Advanced technique to decrease defect density
in molecular-beam-epitaxial silicon film

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Because of the low temperature process, silicon molecular beam epitaxy (SiMBE) can inherently realize a steep impurity profile, which is necessary for high speed devices. Although SiMBE has recently been developed to obtain epitaxial films with a low defect density, the defect density should be decreased to the zero level in order to use MBE Si films in the IC manufacturing.

We have successfully obtained defect-free MBE Si films by an advanced technique of an ozone boiling combined with a Si predeposition process\textsuperscript{1}) for cleaning the substrate.

There were two kinds of lattice defects in MBE films, i.e. stacking faults and dislocations. These defects were counted by etch pits after the Secco etching on 1 \( \mu \)m thick films which were grown with the growth rate of 10 \( \text{Å/s} \) on (111) and (100) oriented substrates.

The present silicon predeposition process was consisted of the following two steps. First, a thin amorphous silicon layer was formed on the boil-cleaned substrate at below 400 \( \text{°C} \) in the MBE growth chamber. Then the substrate was pre-heated for a few minutes at 780 \( \text{°C} \). The thin silicon native oxide film formed on the substrate during the boil-cleaning process can easily be vaporized and removed reacting with the deposited amorphous silicon. As shown in Fig. 1, the stacking fault density varies as a function of the amorphous silicon layer thickness on (111) Si wafers, while, on (100) Si wafers, MBE films contain no stacking fault in a wide range of the amorphous layer thickness. This may be explained as follows. The (111) surface inherently holds impurity atoms more strongly than the (100) surface, which results in more stacking faults on the (111) surface than on the (100) surface. The residual amorphous silicon after the reaction with silicon oxide epitaxially crystallizes much more easily on the (100) surface than the (111) surface. However, there remained dislocations with the density of \( 10^3 - 10^4 \text{ cm}^{-2} \) in either orientation. In the present experiment, a solution of
NH₄OH+H₂O₂+H₂O was used in the boil-cleaning process before the introduction of wafers into the MBE growth chamber. This solution was more effective to decrease the stacking fault density than a solution of HCl+H₂O₂+H₂O.

An ozone bubble-cleaning technique, which was applied at a later stage in the boil-cleaning process, had a remarkable effect on the diminution of defects. For (100) wafers, the remained dislocations were completely vanished, though, for (111) wafers, stacking faults and dislocations were both decreased to the order of 10² cm⁻². This may be due to the fact that radicals originating from the ozone gas attacked the remained contaminants on the substrate surface and removed them.

As shown in Fig. 2, stacking fault density on (111) wafers decreased with decreasing the growth rate. A two-step growth-rate method, typically with a growth rate of 2 Å/s followed by a rate of 10 Å/s, was efficient to decrease the density of defects. This was because the stacking faults originating from the interface between the epitaxial film and the substrate were diminished during the first growth stage with a low growth rate.

In conclusion, using the silicon predeposition method with the preparatory cleaning process by boiling in a solution of NH₄OH+H₂O₂+H₂O and by ozone-bubbling, we were able to obtain defect-free MBE films on (100) wafers. In the case of (111) wafers, an additional technique, that is, the two-step growth-rate method was necessary for decreasing the residual defects.

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