Extended Abstracts of the 2010 International Conference on Solid State Devices and Materials, Tokyo, 2010, pp1309-1310

Epitaxial $NiSi_2$ Buffer Technique for Fluoride Resonant Tunneling Devices on Si

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1. Introduction

Resonant Tunneling Devices composed of ultra-thin fluoride heterostructures on Si such as $CaF_2/CdF_2/CaF_2/Si$ are one of promising candidates for quantum devices co-integrated with Si integrated circuit [1, 2]. However, large chemical reactivity between CdF_2 and Si is a significant problem, which leads instable electrical properties of the devices due to very low growth temperature around room temperature (R.T.) to avoid the chemical reaction.

We propose a new approach in which epitaxial $NiSi_2$ layer is introduced as a buffer layer to control the chemical reaction. From the view point of Gibbs formation energy, reactivity of CdF_2 with $NiSi_2$ is much lower compared to that of CdF_2 with Si. Therefore, use of higher growth temperature to improve quality of the grown layers is expected. Since $NiSi_2$ has fluorite crystalline structure with lattice constant very close to that of Si, this is a suitable material for buffer layer in the heteroepitaxial structures.

Heteroepitaxial growth of $NiSi_2$ on Si substrates was systematically investigated by Tung et al. [3.4], and microscopic growth behaviors related to its growth conditions has been clarified. In this work, based on the knowledge, uniformity of $NiSi_2$ layer in large area and growth characteristics of fluoride layers on the $NiSi_2$ layer are investigated, and potential of the new approach to overcome the problem of chemical reaction is demonstrated.

2. Experimental Procedures

$NiSi_2$ layers were grown by using a solid source molecular beam epitaxy system equipped with an electron beam evaporator of Ni. Heavily doped N-type Si(111) substrates were chemically cleaned and thermal flushing in UHV was carried out to obtain clean surfaces. The following growth methods were carried out and compared. In the first method, Ni is deposited on heated substrate, which is referred as "direct growth method". In the second method, Ni is deposited on the substrate at R.T. and post annealed *in situ* for silicidation, which is referred as "two-step growth method". In the third method, after a thin $NiSi_2$ layer is grown by the two-step growth method, an additional growth is carried out by supplying Ni molecular beam on the heated sample subsequently, which is referred as "additional growth method".

20-nm-thick CdF_2 layers were grown on the $NiSi_2/Si$ structure at 100°C. Not only $CdF_2/NiSi_2/Si$ structures, but also the structures with a 3-nm-thick CaF_2 buffer layer, $CdF_2/CaF_2/NiSi_2/Si$ structures, were grown. The structures without $NiSi_2$ layer were also grown as references to see the effects of the $NiSi_2$ buffer layer.

3. Results and Discussion

Two-Step Growth Method

Surface morphologies of $NiSi_2$ layers grown by the direct growth method at 500°C and by the two-step growth method with 500°C post annealing are shown in Fig. 1, in which Ni of equivalent thickness of 2 nm was deposited. Epitaxial growth of single crystalline $NiSi_2$ was confirmed for both layers by RHEED observations. Agglomeration was occurred and Si surfaces were exposed partially for the direct growth method (Fig. 1(a)). On the other hand, very smooth surface was obtained for the two-step growth method (Fig. 1(b)).

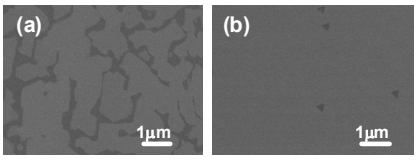

Fig.1 SEM images of $NiSi_2$ surfaces grown by 2 nm Ni deposition. (a) Direct growth method at 500°C. (b) Two-step growth method with 500°C post annealing.

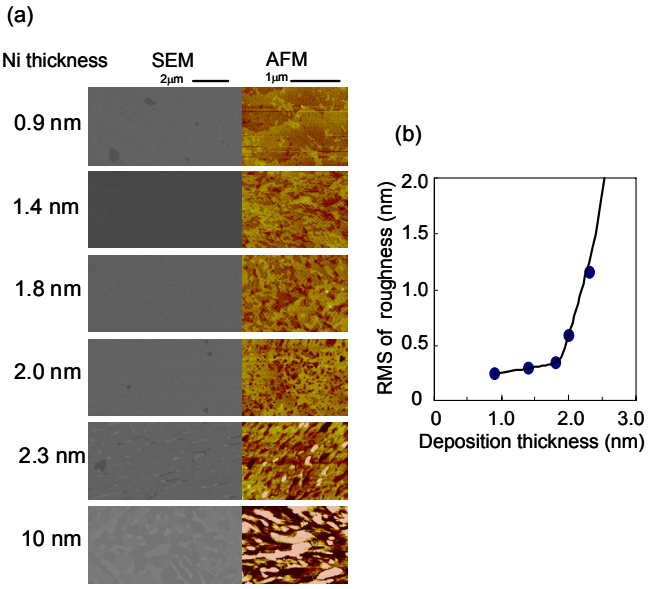

Fig.2 Surface morphologies of $NiSi_2$ layers grown by two-step growth method with 500°C post annealing, depending on thickness of Ni deposited. (a) SEM and AFM images. (b) RMS of surface roughness as a function of Ni thickness.

The thickness of Ni deposited in the two-step growth process was fond to be very critical. Figure 2 shows surface morphologies of $NiSi_2$ grown by the two-step growth method depending on the thickness of Ni deposited. The incomplete coverage of substrate surface or agglomeration of $NiSi_2$ was occurred in the regions of Ni thickness thinner than 0.9 nm and thicker than 2.4 nm. Excess Ni deposition led heavy agglomeration as indicated by increase in surface roughness as shown in Fig. 2(b).

Additional Growth Method

For the enough control of the chemical reaction, $NiSi_2$ layer thicker than that optimized above is desirable. The additional growth method was fond to be useful for the purpose. After the initial $NiSi_2$ layers were grown by the two-step growth method with the optimum condition, Ni of 8 nm in equivalent thickness was supplied on the heated samples. Figure 3 shows morphologies of the grown surfaces as a function of substrate temperature during the additional Ni deposition. All surfaces exhibited epitaxial growth but their morphologies were varied. The very smooth surface was obtained at 500°C.

Growth on CdF_2 Layers on $NiSi_2$ Buffer

In order to see the effects of insertion of $NiSi_2$ buffer layers, 20-nm-thick CdF_2 layers were grown at 100°C on the $NiSi_2$ layer formed by the additional growth method at 500°C described above. It is known that CdF_2 does not grow directly on Si surface but rather etches Si surface at 100°C due to the chemical reaction.

CdF_2 was deposited on the $NiSi_2$ surface even at 100°C, however, the deposited CdF_2 layer exhibited very poor crystallinity. It was found that insertion of a thin (3nm) CaF_2 layer between $NiSi_2$ and CdF_2 was useful to obtain good epitaxial growth of the CdF_2, in which growth condition of the thin CaF_2 was optimized to the two-step growth

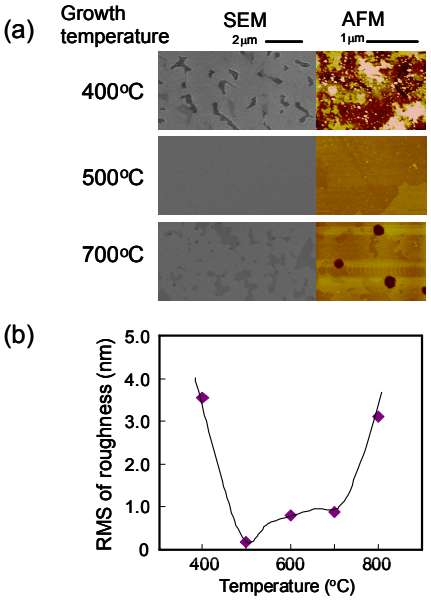

Fig.3 Surface morphologies of $NiSi_2$ grown by additional growth method with 8 nm Ni addition, depending on substrate temperature during the additional growth process.

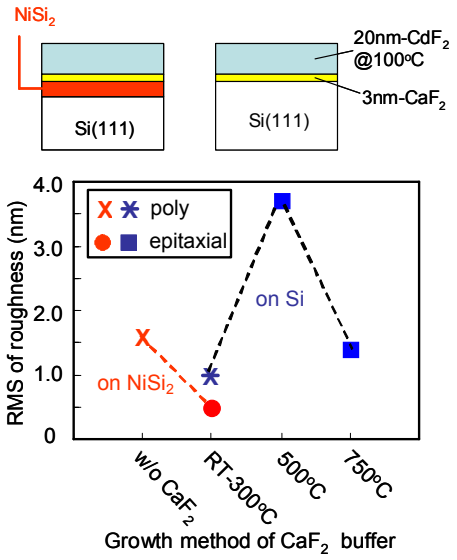

Fig.4 Properties of 20-nm-thick CdF_2 layers grown at 100°C on various structures of substrates. Growth with and without $NiSi_2$ buffer layer is compared for the condition of 3-nm-CaF_2 layer.

composed of RT deposition and post annealing at 300°C.

Figure 4 shows surface roughness and classification of epitaxial growth or polycrystalline growth of the 20-nm-thick CdF_2 layer grown at 100°C depending on the growth condition of the 3-nm-thick CaF_2 buffer layer. The results of direct growth on Si substrate without $NiSi_2$ are also shown for comparison. The various growth condition of the CaF_2 buffer layer were examined because optimum condition was different between on $NiSi_2$ and on Si. As a result, epitaxial CdF_2 grown at 100°C on the $NiSi_2$ buffer layer exhibited obvious advantage in smooth surface compared to on bare Si substrates.

4. Conclusion

Growth condition of epitaxial $NiSi_2$ buffer layer to control chemical reaction between Si and CdF_2 was surveyed, and very uniform $NiSi_2$ layer was realized by using the additional growth method composed of initial growth by the two-step growth method and the following Ni deposition on the heated substrate. Growth of CdF_2 layers at 100°C on the optimized $NiSi_2$ buffer layer was achieved. Growth at the same temperature was not successful on bare Si substrate without $NiSi_2$ buffer layer. The $NiSi_2$ buffer technique is useful to obtain fluoride heterostructures with good quality on Si since it enable higher temperature growth.

Acknowledgement

This work was partially supported by Grant in Aid of Science Research from Ministry of Education, Culture, Sports, Science and Technology.

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