382 \times 10^{-5} \text{ cm}^2/\text{s}$ at 1100 K to the value of $0.492 \times 10^{-4} \text{ cm}^2/\text{s}$. We thus conclude that this condensed phase is not a solid phase but a two-dimensional liquid phase. This is corroborated by the absence of the peaks except for the first peak at 1300 K in Fig. 3. The notion that the GaN surface during the epitaxial growth is 2-dimensional liquid is unrecognized in the past and important to consider mechanism of the epitaxial growth.

Related Publications

- [1] K. Seino and A. Oshiyama, *Appl. Phys. Exp.* **13**, 015506 (2020).
- [2] K. Seino and A. Oshiyama, *Phys. Rev. B* (2020) to be published.
- [3] K. M. Bui, M. Boero, K. Shiraishi and A. Oshiyama, *Jpn. J. Appl. Phys.* **59**, SGGK04 (2020).
- [4] F. Shintaku *et al.*, *Appl. Phys. Exp.*, **13**, 055507 (2020)
- [5] D. Yosho *et al.*, *Phys. Sta. Solidi - Rapid Res. Lett.* 2000142 (2020).
- [6] K. Sawada, J.-I. Iwata, a. Oshiyama, *Appl. Phys. Lett.* **104**, 051605 (2014).