Chemical Trend of Isoelectronic Traps in Si Tunnel FET; First-Principles Study

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Abstract

Isoelectronic impurity complexes, such as Al+N and Mg+O pairs, are key elements to realize the large ON current in Si-based tunnel FETs. We show by the first-principles calculation that such complexes are stable and produce electron-unoccupied localized states made of N/O-3s orbital within the band gap of Si. These states strongly hybridize with Si states and promote the enhanced tunneling current. Chemical trend of complexes is also studied to enable the promising FET design.

1. Introduction

Tunnel field-effect transistor (TFET) is one of the promising candidates in realizing a much steeper switching, compared to conventional metal-oxide-semiconductor field-effect transistors (MOSFETs) [1]. However, the ON current is still low for Si-based TFETs because of the indirect band-to-band transitions in Si [2]. Recently, Mori and his coworkers have succeeded in remarkably enhancing a tunneling current in Si-based TFETs utilizing an Al+N isoelectronic trap (IET), i.e., the co-doping of Al and N impurities around the pn junction [3]. They have shown that the enhancement is caused with the help of localized electronic states of IET, probably by the appearance of pseudodirect tunneling between the valence and conduction bands in Si. However, there have been no theoretical studies on this IET and it has not been clarified what electronic states are produces by the Al+N IET.

In this work, we study how Al and N atoms produce the IET, what electronic states are produced by the IET, and what chemical trend exits with varying the doping atoms, by using the first-principles calculations.

2. Methodology

We consider the IETs made of III+V and II+VI atoms, i.e., made of cation atoms, B, Al, Ga, Be and Mg, and anion atoms, N and O. To simulate the IET in Si, we adopt large cubic unit cells of bulk Si made of 64 to 1000 atoms. Figure 1(a) shows the schematic picture of Si_{216} unit cell. We assume that cation and anion impurity atoms are located at Si sites as substituent atoms.

Electronic structures and atom positions are calculated using the standard first-principles calculations in the density functional theory, by employing the TAPP code [4], where the generalized gradient approximation (GGA) is adopted. The wave functions are expanded by plane waves with the energy less than 36Ry, while the Brillouin-zone integration of charge density is evaluated using $4 \times 4 \times 4$



Fig. 1 (a) Schematic picture of Si_{216} cubic unit cell adopted in the present calculation. IET atoms such as Al and N are substituted into Si sites. (b) Calculated total energy of (cation+anion)-doped system as a function of distance between cation and anion atoms. The smallest distance corresponds to the case of the near-est-neighboring sites.

k-mesh points. The other calculation details are described elsewhere [5].

3. Results and Discussions

First, we consider the stability of IETs. Figure 1(b) shows the total energies of various IET pairs as a function of the distance between cation and anion atoms, where the energy is selected as zero when cation and anion atoms are located at the nearest-neighboring sites. It is seen that the nearest-neighboring pair is the most stable in most of cation-anion pairs.

Then, we consider the reason why cation and anion atoms prefer to locate at the nearest neighboring sites, by using Al+N pair as an example. The most important factor is the energy gain by the direct bonding between Al and N atoms. Since the electro-negativities of Si, Al, and N atoms are 1.9, 1.6, and 3.0, respectively, the energy gain becomes the largest when Al and N are located at the nearest-neighboring sites. In fact, the calculated Mulliken charges of Al and N are respectively 2.06 and 8.28e when both atoms are isolated in Si, while these charges change to 1.86 and 8.39e when both atoms are located nearby, which indicates the production of strong ionic bonding between Al and N. The stability of other IET pairs is also explained by the same scenario. In case of a B+N pair, on the other hand, the total energy shows little change with varying the distance between B and N atoms. This is because B has larger electro-negativity, 2.04, compared to Si, 1.9, thus both B and N becoming negative ions and showing the repulsive interaction.



Fig. 2 Atomic structures around (a) (Al+N) and (b) (B+N) IET pairs in Si, viewed from (001) direction.

It is interesting to note that, as seen in Fig.1(b), the B+N and Be+O pairs have the longer nearest-neighboring distance, compared to the other pairs. This occurs due to the small atomic radius of not only N and O but also B and Be atoms. In fact, as shown in Figs. 2(a) and 2(b), a Al+N pair has the direct bonding, while the bond is broken between B and N atoms and the B-N distance increases. Therefore, we reasonably expect that B+N and Be+O pairs prefer to locate at a single Si site like a single dopant rather than at nearest neighboring sites like a substitutional pair.

Next, we consider what electronic states are produced by the (cation+anion) IET. Figure 3(a) displays the calculated band structure of (Al+N)-doped Si₅₁₂ system for the case of the nearest-neighboring Al and N pair. The band gap of Si is located from around -0.5 to +0.2eV. Most remarkable feature is the appearance of an electron-unoccupied state within the band gap of Si, near 0eV, which we call the IET state. To characterize the IET state, we show in Fig. 3(b) its wave function in the case of Si₁₀₀₀ unit cell. It is seen that the IET state is localized around the doped N atom and is mainly made of N(3s) orbital, but it strongly hybridizes with 3s and 3p orbitals of surrounding Al and Si atoms. Since the excess of valence electron number of N is compensated by the electron deficiency of Al in a zincblende tetrahedral network, the IET state becomes unoccupied.

It is also interesting to note that the localization length (exponential factor) of the IET state is roughly estimated as 10-20Å. Considering that the tunneling current is often realized by the tail of wavefunction, this result indicates that the width of pn junction in TFET should be comparable to this length.

Finally, we consider what chemical trend exists when the IET atoms are changed. Figure 4 shows the calculated energy positions of various IET states within the band gap of Si. These IET states are also made of N(3s) and O(3s) orbitals with the strong hybridization with Si(3s, 3p) orbitals, similar to the case of Al+N complex. Since the O(3s) orbital has the lower energy position than N(3s), the O-originated IET states appear near the valence-band top, thus promising for hole-carrier TFET. On the other hand, with varying cation atom from B to Ga, the energy position of the IET state increases reflecting the electro-negativity. These results are important to select a suitable IET pair.

It should be noted here that the existence of the IET state within the band gap of Si is closely related to the low energies of N(3s)/O(3s) orbitals. In fact, the doping of N and O atoms into III-V and II-VI semiconductors is known to produce localized electronic states near the conduction



Fig. 3 (a) Band structure of (Al+N)-doped Si system when Al and N atoms are located at the nearest neighboring sites. (b) Contour plot of wave function of the (Al+N) IET state in a band gap of Si, viewed from (001) direction. Yellow and blue regions correspond to positive and negative amplitude, respectively. Small dots indicate the Si-atom positions.



Fig. 4 Calculated energy positions of various IET states in the band gap of Si.

bands and promote strong optical transitions useful for the solar-cell application [6].

4. Conclusions

Electronic properties and chemical trend of (cation+anion) isoelectronic traps in Si were studied by the first-principles calculations. It was shown that cation and anion atoms prefer to locate nearby and produce an electron-unoccupied state in the band gap of Si. This state is made of the 3s orbitals of N/O which strongly hybridizes with 3s/3p orbitals of Si, and is located around N/O atoms with the localization length of about 10-20Å. These features are important to enhance the tunneling current.

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