HRTEM Study of an Epitaxial C49-TiSi2 Phase Formed on the Si (100) Substrate

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Ⅰ. Introduction

The Ti-silicide compounds formed by a solid-state reaction of Ti and Si have very important applications such as silicide/active contacts and interconnection materials in microelectronic device technology due to its high conductivity and selective growth on Si [1,2]. A mechanism on the formation of TiSi2 accompanying a phase transformation (unstable and defective C49 phase stable C54 phase) in thermal treatment at a relatively low temperature has been extensively studied.

Recently, the epitaxial C49-TiSi2 phases were observed by a retarded interdiffusion of Ti and Si atoms, and it was found that the C49 phase was thermally stable even at the high temperature of above 900℃ without transforming to the C54 phase [3,4]. However, the formation mechanism of epitaxial C49-silicides and the interfacial structure have not yet been clarified. In this study, the crystallographic characteristics between the epitaxial C49-TiSi2 phase and the Si (100) substrate are investigated by HRTEM study. We discuss the formation mechanism of the epitaxial C49 phase and stacking faults lying on the C49 (020) plane through the atomic modeling and HRTEM simulation based on the experimental HRTEM images.

Ⅱ. Experiment

The preparation procedure of an epitaxial C49-TiSi2 island is as follows. The Si (100) substrate surface was cleaned by a dilute-HF last and exposed to a N2 plasma nitridation under the RF power of 410 W. And then, Ti film 20 nm was deposited on the Si substrate by ionized metal plasma. Silicidation was carried out by 2-step rapid thermal annealing (RTA) at the temperature of 670℃ and 850℃ (for 20 s under a N2 ambient).

TEM study for the crystallographic characterization of the epitaxial C49-TiSi2 phase on the Si substrate and stacking faults in the C49 phase was performed using a JEM-2010UHR TEM (JEOL) having a point-to-point resolution of 0.20 nm at the accelerating voltage of 200 kV. The incident electron beams were parallel to the [011] and [100] directions of the Si substrate for the cross-sectional and plan-view observations, respectively. The simulation of HRTEM images for the stacking fault formed on the C49 (020) plane was carried out by the multislice method using the Cerius2 software package.

Ⅲ. Results and Discussion

Figure 1 shows TEM images of an epitaxial C49-TiSi2 island produced with a N2 treatment on the Si (100) substrate prior to the Ti deposition. The cross-sectional TEM image of Fig. 1(a) indicates that the side and bottom planes of the epitaxial C49 island are almost parallel to the (111) and (100) plane of the Si substrate, respectively. The conventional C54-TiSi2 film, which is polycrystalline and random oriented to the substrate, was formed with a continuous layer as prepared by the same annealing condition however, it was morphologically agglomerated as shown in the inset of Fig. 1(a). It was also observed that the epitaxial C49-TiSi2 phase was formed by the mobility reduction of Ti and Si atoms with the TiNx precursor or the SiNx buffer layer produced by the N2 treatment [3,4]. This epitaxial C49 phase was not transformed to the C54 phase even at the high temperature of ~900℃. Note that the thicker TiN film was observed in the case of the N2 treatment [Fig. 1(a)]. Based on the TEM results, the epitaxial relationship between the C49-TiSi2 island and the Si substrate is found to be [001]C49 // [011]Si and (010)C49 // (100)Si.

The formation of epitaxial C49-TiSi2 on the Si substrate is explained with the atomic models. The Si atomic model projected to the [011] direction and the C49-TiSi2 atomic model to the [001] one are represented in Figs. 2(a) and 2(b), respectively. From the comparison of the models, it is observed that the C49-TiSi2 structure is basically formed by the substitution of one atom in a dumbbell site of the Si structure to the Ti atom. Also, it is found that the $\sqrt{2}a$ $\sqrt{2}a$ $5a$ structure of Si is well matched with the $2a$ $2c$ $2b$ one of C49-TiSi2. Suppose that the family plane in the Si structure is considered (90° rotation), the atomic arrangement of the C49-TiSi2 (100) zone is also possible as indicated in Fig. 2(c).

The C49-TiSi2 phase include many defects, especially on the (020) plane. The stacking faults on the C49 (020) plane are clearly observed in Fig. 3(a) (regions indicated by the arrows). From the enlarged HRTEM images obtained in the another island, it is clearly observed that the stacking fault was formed by the lattice translation of 1/2[001] as considered in two-dimension [Fig. 3(b)], and further the continuous translated region exists [Fig. 3(c)]. Through the investigation of their atomic arrangement, it was found that the non-faulted region (A) corresponds to the (100) plane, and the faulted region (B) the (001) one.

The atomic arrangements of the C49-TiSi2 (001) and (100) planes can be interchanged each other due to the similarity of the lattice geometry such as plane spacings and interplanar angles. The atomic arrangement in the C49 (100) plane can be made by the lattice translation of 1/2[100] and

1/2[001] in the A1* and C1* atomic layers of the (001) plane as indicated in Figs. 2(b) and 2(c). Shown in Fig. 4 is an HRTEM image of the atomic structure in the [100] zone, where the atomic rows indicated by arrows correspond to the stacking faults. The atomic structure of the stacking faults is similar to the atomic structure in the [001] zone. Based on the results, the HRTEM image of the stacking fault simulated with the same magnification is shown in the inset of Fig. 4. The atomic model and the simulated image of the stacking faults are well matched to their experimental HRTEM image.

IV. Conclusion

From the HRTEM study on the formation of the epitaxial C49-TiSi2 phase on the Si (100) substrate, we have concluded that the TiSi2 phase and the Si substrate have the orientation relationship of [001]C49 // [011]Si and (010)C49 // (100)Si, and the formation of epitaxial C49-TiSi2 on the Si (100) substrate could be explained with the lattice correspondence of the Si $\sqrt{2}a$ $\sqrt{2}a$ $5a$ and C49-TiSi2 $2a$ $2c$ $2b$ structures. Furthermore, it was suggested that stacking faults lying on the C49 (020) plane is formed by the interchange of the C49-TiSi2 (001) and (100) planes due to the similarity of the lattice geometry.

References

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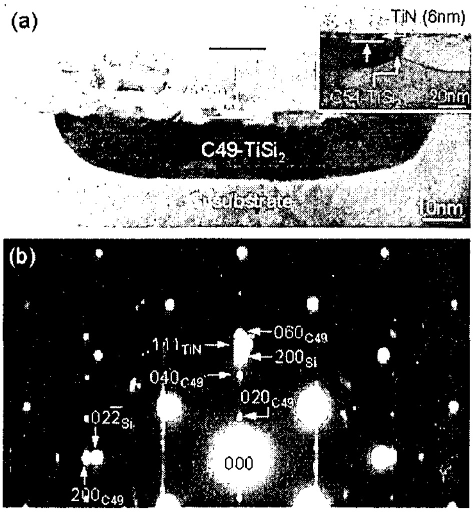

Fig. 1. Cross-sectional TEM image (a) and electron diffraction pattern (b) showing an epitaxial C49-$TiSi_2$ island formed on the Si (100) substrate with a N_2 treatment. The electron incident beams were parallel to the [001] direction in C49-$TiSi_2$ and the [011] direction in Si. The C54-$TiSi_2$ film formed by conventional silicidation is shown in the inset of Fig. 1(a).

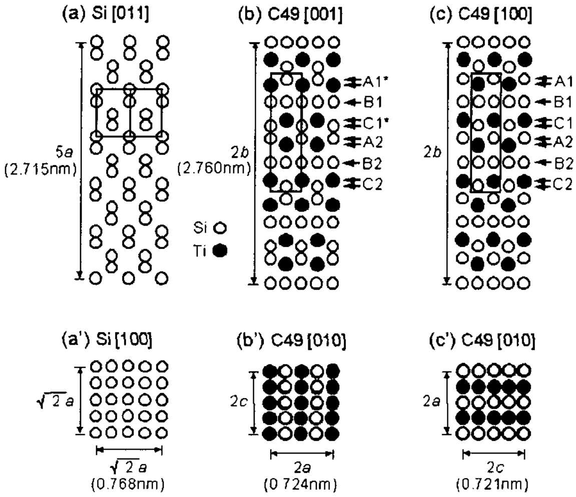

Fig. 2. (a) and (a') Si atomic models projected to the [011] and [100] directions. (b) and (b') C49-$TiSi_2$ atomic models projected to the [001] and [010] directions. (c) and (c') C49-$TiSi_2$ atomic models projected to the [100] and [010] directions. In the models, the rectangles correspond to the unit cells.

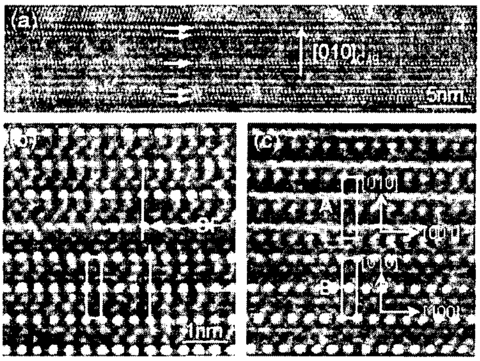

Fig. 3. (a) HRTEM image showing the stacking faults lying on the C49-$TiSi_2$ (020) plane. Enlarged HRTEM images obtained in other regions are shown in (b) and (c). The rectangles in (b) and (c) correspond to the unit cell of the C49-$TiSi_2$ phase.

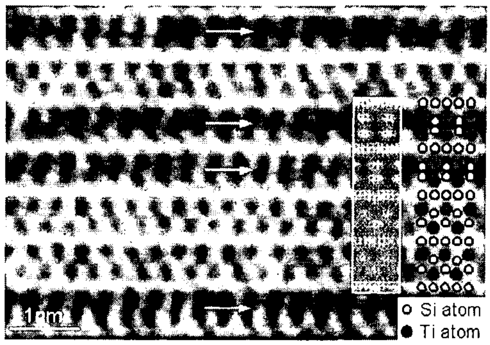

Fig. 4. HRTEM image showing the atomic structure of the stacking fault in the C49-$TiSi_2$ phase. The atomic model and the simulated HRTEM image are indicated in the image with the same magnification. The HRTEM simulation was carried out in the condition corresponding to the specimen thickness of ~27 nm (75 slices) and the defocus of −60 nm.