Effective approach for accurately calculating individual energy of polar heterojunction interfaces

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We propose a direct approach for calculating individual energy of polar semiconductor interfaces using density functional theory calculations. This approach is applied to polar interfaces between group-III nitrides (AlN and GaN) and SiC and clarifies the interplay of chemical bonding and charge neutrality at the interface, which is crucial for the stability and polarity of group-III nitrides on SiC substrates. The ideal interface is stabilized among various atomic arrangements over the wide range of the chemical potential on Si-face SiC, whereas those with intermixing are favorable on C-face SiC. The stabilization of the ideal interfaces resulting in Ga-polar GaN and Al-polar AlN films on Si-face SiC is consistent with experiments, suggesting that our approach is versatile to evaluate various polar heterojunction interfaces as well as group-III nitrides on semiconductor substrates.

I. INTRODUCTION

Semiconductor heterojunctions often exhibit unusual phenomena and occasionally induce local dipoles, which affect the band offset at the interface [1,2]. Therefore, understanding and optimizing the structure and stability of semiconductor interfaces are of importance for the control of band offsets in semiconductor heterostructures. The atomic structures and electronic properties of polar interfaces for crystalline materials with cubic (zinc blende) structure have been intensively studied through the electronic-structure calculations within density functional theory (DFT) [2,3]. However, those for the wurtzite structure still remain unclear due to the intrinsic difficulty of treating asymmetrically bonded surface atoms.

In group-III-nitride semiconductors, which are widely used for optoelectronics, polar heterojunctions between nitrides and SiC have attracted considerable interest, and abrupt GaN/SiC and AlN/SiC heterojunctions with a low density of dislocations have been successfully fabricated owing to the negligible lattice mismatch between SiC and AlN (less than 1%) and the relatively low misfit for GaN on SiC (∼3%). It has been experimentally reported that Ga-polar GaN and Al-polar AlN are epitaxially grown on Si-face SiC, and N-polar nitrides are formed on C-face SiC [4–13]. The structure and polarity of group-III-nitrides on SiC substrates have been intuitively explained in terms of the dipole contribution and charge neutrality between group-III-nitrides and SiC interface [5,8,14–16]. However, *quantitative* analysis for these polar interfaces on the basis of absolute interface energies is still lacking. Polar surfaces and interfaces for low-symmetry crystalline materials including wurtzite structure cannot be individually treated in conventional slab geometries, and therefore absolute surface and interface energies are fundamentally ill defined [17,18]. Despite several theoretical investigations for group-III nitrides on SiC substrates [19–23], the accurate values of interface energies for polar orientations are not yet available.

The first attempt to calculate individual polar surface and interface energies was demonstrated by Chetty and Martin on the basis of a local energy density approach [18]. However, the method suffers from nontrivial calculations of the local energy density. The calculated energies for GaAs(111) surfaces by Moll *et al.* [24] are quite different from those by Chetty and Martin, even though the exactly same approach has been used. For accurately calculating individual energy for polar semiconductor surfaces, a direct approach using the total energy difference between two identical structures of different size has been proposed [25] and applied to absolute surface energies of GaN polar planes by invoking the similarity between the polar $(0001)/(000\bar{1})$ surface in the wurtzite structure and the $(111)/(\bar{1}\bar{1}\bar{1})$ surface in the zinc blende structure [26,27]. These theoretical investigations inspire us to extend this approach to calculate the accurate values of interface energies.

In this paper, we propose a direct approach to calculate absolute interface energies of polar orientations on the basis of the method using slab models with polar heterojunctions between two different materials. Our approach is successfully applied to clarify the stability and polarity of interfaces consisting of group-III-nitride semiconductors coherently grown on SiC substrates. The interface energies for various atomic configurations with different polarity are related to each other by considering the formation of stable bonds and charge neutrality at the interface.

II. COMPUTATIONAL DETAILS

The method to calculate polar interface energies is based on an effective approach using a wedge-shaped geometry [25]. The slab models of surfaces and interfaces terminated by polar planes in group-III nitrides inevitably exhibit inequivalent surfaces, such as (0001) and $(000\bar{1})$ planes. The relative stability among various atomic configurations can be determined by passivating the surface of the slab with artificial hydrogen atoms with fractional atomic number [28], but the absolute energies of surfaces and interfaces cannot be determined with the knowledge of the absolute surface energy of the passivated surfaces. One of schemes to calculate the absolute surface energy of the passivated surfaces is the use of one-dimensional wire nanostructures with triangular cross section. The nanostructures consist of either two equivalent (111) facets and one $(00\bar{1})$ facet or two equivalent $(\bar{1}\bar{1}\bar{1})$ facets and one (001) facet, so that the difference in surface energy

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between (111) and $(\bar{1}\bar{1}\bar{1})$ surfaces, $\sigma_{(111)} - \sigma_{(\bar{1}\bar{1}\bar{1})}$, is given by

$$
\sigma_{(111)} - \sigma_{(\bar{1}\bar{1}\bar{1})} = \frac{1}{2A^{(111)}} \Big\{ \big[E_{\text{wedge}}^{(111)}(36) - E_{\text{wedge}}^{(\bar{1}\bar{1}\bar{1})}(36) \big]
$$
$$
- \big[E_{\text{wedge}}^{(111)}(28) - E_{\text{wedge}}^{(\bar{1}\bar{1}\bar{1})}(28) \big]
$$
$$
- \frac{1}{2} \big[E_{\text{slab}}^{(001)} - E_{\text{slab}}^{(00\bar{1})} \big] + \frac{1}{2} [\mu_{\text{N}} - \mu_{\text{Ga}}] \Big\}, \quad (1)
$$

where $A^{(111)}$ is the area of the (111)-(1×1) surface, $E_{\text{wedge}}^{(111)}(n)$ and $E_{\text{wedge}}^{(\bar{1}\bar{1}\bar{1})}(n)$ are the total energies of the wedges with passivated (111) and $(\bar{1}\bar{1}\bar{1})$ surfaces containing n formula units, and $E_{\text{slab}}^{(001)}$ and $E_{\text{slab}}^{(00\bar{1})}$ are the total energies of slabs with (001) and $(00\bar{1})$ surfaces, and μ_{Ga} and μ_{N} are Ga and N chemical potentials, respectively. The contribution of ridges can be removed by subtracting energies for different wedge sizes. It has also been shown that a better convergence can be obtained if we take an energy difference between structures of the same size in which cations and anions are interchanged [29]. The total energies for (001) and $(00\bar{1}))$ surfaces are obtained by using slabs with two equivalent surfaces. The sum of surface energies for passivated (111) and $(\bar{1}\bar{1}\bar{1})$, $\sigma_{(111)} + \sigma_{(\bar{1}\bar{1}\bar{1})}$, is easily obtained from a slab calculation. The individual absolute energies for passivated surfaces are thus achieved by combining Eq. (1) with $\sigma_{(111)} + \sigma_{(\bar{1}\bar{1}\bar{1})}$.

In the case of the GaN/SiC interface, which results in the formation Ga-polar GaN films on the Si-face SiC substrate, the absolute interface energy is then given by using the absolute energies of top- and bottom-passivated surfaces $\sigma_{\text{GaN}(0001)}$ and $\sigma_{\text{SiC}(\bar{1}\bar{1}\bar{1})}$ as

$$
\sigma_{\text{int}} = \frac{1}{A^{\text{SiC}(111)}} \Big[E_{\text{int}}^{(000\bar{1})/(111)} - (n_{\text{Ga}} - n_{\text{N}})\mu_{\text{Ga}}
$$
$$
- n_{\text{N}} E_{\text{GaN}} - (n_{\text{Si}} - n_{\text{C}})\mu_{\text{Si}} - n_{\text{C}} E_{\text{SiC}} \Big]
$$
$$
- \sigma_{\text{GaN}(0001)} - \sigma_{\text{SiC}(\bar{1}\bar{1}\bar{1})}, \quad (2)
$$

where $A^{\text{SiC}(111)}$ is the area of 3C-SiC(111)-(1 × 1) substrate, $E_{\text{int}}^{(000\bar{1})/(111)}$ is the total energy of a slab with both the polar GaN(0001) top-surface passivated by artificial H atoms with $1.25e$ [28] and the C-face SiC$(\bar{1}\bar{1}\bar{1})$ bottom-surface passivated by H atoms, n_i is the number of ith type atoms in the slab, μ_{Si} is Si chemical potential, E_{GaN} (E_{SiC}) is the total energy per formula unit of bulk GaN (SiC). The relationship between μ_{Ga} and μ_{N} (μ_{Si} and C chemical potential μ_{C}), expressed as $\mu_{\text{Ga}} + \mu_{\text{N}} = E_{\text{GaN}}$ ($\mu_{\text{Si}} + \mu_{\text{C}} = E_{\text{SiC}}$), is used as an equilibrium condition. The interface energies are thus evaluated as functions of μ_{Ga} and μ_{Si}, which can vary in the thermodynamically allowed range. This range corresponds to the heat of formation (formation enthalpy), and the calculated values for GaN, AlN, and SiC are -1.15, -2.80, and -0.56 eV, respectively. Therefore, the ranges for μ_{Ga}, μ_{Al}, and μ_{Si} are $\mu_{\text{Ga}}^{\text{bulk}} - 1.15$ eV $\leqslant \mu_{\text{Ga}} \leqslant \mu_{\text{Ga}}^{\text{bulk}}$, $\mu_{\text{Al}}^{\text{bulk}} - 2.80$ eV $\leqslant \mu_{\text{Al}} \leqslant \mu_{\text{Al}}^{\text{bulk}}$, and $\mu_{\text{Si}}^{\text{bulk}} - 0.56$ eV $\leqslant \mu_{\text{Si}} \leqslant \mu_{\text{Si}}^{\text{bulk}}$, where $\mu_{\text{Ga}}^{\text{bulk}}$, $\mu_{\text{Al}}^{\text{bulk}}$, and $\mu_{\text{Si}}^{\text{bulk}}$ are the chemical potentials of bulk Ga, Al, and Si, respectively. These calculated values of heat of formation agree with those obtained by experiments [30].

Figure 1(a) illustrates the cross-sectional views of wedge consisting of 28 and 36 formula units to calculate the energy difference $\sigma_{(111)} - \sigma_{(\bar{1}\bar{1}\bar{1})}$ in Eq. (1). By maintaining
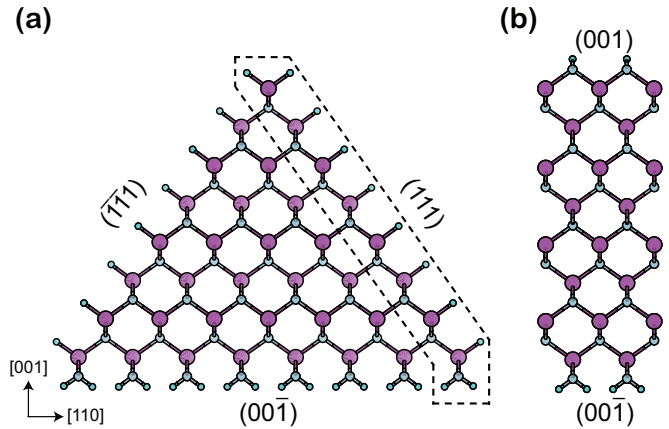

FIG. 1. Cross-sectional views of (a) a triangular wedge consisting of 36 formula units to calculate the difference in surface energy between (111) and $(\bar{1}\bar{1}\bar{1})$ surfaces, and (b) a slab model to calculate the total energy of (001) and $(00\bar{1})$ surfaces with two equivalent surfaces. Large, small, and tiny circles correspond to cation (Al, Ga, or Si), anion (N or C), and artificial H atoms, respectively. The wedge consisting of 28 formula units is constructed by removing the atoms enclosed by dashed lines and passivating the resultant dangling bonds by artificial H atoms. Note that the unit cell along the [110] direction in panel (b) is multiplied for visual understanding.

the geometry of passivated (111) and $(\bar{1}\bar{1}\bar{1})$ facets in the wedge to that of slab geometry, the artificial hydrogen atoms on the wedge surfaces are allowed to relax while the other atoms are fixed. To calculate the energies for (001) and $(00\bar{1})$ surfaces, the 1×1 slab models consisting of eight bilayers and 12 Å of vacuum region shown in Fig. 1(b) are employed. In addition, the 1×1 slab models consisting of six bilayers and 12 Å of vacuum region are used to obtain the sums of the surface energies of passivated (111) and $(\bar{1}\bar{1}\bar{1})$ surfaces for GaN, AlN, and SiC. It should be noted that the effect of lattice strain on the absolute energy of passivated surfaces must be included due to the lattice mismatch between group-III nitrides and SiC (3% for GaN and 1% for AlN). To take this effect into account, calculated lattice parameters ($a = 3.10$ Å and $c = 5.06$ Å) of the 3C-SiC substrate are used to obtain the absolute energies of passivated (111) and $(\bar{1}\bar{1}\bar{1})$ surfaces even for GaN and AlN. Actually, we estimate the critical thickness of dislocation formation for GaN (AlN) films on SiC substrates by using the People–Bean formula [31] to be 103 (2403) Å. This suggests that the interfaces with coherently grown group-III nitrides could be formed during the growth and play an important role to determine the polarity on SiC substrates. For calculations including polar heterojunctions, we adopt slab models with 2×2 and $\sqrt{3} \times \sqrt{3}$ unit cells consisting of four bilayers of GaN/AlN with a wurtzite structure along the [0001] direction and six bilayers of 3C-SiC along the [111] direction and 13 Å of vacuum region. The calculations using slab models with large numbers of bilayers and vacuum region thickness including different stacking sequences at the interface are also performed. The difference of interface energies depending on the calculation model is found to be less than 0.005 eV/Å^2. The small energy difference manifests the absence of a macroscopic field [32],
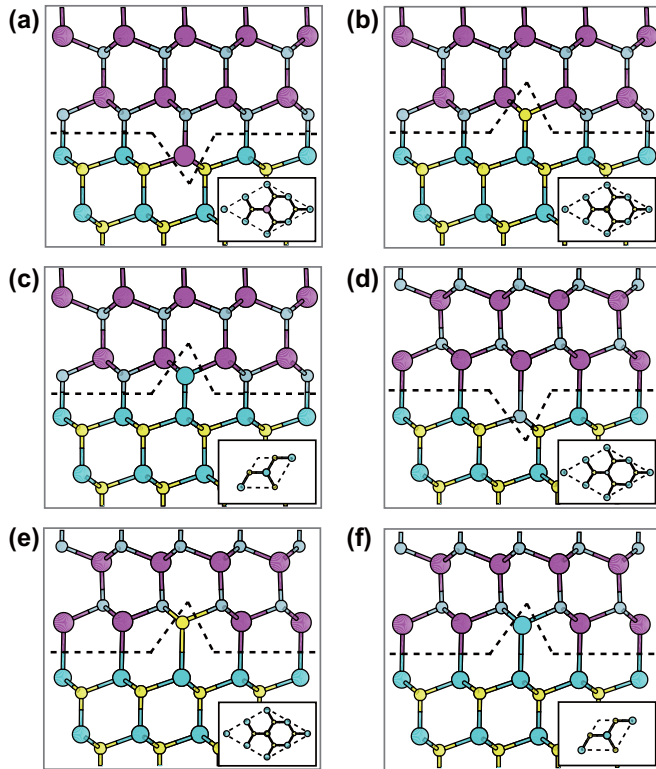
FIG. 2. Schematics of possible atomic arrangements at the interface between group-III nitrides and the Si-face SiC substrate. In addition to the ideal interface, we consider the interfaces resulting in Ga/Al polar films with substitutional (a) Ga/Al atoms in SiC (Ga_{Si}/Al_{Si}), (b) C atoms in GaN/AlN (C_N), and (c) Si atoms in GaN/AlN (Si-face Si_N), and those resulting in N-polar nitrides with substitutional (d) N atoms in SiC (N_{Si}), (e) C atoms in GaN/AlN (C_{Ga}/C_{Al}), and (f) Si atoms in GaN/AlN (Si-face Si_{Ga}/Si_{Al}). Large purple, large blue, small blue, and small yellow circles represent group-III (Al or Ga), Si, N, and C atoms, respectively. The insets show top views of SiC substrate with substitutional atom in the 2×2 (for Ga_{Si}/Al_{Si}, C_N, N_{Si}, and C_{Ga}/C_{Al}) and $\sqrt{3} \times \sqrt{3}$ (for Si-face Si_N and Si-face Si_{Ga}/Si_{Al}) unit cells, respectively.

so that the energies of polar interfaces can be well defined by employing the present approach.

Figures 2 and 3 show the schematics of atomic arrangements at the polar interface for group-III nitrides on Si-face and C-face 3C-SiC substrates, respectively. In addition to the models for the ideal abrupt interfaces (not shown here), we adopt several models satisfying the charge neutrality at the interface, which correspond to the intermixing proposed by previous investigations [5,8,14]. We note that the models with substitutional Si atoms shown in Figs. 2(c), 2(f), 3(b), and 3(d) correspond to group-III nitrides directly deposited on the reconstructed SiC surfaces, such as the $(\sqrt{3} \times \sqrt{3})R30°$ surface with a Si adatom on the Si-face and the 2×2 surface with a Si adatom on the C-face SiC [33–35].

The total-energy calculations within the DFT are performed by using the plane-wave pseudopotential approach with the generalized gradient approximation [36]. We employ norm-conserving pseudopotentials for Si, Ga, Al, and H atoms [37] and ultrasoft pseudopotentials for C and N atoms [38]. The valence wave functions are expanded by the plane-wave basis
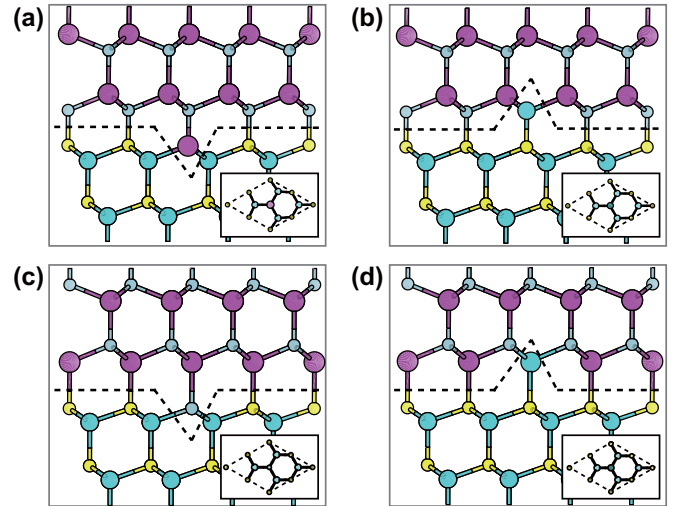

FIG. 3. Schematics of possible atomic arrangements at the interface between group-III-nitrides and C-face SiC substrate. In addition to the ideal interfaces, we consider the interfaces resulting in Ga/Al-polar films with substitutional (a) Ga/Al atoms in SiC (Ga_C/Al_C) and (b) Si atoms in GaN/AlN (C-face Si_N), and those consisting of N-polar nitrides with substitutional (c) N atoms in SiC (N_C) and (d) Si atoms in GaN/AlN (C-face Si_{Ga}/Si_{Al}). The insets show top views of a SiC substrate with a substitutional atom in the 2×2 unit cell. Notations of circles are same as those in Fig. 2.

set with a cutoff energy of 30.25 Ry, and the conjugate gradient technique is utilized for both electronic structure calculations and geometry optimization. Ga-$3d$ electrons are treated by partial core corrections [39]. The geometry is optimization until the remaining forces acting on the atoms are less than 5.0×10^{-3} Ry/Å. We use the k-point sampling corresponding to 36 points in the irreducible part of the 1×1 surface Brillouin zone, which provides sufficient accuracy in the total energies. The computations are carried out the using Tokyo *ab initio* Program Package [40–42].

III. RESULTS AND DISCUSSION

A. GaN/SiC interface

Figure 4 shows the calculated interface energy σ_{int} of GaN on a 3C-SiC(111) substrate for various atomic configurations obtained using Eq. (2) as a function of μ_{Ga}. The atomic configuration with the lowest interface energy for a given μ_{Ga} is definitely determined. For Ga-polar films on Si-face SiC, the energy of the ideal interface without intermixing is the lowest over the entire range of μ_{Ga}, as shown in Fig. 4(a). The stabilization of the ideal interface originates from the formation of stable Si–N bonds, which prevails the charge neutrality at the interface, is consistent with the observations by the polarization-dependent x-ray absorption spectroscopy [16]. It should noted that the energy of the ideal interface takes a negative value, especially under N-rich conditions owing to the formation of stable Si–N bonds. The negative value implies that the stability of the ideal interface may contribute to the formation of Ga-polar GaN films on the SiC substrate in addition to a small surface energy on the Ga-polar surface [26]. In contrast, for N-polar films, the interface with substitutional
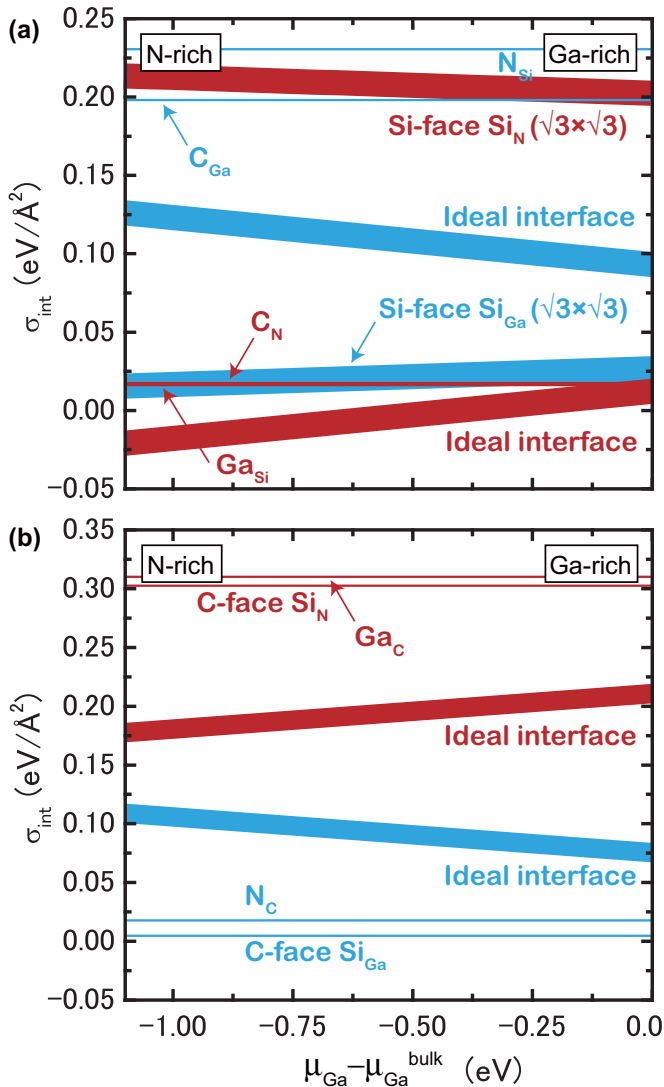
FIG. 4. Calculated interface energy σ_{int} between GaN and (a) Si-face and (b) C-face 3C-SiC substrates with various atomic configurations as a function of the Ga chemical potential. Red and blue lines represent the interface energies corresponding to Ga-polar and N-polar GaN, respectively. Thick lines represent the range of interface energy, which depends on the Si chemical potential. Schematics of interfaces on Si-face and C-face SiC are shown in Figs. 2 and 3, respectively.

Si [Si-face Si$_{Ga}$ with $(\sqrt{3} \times \sqrt{3})R30°$ periodicity] shown in Fig. 2(f) takes the lowest value, reflecting the stable surface reconstruction on the Si-face SiC surface. Furthermore, our results allow a comparison of interface energies for different planes. On the Si-face SiC, the ideal interface resulting in Ga-polar films is stable compared with that of the Si-face Si$_{Ga}$ in N-polar films, indicating that the ideal interface resulting in Ga-polar films is always formed irrespective of epitaxial growth conditions. This result is consistent with the fabrication of Ga-polar GaN on Si-face SiC substrate in molecular beam epitaxy (MBE) growth [4,8–10]. Furthermore, the calculated interlayer distances [43] qualitatively agree with those obtained by high-resolution transmission-electron microscopy [8].

The results of GaN on a C-face 3C-SiC(111) substrate as a function of μ_{Ga} are presented in Fig. 4(b). For Ga-polar films, the ideal interface without intermixing is stabilized over the entire range of μ_{Ga}. However, its interface energy is larger than those of N-polar films. Furthermore, in contrast to the Si face, the interfaces with substitutional N (N$_C$) and Si (C-face Si$_{Ga}$) atoms shown in Figs. 3(c) and 3(d), respectively, are more stable than the ideal interface. This is because charge neutrality is maintained by these substitutional atoms and stable Ga–N and Si–C bonds are formed at the interface instead of less stable Ga–C bonds: The bond energy of Ga–C is 2.0 eV, while that of Ga–N and Si–C is 2.3 and 3.2 eV, respectively [44]. Since the number of Si–N bonds formed near the interface at the C-face Si$_{Ga}$ is same as that in N$_C$, the energy difference between C-face Si$_{Ga}$ and N$_C$ is interpreted in terms of the energy difference between Si–C and Ga–N bonds. It is thus suggested that the interfaces resulting in N-polar GaN films with intermixing are stabilized on the C-face SiC substrate. Indeed, this result is consistent with the experimental results of the fabrication of N-polar GaN on a C-face SiC substrate in the MBE growth [4,9].

B. AlN/SiC interface

Owing to the difference in the thermodynamically allowed range between μ_{Ga} and μ_{Al}, the calculated results of the interface energy σ_{int} as a function of μ_{Al} for AlN/SiC interfaces shown in Fig. 5 are slightly different from those of GaN/SiC interfaces. When $\mu_{Al} - \mu_{Al}^{bulk}$ is less than -1.5 eV, as shown in Fig. 5(a), the energy of the ideal interface without intermixing is the lowest among the interfaces resulting in Al-polar AlN films on Si-face SiC. On the other hand, the interface with substitutional Al atom (Al$_{Si}$) shown in Fig. 2(a) is favorable under Al-rich conditions for $\mu_{Al} - \mu_{Al}^{bulk}$ larger than -1.5 eV. It is thus suggested that the atomic arrangements and resultant electronic states depend on the growth condition. The stabilization of Al$_{Si}$ originates from the charge neutrality at the interface as well as from the formation of stable Al–N bonds, whose bond energy (2.7 eV) is larger than the Ga–N bond energy by 0.4 eV. [44] For N-polar films the interface with substitutional Si [Si-face Si$_{Al}$ with $(\sqrt{3} \times \sqrt{3})R30°$ periodicity] shown in Fig. 2(f) always takes the lowest value. By comparing the interface energies among different planes, the interfaces resulting in Al-polar films are found to be stabilized compared with that in N-polar films on Si-face SiC. The stabilization of Al-polar films on the Si-face is consistent with the experimental results of the fabrication of Al-polar AlN on the Si-face SiC substrate in the MBE [6], metal-organic vapor phase epitaxy [5,11,12,14], and hydride vapor phase epitaxy growth [13]. Moreover, the calculated interlayer distances [43] qualitatively agree with those observed by high-resolution transmission-electron microscopy [14].

On the C-face SiC substrate, as shown in Fig. 5(b), the energy of the ideal interface resulting in Al-polar films is larger than that of N-polar films. Among the interface structures resulting in N-polar films, the interfaces with substitutional N (N$_C$) and Si (C-face Si$_{Al}$) atoms shown in Figs. 3(c) and 3(d), respectively, are stabilized compared with the ideal interface over the entire range of μ_{Al}. Instead of Al–C bonds, stable Al–N and Si–C bonds are formed at the interface in N$_C$ and C-face
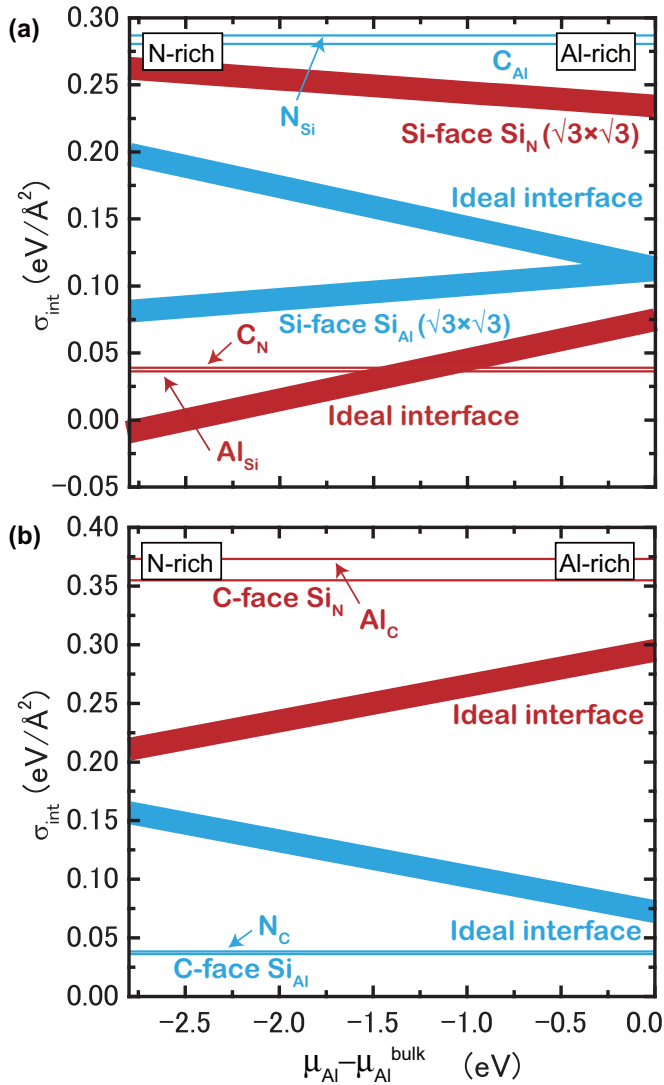
FIG. 5. Calculated interface energy σ_{int} between AlN and (a) Si-face and (b) C-face 3C-SiC substrates with various atomic configurations as a function of Al chemical potential. Red and blue lines represent the interface energies corresponding to Al-polar and N-polar AlN, respectively. Thick lines represent the range of interface energy, which depends on the Si chemical potential. Schematics of interfaces on Si-face and C-face SiC are shown in Figs. 2 and 3, respectively.

Si_{Al}, respectively, so that charge neutrality is maintained by the intermixing atoms. The small energy difference between N_C and C-face Si_{Al} (within 0.003 eV/Å^2) comes from the energy difference between Al–N and Si–C bonds (by 0.4 eV), which is smaller than that between Ga–N and Si–C bonds of 1.0 eV.

It is thus implied that the interface resulting in N-polar AlN films with intermixing is always stabilized on the C-face SiC substrate.

Finally, we comment on the versatility of present approach. Although further investigations incorporating the formation of dislocations and interfacial layers are necessary, this approach is feasible to evaluate the stability of various polar heterojunction interfaces as well as those consisting of group-III nitrides on lattice-matched substrates such as ZnO [45–50], ZrB$_2$ [51,52], and ScAlMgO$_4$ [53]. Indeed, we have successfully applied this approach to clarify the stability of polar interfaces between GaN and ZnO substrates [43] and are now examining the interfaces between GaN films on ScAlMgO$_4$ substrates, which have recently been fabricated. This approach can also be applied to clarify microscopic mechanisms of various phenomena related to polar heterojunction interfaces, including polarity inversion [54,55] and inversion domain boundaries [56]. Furthermore, this approach may be applied not only to semiconductor interfaces but also to other novel polar interfaces including topological insulators.

IV. SUMMARY

We have proposed an effective approach to calculate the individual energy of polar semiconductor interfaces and applied to polar interfaces between group-III nitrides and SiC substrates. We have found that the ideal interface has the lowest interface energy among various atomic arrangements on the Si-face SiC over a wide range of chemical potential. On the other hand, the energy of interface with intermixing is lowest on C-face SiC to maintain charge neutrality at the interface. Moreover, the interfaces resulting in Ga-polar GaN and Al-polar AlN films are found to be stable compared with those in N-polar films on Si-face SiC, consistent with experiments. Our approach has identified the polarity and stable structures of semiconductor interfaces, suggesting that the interplay of chemical bonding and charge neutrality at the interface is crucial for polar interfaces between group-III nitrides and SiC substrates.

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[44] The bond energies are estimated by calculated cohesive energies of bulk AlN, GaN, SiC, and GaC. The calculated cohesive energies of AlN, GaN, and SiC agree well with the experimentally reported ones. See *Physics of Group IV Elements and III-V Compounds*, edited by K.-H. Hellwege and O. Madelung, *Landolt-Börnstein*, New Series, Group III, Vol. 17, Pt. a (Springer, Berlin, 1982). In the case of bulk GaC, we assume hypothetical 3C structure in order to calculate the energy of tetrahedrally coordinated Ga–C bonds.

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