Extended Abstracts of the 2010 International Conference on Solid State Devices and Materials, Tokyo, 2010, pp1000-1001

Interfacial atomic structure between Pt-added NiSi and Si (001)

Nobuyuki Ikarashi, Mitsuru Narihiro and Takashi Hase

LSI Research Laboratory, Renesas Electronics Corporation

1120 Shimokuzawa, Chuou-ku, Sagamihara, 252-5298, Japan

E-mail: nobuyuki.ikarashi.xz@renesas.com

1. Introduction

NiSi is used as contact to the source and drain in advanced metal-oxide-semiconductor field effect transistors [1]. In terms of the device production technology, the formation of NiSi2 has been serious concern because of the high-resistivity of NiSi2, which results in degradation of the transistor performances.

Various countermeasures have been proposed to suppress the transformation of NiSi to NiSi2: previous studies indicated that Pt when added to NiSi increases the reaction temperature of NiSi+Si→NiSi2 at the NiSi/Si interface, stabilizing NiSi [2-5]. Also, added Pt reportedly changes the texture of the NiSi layer and segregates near the NiSi/Si interface. These findings suggest that the added Pt probably affects the stability of the NiSi layer. However, the details of the Pt-added NiSi/Si interfacial structure, as well as how the added Pt changes the NiSi stability, have not been clarified.

Accordingly, we examined a Pt-added NiSi/Si (001) interface using a cross-sectional observation by high-angle annular dark-field scanning transmission electron microscopy (HAADF-STEM). The observation revealed the atomic structure of the interface and indicated that the added Pt segregates to reduce the interfacial strain and plays an important role in stabilizing the NiSi layer.

2. Experiments

We deposited Ni and Pt on a p-type Si (001) substrate, and sintered the sample at 500°C to form NiSi. The Pt composition of the film was 10 atomic %. In the HAADF-STEM observations, the electron probe convergence angle was 20 mrad, and the detector was set to collect the electrons scattered at angles between 45 and 110 mrad.

3. Results

A representative STEM image of the NiSi/Si interface is shown in Fig. 1. We found that the interface was atomically abrupt and that markedly bright spots appeared at the NiSi/Si interface. The bright spots bunch together and groups of bright spots are regularly spaced.

A Fourier transform of the STEM image (inset in Fig. 1) indicates that the crystal orientation of the NiSi matches one of the preferential alignments at the interface [2-4]. The NiSi film was poly-crystal and other alignments were also observed, but the interface was atomically abrupt and groups of the interfacial bright spots were observed in the large part of the interface regardless of the alignment. We thus describe the interfacial structure seen in Fig. 1 as a typical structure of the interface.

A close-up view of the interface (Fig. 2) shows that markedly bright atomic-column images are observed at the first interfacial atomic layer of NiSi and that they appear at the intervals of the two-dimensional unit cell. In addition, in the interfacial areas without the bright atomic-column images, Si atomic-column images were unclear and the interval of the unclear Si atomic-column images was 2.1 nm.

The unclear Si atomic-column images should be attributed to misfit dislocations at the interface. This is because their 2.1-nm interval agrees with average spacing of misfit-dislocations that is expected from the 15.4 % misfit at the interface when the lattice misfit is totally accommodated by 90° dislocations [9]. This finding also indicates that NiSi and Si are lattice matched locally in the areas between the misfit dislocations and that the interfacial bright atomic-column images appear in such lattice-matched areas.

Our STEM image simulation indicated that the observed interfacial bright atomic-column image is generated by substitution of Pt atoms for Ni atoms in the atomic-column. In Fig. 3, we replaced some of the Ni atoms with Pt atoms in atomic columns p1 and p2. They become brighter as the Pt composition increases and atomic-column p2 is the brightest. As a result, markedly bright atomic-column image appear at the interval of the two-dimensional unite-cell, reproducing the observed images in Fig. 1 and 2.

The STEM image intensity analysis indicates that Pt segregated only in the first interfacial atomic layer of NiSi. Figure 4(a) shows measured intensity distribution in a NiSi (010) plane that contains the markedly bright interfacial atomic column. The corresponding intensity distribution in the simulated image is shown in Fig. 4(b). The peak height of interfacial atomic column-image is clearly larger than those of atomic-column images in the second and following interfacial atomic layers, indicating that Pt atoms segregate only in the first interfacial atomic layer of NiSi.

4. Discussion

The in-plane distribution of Pt and misfit dislocations at the NiSi/Si interface (Figs. 1 and 2) is a direct evidence that Pt segregates at the interface to decrease the interface energy. We showed that Pt segregated in the interfacial area where the NiSi lattice matched the Si lattice (Fig. 5). Because the distances of these lattice-plane are 0.325 and 0.384 nm, respectively, and the PtSi (010) lattice-plane distance is 0.360 nm [6, 7], Pt segregation lowers the interfacial strain, reducing the interface energy, which linearly decreases as the interface strain decreases [8].

The activation energy of the NiSi2 formation, ΔG^*, is given by $\Delta G^*=\Delta\sigma^3/\Delta G^2$, where $\Delta\sigma$ and ΔG are the increases in the interface energy and Gibbs free energy, respectively [9]. Previous studies suggested that Pt addition probably

affected ΔG to increase ΔG* [3, 4]. In the present study, we showed that the Pt addition lowers the NiSi/Si interface energy, i.e., the interface energy before the NiSi2 nucleation. This strongly suggests that the Pt addition increases Δσ and raises the reaction barrier, ΔG*. Therefore, the changes in the interface energy should also play an important role in suppressing NiSi2 formation.

5. Summary

HAADF-STEM was used to analyze the Pt-added NiSi/Si interfacial structure. The observation revealed that Pt segregates at lattice-matched areas of the interface and occupied the Ni sites at the first interfacial atomic layer of NiSi. This finding shows that the added-Pt segregates to lower the interfacial strain and reduces the interface energy. Thus, we infer that the lowering the interface energy by the Pt-addition results in the NiSi layer being stabilized.

Acknowledgement

The authors thank Dr. N. Kasai from NEC and Dr. H. Watanabe for their helpful comments. We also thank Ms. M. Oshida for preparing the STEM specimens.

References

1. L. Chen, 'Silicide tech. for integ. circuits' (IEE, London, 2005)..
2. D. Mangelinck, et al., Lahiri, Appl. Phys. Lett. 75, 1736 (1999).
3. C. Lavoie et al., Micro. Electronic. Eng. 70, 144 (2003).
4. C. Detavernier and C. Lavoie, Appl. Phys. Lett. 84, 3549 (2004).
5. H. Akatsu, et al,. Mater. Res. Soc. Symp. Proc. 1070, 79 (2008).
6. F. d'Heurle, et al., J. Appl. Phys. 55, 4208 (1984).
7. R. W. G. Wyckoff, 'Crystal Structures' (John Wiley & Sons, New York, London, 1963).
8. A. Zangwill, 'Physic at Surfaces' (Cambridge University Press, London, 1988).
9. F. d'Heurle, J. Mat. Res. 3, 167 (1988).

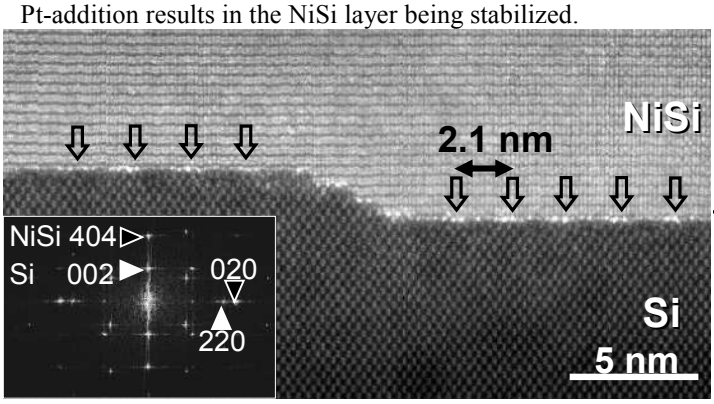

Fig. 1 Cross-sectional HAADF-STEM image of NiSi/Si interface. Fourier transform of the image is shown in the inset, where open and filled triangles indicate spots due to NiSi and Si, respectively. Markedly bright spots bunch together at the interface (denoted by open arrows).

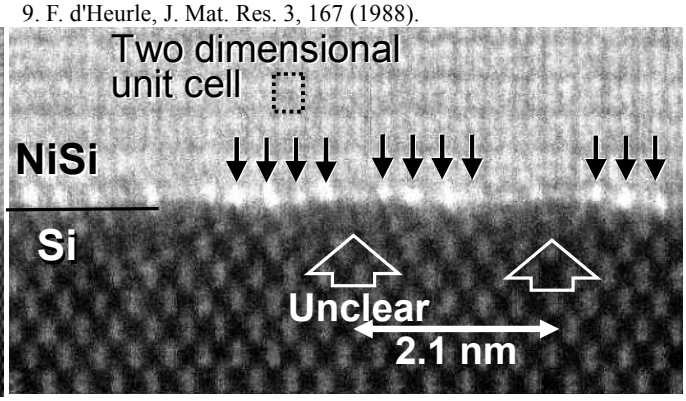

Fig. 2 Close-up view of NiSi/Si interface. A rectangle shows the two-dimensional unit cell of NiSi. Markedly bright atomic-column images denoted by arrows were observed in the first interfacial layer of NiSi. The Si atomic-column image is unclear in the interfacial areas that are denoted by open arrows.

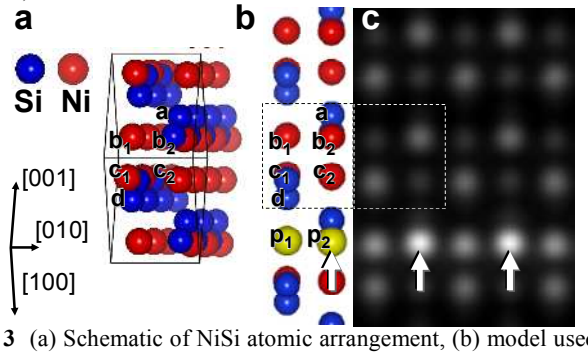

Fig. 3 (a) Schematic of NiSi atomic arrangement, (b) model used in simulation, and (c) example of simulated STEM image of NiSi. Rectangle in (b) and (c) shows two-dimensional unit cell. One third of Ni is replaced by Pt in atomic columns p1 and p2 in (c).

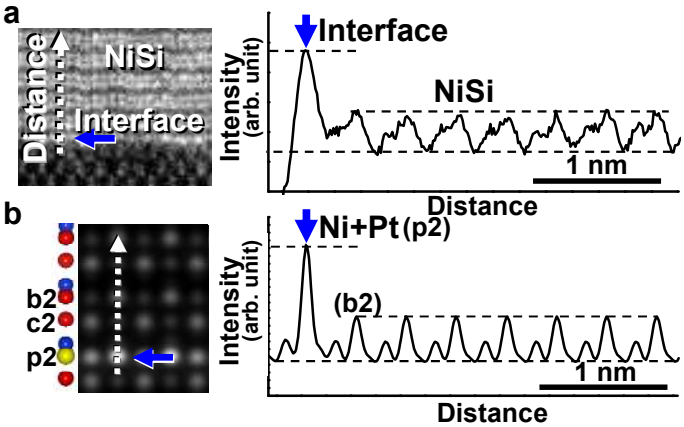

Fig. 4 (a) Intensity distribution in the STEM image in Fig. 2. (b) Corresponding simulated intensity distribution in Fig. 3(c). In (a), the peak height of the interfacial bright atomic-column image is clearly larger than that of the atomic-column images in NiSi. Intensity distribution in (b) reproduces that in (a).

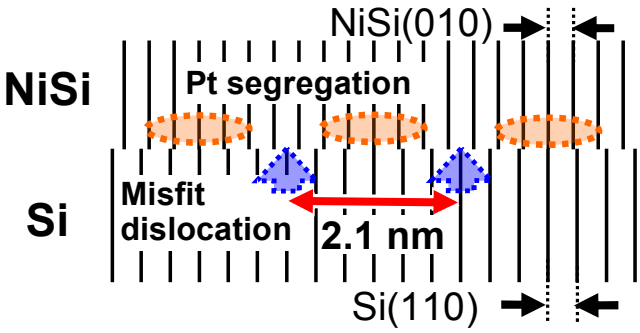

Fig.5 Schematic of relative positions of Pt segregation (denoted by circles) and misfit dislocations (denoted by arrows) at NiSi/Si interface. Vertical lines show lattice planes of NiSi and Si.