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Limiting conditions of Si selective epitaxial growth in Si_2H_6 gas-source molecular beam epitaxy

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The limiting conditions are presented of selective epitaxial growth (SEG) on a SiO_2-patterned Si (001) substrate for Si gas-source molecular-beam epitaxy by use of 100% Si_2H_6. In the initial stage of growth, epitaxial Si was selectively grown on a Si surface in the wide temperature range of 500–850 °C. On the other hand, polycrystalline Si nucleation on a SiO_2 surface was intimately related to the total volume of supply gas. At a substrate temperature of 700 °C and a Si_2H_6 flow rate of 60 sccm, a SEG layer could be deposited at a rate as high as 645 Å/min.

Si gas-source molecular-beam epitaxy (MBE) using SiH_4 or Si_2H_6 has many advantages, such as a low process temperature, no spitting defects, a high growth rate, and selective epitaxial growth (SEG) on SiO_2-patterned Si.[1,2] In particular SEG is one of the most important technologies for fabricating future ultra-large-scale integrated circuits (ULSIs). Yew and Reif reported that the SEG temperature using HCl should be higher than 900 °C by chemical vapor deposition (CVD).[3] On the other hand, Gas-source MBE is one of the most promising methods for low-temperature SEG. However, Hirayama and co-workers reported that SEG conditions using Si_2H_6 were restricted to the low-molecular-beam intensity[2] and consequently the growth rate was very low. In this study, we tried to find the critical condition of Si-SEG on a SiO_2-patterned Si(001) substrate using reflection high-energy electron diffraction (RHEED) observations in the wide temperature range of 500–850 °C using pure Si_2H_6.

The Si SEG layers were grown with a gas-source MBE system (ANELVA GBE-620) which consists of a loadlock chamber and a growth chamber with liquid–nitrogen shrouds. The growth chamber is evacuated to the background pressure of 1.5×10^{-9} Torr by a 1000 l/s turbomolecular pump (SEIKO SEIKI STP-H1000C) and liquid-nitrogen shrouds. According to the change of Si_2H_6 flow rate from 1 to 60 sccm, the steady-state pressure in the growth chamber varied from 2×10^{-6} to 5×10^{-5} Torr. The substrate was a 4-in. (001) Si wafer patterned with CVD SiO_2 and rinsed in an etching solution (H_2O:H_2O_2:NH_4OH = 20:6:1) before loading. After thermal cleaning in the growth chamber at 850 °C for 10 min, films were grown at several temperatures. The presence of SEG was observed using the RHEED pattern. When the RHEED pattern showed 2×1 with a halo, polycrystalline Si was not observed on SiO_2 by scanning electron microscopy (SEM) and the atomic Si signal was not detected by auger electron spectroscopy (AES), either. However, when the RHEED pattern changed to 2×1 overlapped with rings, polycrystalline Si on SiO_2 was clearly observed by SEM and Nomarsky microscopy. The experiment will be described in more detail elsewhere.[4]

Periodic RHEED observations during growth showed that polycrystalline Si nucleation started after an initial incubation time. For example, for growth at 600 °C and a Si_2H_6 flow rate of 15 sccm the transition between perfect and imperfect SEG growth occurred between 14 and 18 min after the start of growth. As shown in Fig. 1, the incubation time was decreased with increasing the gas flow rate at 600 °C. The curve shows that the incubation time was inversely proportional to the gas flow rate. Therefore, a product of the incubation time and the gas flow rate, i.e., the total volume of gas supplied during the incubation time, is a constant at the fixed temperature. This implies that the total volume of gas supplied during the incubation time is a critical volume above which polycrystalline Si nucleation started.

Figure 2 shows the critical volume of supply gas as a function of the substrate temperature. In the low-temperature region below about 650 °C, the critical volume of supply gas decreases with increasing substrate temperature independent of the gas flow rate, whereas above about

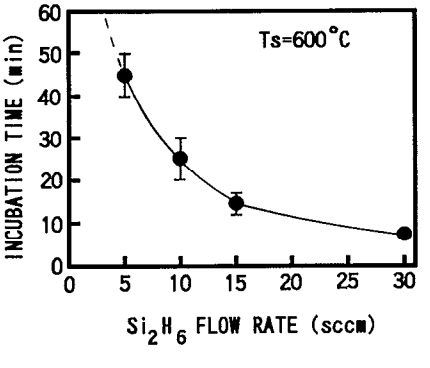

FIG. 1. Flow rate dependence of incubation time. When Si_2H_6 was supplied for longer than the incubation time, polycrystalline Si was nucleated on the SiO_2.

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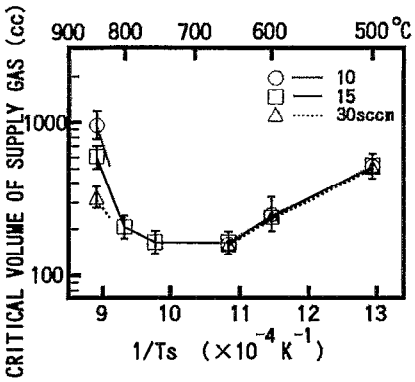

FIG. 2. Critical volume of supply gas for polycrystalline Si nucleation on SiO_2 vs substrate temperature. The critical volume of supply gas is equivalent to the product of the incubation time and the gas flow rate.

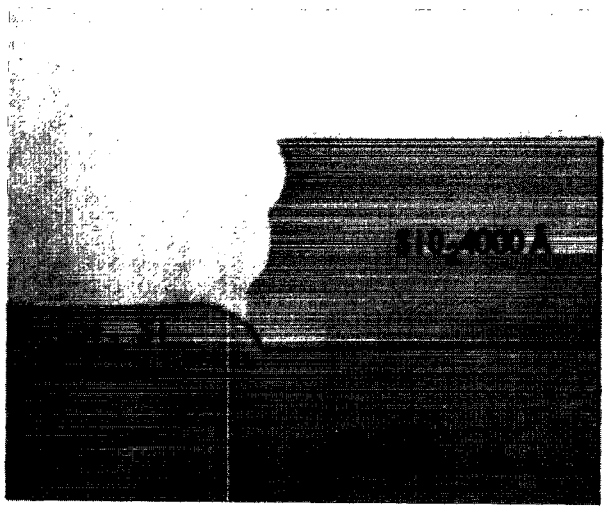

FIG. 3. Cross-sectional TEM image showing an epitaxial layer grown selectively on the exposed Si window without polycrystal line Si grown on SiO_2. The film was deposited at a growth rate of 645 Å/min with a thickness of 1290 Å at 700 °C and a gas flow rate of 60 sccm.

750 °C the critical volume increases with the substrate temperature. The temperature dependence of the critical volume is thought to change gradually from decreasing to increasing between 650 and 750 °C. Moreover, at 850 °C the critical volume decreases with increasing gas flow rate.

The critical volume of supply gas suggests that there is a critical coverage of reacted species on the SiO_2 surface to start polycrystalline Si nucleation, since the number of reacted species decomposed from impinged Si_2H_6 molecules is proportional to the volume of gas supplied under molecular flow conditions. While Si_2H_6 molecules are decomposed and contribute to the epitaxial growth on the Si surface, most of the molecules impinging on the SiO surface are reflected with a small portion decomposing and remaining on the SiO_2. As far as the density of reacted species on SiO_2 does not exceed the critical coverage, the polycrystalline Si nucleation does not start and SEG continues on the Si surface.

In the low-temperature region below 650 °C, the surface reaction on SiO_2 is explained by the mechanisms described above. The surface decomposition rate of Si_2H_6 increases with temperature, and thus the critical volume of the supply gas decreases with increasing temperature. In the high-temperature region over 650 °C, etching of the SiO_2 surface by decomposed Si_2H_6 must also be considered. Tabe reported[5] that at high temperature, SiO_2 and Si evaporated from a solid source react as

$$Si + SiO_2 \rightarrow 2SiO,$$

and that the volatile SiO is evaporated at the growth temperature. Since the reacted species necessary for Si island nucleation is lost by the above reaction, the critical volume of supply gas is increased with temperature. By increasing the gas flow rate at a constant temperature, the polycrystalline Si nucleation rate becomes higher than the SiO evaporation rate. Therefore, the critical volume of supply gas decreases with increasing the gas flow rate at 850 °C. In the temperature region where SiO evaporation is significant, the critical volume of supply gas depends on the gas flow rate.

The results above show that the integrated flux of Si_2H_6 molecules impinging on the surface, from which the system-dependent critical volume of Fig. 2 is derived, determines the conditions for SEG. At high deposition temperatures the growth rate is also important. The quality of epitaxial growth was investigated using transmission electron microscopy (TEM). Figure 3 shows a cross-sectional TEM image of a 1290-Å SEG film deposited at 700 °C with a gas flow of 60 sccm. The growth rate of 645 Å/min was the highest achieved in this study. It can be seen that the contact of the epitaxial Si layer with the side wall of the SiO_2 is satisfactory.

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