Investigation of Effect of Sputtering Gases on Ion-Beam-Sputtering Growth of Si and Ge

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Sputtering gas effects on Si and Ge homo- and hetero-epitaxy by ion-beam-sputtering technique are investigated. A Mote Carlo sputtering simulation was developed and the kinetic energy distributions of sputtered atoms were simulated for the case of Ar, Kr and Xe sputtering gases. The larger atomic mass, the smaller kinetic energy. Moreover, Si and Ge epitaxy experiments were carried out and film crystallinity was analyzed. A better crystallinity was obtained for Kr and Xe than that of Ar. The kinetic energy was clarified to significantly affect the crystallinity.

Key words: Si Ge epitaxy, sputtering simulation, hetero-epitaxy, strained growth

1. INTRODUCTION

SiGe is attracting great attention as one of the key material for developing future high-speed devices and high performance ultra-large scale integration(ULSI). Heterojunction bipolar transistor(HBT) with a SiGe graded base have achieved a cut off frequency of 350GHz[1], which must not be realized in Si homojunction transistors and is comparable with compound semiconductor HBTs.

On another application, a strained Si which is usually prepared on relaxed SiGe substrates is anticipated to generate about twice large carrier mobility[2], which contributes increase of the current drivability of scaled MOSFETs, resulting in high speed operation of the ULSI system. Moreover, SiGe is useful for a gate electrode instead of poly-Si and an ohmic contact buffer to reduce parasitic capacitance and resistance[3].

We have been developing ion-beam sputtering technique as a tool of epitaxial growth of SiGe thin films[4]. Distinctive features of the sputtering technique are that some of emitted atoms from a target and recoiled Ar atoms have large kinetic energy of more than several tens eV. The bombardment would enhance crystalline growth due to increase of surface migration, while it would induce crystalline defects due to radiation damage depending on the impact energy. Thus, to control the kinetic energy is a significant issue in the sputtering film preparation.

In this paper, first we present a simulation result of the sputtering physical process employing Monte Calro technique. We found in the simulation that the kinetic energy is decreased by using sputtering gases with large atomic mass. We demonstrate that high quality Si films are obtained in the case using sputtering gases with large atomic mass and indicate the significance of the energy control in the sputtering process.

2. EXPERIMENTS

A Kaufmann type ion source (SINCRON, KIS-50P, 90mm caliber) and a rotary target holder on which Si and Ge disk targets with 3-4 inch diameters were fixed were equipped in a vacuum system. An ion-beam (approximately 30mm dia.) was focused on the targets by a dish shape acceleration electrode made by graphite. The target was tilted against the incident ion-beam and the substrate holder. The back ground pressure and the gas pressure during the film deposition were $<5x10^{-8}$ and $2x10^{-4}$ Torr, respectively. Schematic of geometry of the IBS system is shown in Fig.1.

Si(100) wafer substrates were loaded in the ionbeam sputtering system after the chemical cleaning by dipping in an aqueous HF solution. The substrate was heated by an alumina heater block. The substrate temperature was measured in advance by using a dummy substrate with a thermocouple attached on the dummy substrate surface. Unlike the conventional sputtering technique, substrate heating by the plasma radiation can be ignored in the ion-beam sputtering because the substrates are isolated from the plasma.



Fig.1. Schematic of geometry of incident ion-beam, sputtering target and substrate.

Substrate pre-heating at 550° C was carried out in the vacuum chamber. By means of this heat treatment, the adsorbing contaminants and the surface-terminating hydrogens are considered to be removed. If we omit this process, epitaxial growth have not taken place at any substrate temperature lower than 450° C.

Si/Ge multi-layered films were prepared by sputtering the Si and Ge targets alternately. The film thickness and the average Si/Ge composition were evaluated from the each sputtering time. The typical Si and Ge film growth rates were 0.05 and 0.066nm/s, respectively when Ar ion acceleration voltage is 500V and current is 10mA.

The film crystallinity and surface roughness were characterized by X-ray diffraction (XRD), reflection high-energy electron diffraction (RHEED, and atomic force microscope (AFM).

3. RESULTS AND DISCUSSION

3.1 Sputtering simulation

A particle simulation employing Monte Calro technique was performed. Physical process based on the LSS theory was taken into account for the simulation. Details are appeared elsewhere [5].

An example of the simulation on energy distribution of sputtered Si atoms is shown in Fig.2. Where, the primary incident ions are Ar, Kr and Xe and the acceleration energy is 500eV. Any distribution spectra are commonly seen to peak at around 10eV and in the higher energy region exponentially decrease with energy increase. Nevertheless, closely observing the spectra, that of Ar deviates to higher energy side comparing with those of Kr and Xe. Average energy was calculated, as a result, those of Kr and Xe were 30% and 50% smaller than that of Ar, respectively. The reason why Ar sputtering induces high energy sputtered particles is that the atomic mass of Ar is near to that of Si so that kinetic energy transfer takes place effectively.

Simulation was performed also on recoiled sputtering atoms on the target as shown in Fig.3. Unlike the target atoms, clearly as the atomic mass becomes larger, the kinetic energy decreases.



Fig.2. Energy distribution of sputtered Si atoms. Sputtering gases are Ar, Kr and Xe. Acceleration energy of incident ions is 500eV.



Fig.3. Energy distribution of recoiled atoms (Ar, Kr and Xe) on the Si target surface. Acceleration energy of incident ions is 500eV.

As we have reported before[4], it is impossible to lower the kinetic energy of sputtered particles by decreasing the incident energy of sputtering gas. However, it was possible to decrease it by choosing sputtering gas with a large atomic mass.

3.2 Crystallinity of Si films

Experiments of Si film growth were carried out using Ar, Kr and Xe gases. The substrate temperature was 600° C and the thickness was 50nm.

RHEED images are shown in Fig.4. Any case shows a streak pattern revealing good epitaxial growth. As for Kr case, the Kikuchi-line is observed obviously and also for Xe case it is somewhat observed. While for Ar case, no such a pattern. Because the Kikuchi-line appears when crystalline integrity is very high, it can be said that Si films grown by Kr and Xe have better crystallinity than that by Ar. In any our experiment using Ar in past Kikuchi-line has never been observed, thus this difference is due to Ar itself.

As discussed in previous section, it is reasonable to correlate the crystallinity to the kinetic energies of sputtered and recoiled atoms, although it is unknown



Fig.4. RHEED images of Si films prepared by using Ar, Kr and Xe as sputtering gases.

that which contribution of them is essential to the crystallinity.

3.3 On Ge film growth

According to the similar simulation on Ge sputtering, unlike Si case little significant difference of energy distribution of sputtered atoms was seen. This would be because the atomic mass of Ge is comparable with those of Kr and Xe.

Ge epitaxial growth using Kr and Xe sputtering gases carried out as well as Ar. Distinguishable difference of crystalinity of the films was not found because the heteroepitaxial growth of Ge films on Si substrates was likely to induce crystalline defects due to the lattice miss-mach. From RHEED images of the Ge films epitaxial growth was confirmed. For Ar the RHEED image showed streaky pattern while for Kr and Xe showed spotty pattern as shown in Fig. 5. These results suggested that the surface roughness of the films



Fig.5. RHEED images of Ge films prepared on Si substrates by using Ar, Kr and Xe as sputtering gases.

prepared by Kr and Xe was larger than that by Ar. In fact, the root mean square values of surface roughness measured by AFM were 0.5, 2.4 and 3.6nm for the cases of Ar, Kr and Xe, respectively. It is known that the strained growth of Ge on a Si substrate continues until 6 atomic-layers(=0.85nm)[6], over that the elastic deformation of Ge collapses and crystalline defects such as lattice dislocation takes place abruptly, resulting in surface roughness. Such a phenomena is observed in ideal epitaxial growth, however, in defective crystalline growth, for example low temperature growth, would not always take place because crystalline defects function to absolve the lattice strain. Standing on the above consideration, crystallinity of the films prepared by Kr and Xe comes to be superior to that by Ar.

4.CONCLUSIONS

We developed sputtering process simulator and showed that the energy can be decreased by using sputtering gases with large atomic mass. Moreover, we found that crystallinity of Si films was improved by using the sputtering gas with large atomic mass. Therefore we conclude that energy control of sputtered atoms is a main issue to grow high quality Si and Ge epitaxial films by sputtering technique.

5. REFERENCES

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