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Defect distribution and MIGS at metal/Ge interfaces; first-principles study

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Abstract

Distributions of point defects like vacancy are studied around metal/Ge interfaces by the first-principles calculation. It is shown that the defect density remarkably increases at the interface, while the Schottky barrier shows the Fermi-level pinning not depending on the kind of defects. We show that these features reflect the hybridization of defect electronic states with the metal induced gap states (MIGS).

1. Introduction

Because of the large carrier mobility, germanium (Ge) is expected as one of promising materials for next-generation high-speed devices. However, due to its small cohesive energy, Ge is believed to have many defects compared to Si, especially near metal/Ge interfaces. The defects like vacancy are key elements to determine the interface properties such as Schottky barrier. However, our knowledge is still limited for metal/Ge interfaces [1].

In this work, we study the fundamental properties of point defects around metal/Ge interfaces by the first- principles theoretical calculations, i.e, how many point defects such as vacancy and interstitial impurities are present and distributed around metal/Ge interfaces and how they change the Schottky barrier (SB).

2. Methodology

To simulate metal/Ge interfaces with point defects, we adopt (2x2) Al/Ge (111) repeated slabs made of 5 monolayer (ML) Al and 13-25 ML Ge (Fig.1), while a vacuum region having more than 10Å thickness is employed between slabs. The back-surface of Ge is terminated with H atoms and 2 ML Ge atoms of the back-surface are fixed at bulk positions during the structure optimization. Interstitial atoms are inserted at stable tetrahedral (T_d) sites in Ge layers, while Ge vacancies are arranged at various positions around the interface.

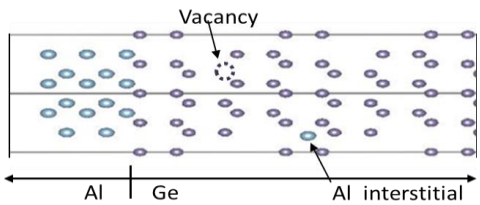


Fig.1. Repeated slab model adopted in this work to simulate defective Al/Ge(111) interfaces. Vacancy and interstitial atoms are inserted at various positions around the interface.

Electronic structures and atom positions are calculated using the standard first-principles calculations based on the density functional theory, by employing Vienna ab initio simulation package (VASP) [2], where the Perdew-Wang generalized gradient approximation is adopted for the exchange-correlation energy. The wave functions are expanded by plane waves with the energy less than 250-300 eV, while the Brillouin-zone integration of charge density is evaluated using 16 Monkhorst– Pack k-mesh points. The calculation details are described elsewhere [3].

3. Results and Discussions

We first consider the stability of point defects. Figures 2(a) and 2(b) show calculated formation energies of Ge vacancies and Al interstitials around Al/Ge interface as a function of the distance from interface. Here, the energy origin is selected to be the formation energies in inner bulk layers, which are about 2.0 and 2.96 eV for Ge vacancy and Al interstitial, respectively. Using these values, for example, we can estimate the vacancy density in bulk layers as 10^{10} cm^{-3}, which is in good agreement with recent experiments [4]. These formation energies in inner bulk layers mainly originate from the elastic energy loss produced by the insertion of foreign atoms in bulk crystal structure [5].

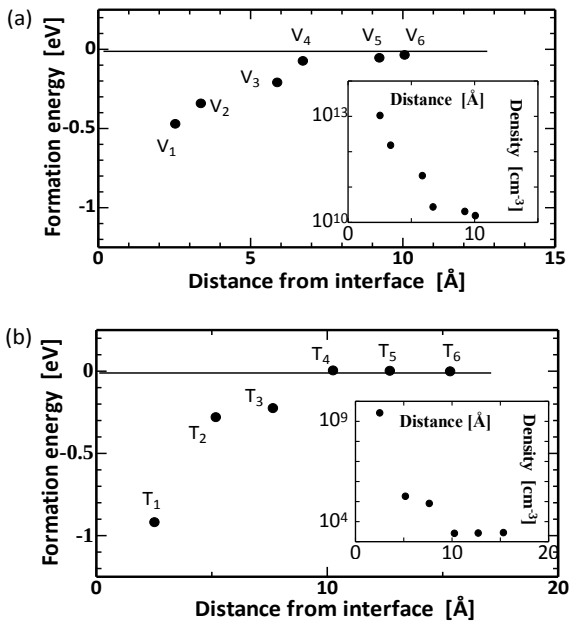


Fig.2. Calculated formation energy and defect density (inset) of (a) Ge vacancy and (b) Al interstitials around Al/Ge interface, as a function of the distance from interface.

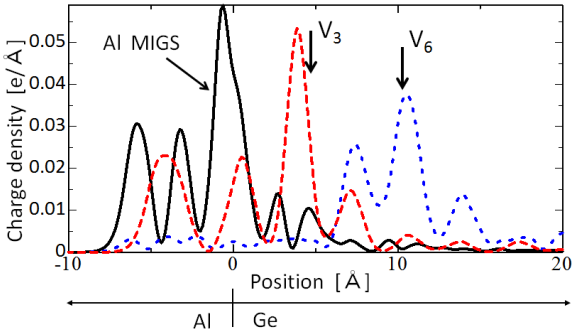


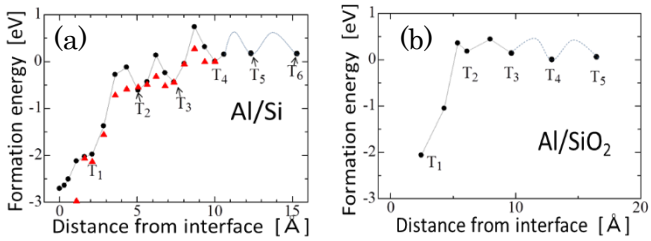
Fig.3. Charge density of vacancy-related states when the vacancy is located at third V_3 (red dashed line) and sixth V_6 (blue dotted line) sites from the Al/Ge interface. Original MIGS state of Al layers is shown by a black line.

It is noted here that the formation energy decreases as the point defect approach the interface. Such energy decrease is about 0.5eV for vacancy defect, which indicates that the vacancy density is three-figure larger than that in bulk layers; around 10^{13} cm^{-3} at the metal/Ge interface (Fig.2 inset).

Then, we consider why the formation energy decreases around the interface. It is well known that the metal induced gap states (MIGS) appear around metal/Ge interfaces [6]. Figure 3 shows the charge density map of the MIGS and vacancy-related states along the (111) direction. It is seen that the MIGS state (black line) is extended in Al layers and penetrates into Ge layers by about 5Å. When the vacancy is located at sixth Ge site (V_6) from the interface, the vacancy-related state (blue dotted line) is localized only around the vacant site. On the other hand, when the vacancy is located at third site (V_3), we can clearly recognize the hybridization between the MIGS and vacancy-related states. This hybridization promotes the energy decrease of vacancy formation around the interface. We have also analyzed the formation-energy variation for Al interstitials and found the same scenario; the defect density is large around the interface due to the decrease of formation energy caused by the hybridization of defect states with the MIGS.

To demonstrate the correlation of defect formation and the MIGS, we calculate the formation energy of Al interstitial defect at Al/Si, Al/SiO_2, and Al/Sn interfaces, the results being shown in Figs. 4(a) to 4(c). It is clearly seen that the variation range of formation energy is short for SiO_2, while long for Sn. This is because MIGS penetration length is roughly proportional to the inverse of band-gap energy and thus it is short for SiO_2 (band gap= about 9.0eV), while long for Sn (gap= about 0.1eV).

Finally, we consider what changes occur in SB height when the point defects exist around the metal/Ge interfaces. Figure 5 shows the calculated SB for hole carriers when various point defects are located at the most stable positions around Al/Ge interface. Here, the blue horizontal line around 0.1eV corresponds to the SB for clean Al/Ge interface without defects. It is seen that the SB does not change even when vacancy, interstitial, and substitution defects exist. This is because most defects prefer to locate in a region where the MIGS penetration occurs and the electronic perturbation by



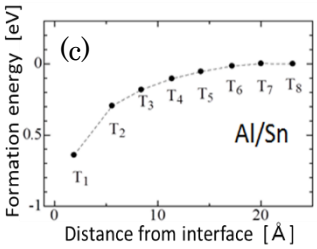


Fig.4. Calculated formation energy of Al interstitial defect as a function of the distance from the interface, for (a) Al/Si, (b) Al/SiO_2, and (c) Al/Sn interfaces.

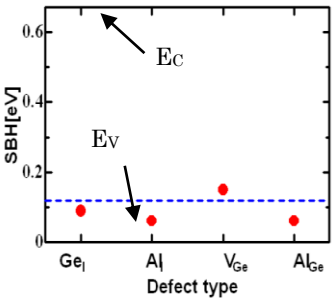


Fig.5.Calculated Schottky barrier height for hole carrier at Al/Ge interfaces having Ge interstitial (Ge_I), Al interstitial (Al_I), Ge vacancy (V_{Ge}), and Al substitution (Al_{Ge}) point defects. Blue horizontal line corresponds to the barrier at clean interface without defects.

the defects is screened and weakened by the hybridization of defect states with the MIGS.

4. Conclusions

We have studied the defect distribution around metal/Ge interfaces by using the first-principles calculation. It was shown that the defect density increases around the interface because the hybridization of defect states with the MIGS stabilizes the defects; e.g, the vacancy density is about three figure larger than that in bulk layers. We also showed that the MIGS screens the defect states and thus the Schottky barrier has similar values for both clean and defective interfaces. These results indicate that the MIGS is important for determining not only the Schottky barrier but also the defect distribution around the metal/Ge interfaces.

Acknowledgements

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