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Dopant Redistribution at Nickel Silicide/Silicon Interface

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1. Introduction

In the trend of scaling down MOSFET, the reduction of contact resistance at the metal/silicon (Si) interface will be inevitable to achieve its higher performance. Since this resistance is inversely proportional to the transmission probability through the Schottky barrier, it will be fulfilled by enhancing the band bending of the Si layer. That could be possible only if we can fabricate a fully-depleted and extremely thin doping layer near the interface. The technique with dopant segregation (snowplow) effect (substitutional dopants beyond solubility limit), which was proposed recently [1,2], may be very promising. Figure 1 shows both boron (B) and arsenic (As) profiles of the nickel silicide (NiSi)/Si junction formed by the dopant segregation technique, which was obtained by backside SIMS. Although the impurities are distributed near the NiSi/Si interface, the distribution around the interface region is quite different. In particular, it has been found from the measurement of the I-V characteristics of the Schottky junction that the effective Schottky barrier height is not lowered for (B-doped) p-type Si as largely as for (As-doped) n-type Si. This dopant-dependence may reflect the difference of redistribution near the interface after silicidation. The aim of this study is to obtain physical insights into these dopant segregation phenomena at the NiSi/Si interface by using the first-principles calculation method. Then, we promote understandings on dopant segregation mechanisms in order to obtain superior Schottky junctions for realizing ultimately low contact resistance.

2. Calculation Methods

Our calculations are based on density functional theory, including spin-polarization and using generalized gradient approximations. The calculations were performed using ultrasoft pseudopotentials[3] for the atoms. Here, we used the unit cell including 64 atoms. We found that the cut-off energies of 25 Ry for the wave functions, 196 Ry for the augmented electron densities and 8 k points for Brillouine-zone samplings are sufficient for converging total energies.

3. Results and Discussions

First, we calculated the formation energies E_f of NiSi with an impurity atom in the interstice (E_f^{int}) or the substitutional site for a Ni atom (E_f^{Ni}) or that for a Si atom (E_f^{Si}), respectively and found the energetically most stable structure in each case. For example, the formation energy E_f^{Si} is defined as follows, as shown in Fig. 2.

$$E_f^{Si} = E_{\mathrm{Imp}} + E_{\mathrm{NiSi}} - E_{\mathrm{Si\,atom}} - E_{\mathrm{sub,Si}} \qquad (1)$$

, where E_{Imp}, E_{NiSi}, $E_{\mathrm{Si\,atom}}$ and $E_{\mathrm{sub,Si}}$ represent the energy of an impurity atom in vacuum, the total energy of NiSi unit cell in this calculation, the bulk silicon energy per Si atom and the total energy of NiSi cell with an impurity atom in the substitutional site for a Si atom, respectively.

Next, for the comparison of formation energies, we applied the same method for the calculation in the case of the bulk Si layer. We used the unit cell including 64 Si atoms. We also performed the calculation for Ni_2Si using the unit cell including 12 atoms. Here, we cannot neglect the formation energies of Ni_2Si, because the Ni_2Si phase appears first in the silicidation process with increasing RTA temperature [4]. The calculated results are listed in Table 1. B atoms exist in both the interstice and the substitutional site in the highly B-doped Si layer. We can also find that the formation energies (E_f^{int} and E_f^{Si}) in the case of both NiSi and Ni_2Si are much larger than those in the case of Si. Therefore, as shown in Fig. 3a, while Ni atoms move to the interface in the silicidation process, a B atom either in the interstice or in the substitutional site of the Si layer remains in the NiSi layer. B atoms around the interface in the unsilicidated Si layer may be absorbed in the NiSi layer. On the other hand, since the formation energy E_f^{int} for an As atom is a negative value, it cannot stay in the interstice in all cases, as shown in Fig. 3b. However, as shown in Fig. 4, the large difference in the formation energy E_f^{int} between the layers may drive an As atom migration into the unsilicidated Si layer through the interface in the silicidation process. Therefore, since the difference of the formation energy E_f^{Si} between the layers is small, As segregation definitely occurs on the both sides of the NiSi/Si interface.

4. Conclusions

By comparing the formation energies (E_f^{int} and E_f^{Si}) of both NiSi and Ni_2Si with those of Si, it was found that the Schottky junction is formed in the silicidation process with B atoms distributed on the NiSi side of the interface, on the other hand, with As atoms on the both sides. The impurity profile around the interface shown in Fig. 1 reflects possible stable structures with a larger formation energy as identified in our calculations. For appropriate regulation of the profile broadness, we need to know the migration potential

for the impurity atom around the interface. Our approach will lead to a new silicidation process to control the ultimate dopant profile realizing the effective lowering of the Schottky barrier height for ultimately low contact resistance.

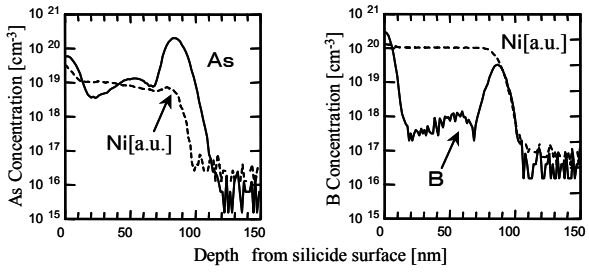

Fig. 1 Impurity and Ni profiles taken by backside SIMS.

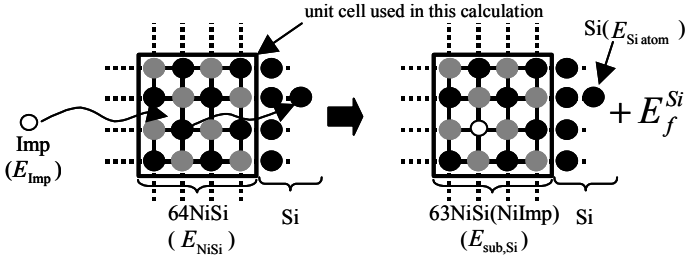

Fig. 2 The formation process of the NiSi cell where an impurity atom is substituted for a Si atom. Black, gray and white circles stand for Si, Ni and impurity atoms, respectively. We assumed that the Si atom in the site moves in the bulk silicon layer, namely, 64NiSi + Imp → 63NiSi(Ni Imp) + NiSi + Si.

Table 1 The calculation results of the formation energies.

a) B

	E_f^{Int}	E_f^{Si} (eV)	E_f^{Ni} (eV)
Ni_2Si	4.48	5.88	5.04
NiSi	4.28	5.24	4.55
Si	2.61	5.19	

b) As

	E_f^{Int}	E_f^{Si} (eV)	E_f^{Ni} (eV)
Ni_2Si	-2.86	2.84	1.68
NiSi	-2.66	2.65	0.49
Si	-0.61	2.33	

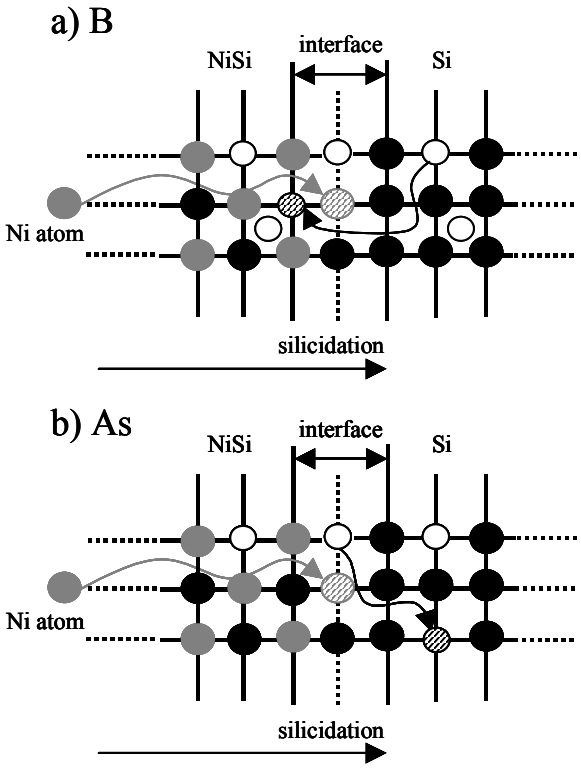

Fig. 3 The diagram that schematically shows the movements of a B or As atom through the NiSi/Si interface in the silicidation process, respectively. The circles mean the same as those in Fig.2. Arrows mean atom movements to the site shown as hatched circles.

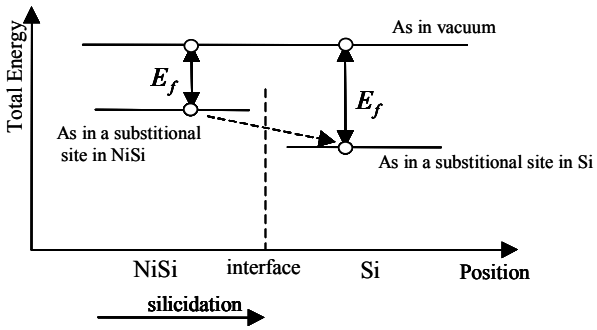

Fig. 4 This figure shows the As atom movement through the interface due to the difference of the formation energy between the layers.

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