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A Hydrogen Pre-bake Process for Si Epitaxy on SiGe Surface

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A typical method for removing native oxide from Si substrate for high-quality Si and SiGe epitaxy, is annealing the substrate at high temperature (>1000°C) in a hydrogen environment (hydrogen pre-bake). Alternatively, an ex-situ HF acid etch of the substrate can be used to remove most of the native oxide before hydrogen pre-bake. The HF will passivate the surface with Si-H bonds, which slows down the native oxide growth. Only a moderate hydrogen pre-bake (≤900°C, 30sec-2min) is required to remove the remaining sub-monolayer oxide following the HF etch. However, in the development of strained Si materials, it is often required to deposit Si on partially relaxed or fully relaxed SiGe. This paper address a unique problem associated with hydrogen pre-bake of SiGe substrates.

It is found that while a hydrogen pre-bake, such as an 800°C, 2min pre-bake, following an ex-situ HF etch is an effective method to completely remove the remaining oxide on the SiGe surface, the SiGe surface quickly becomes rough when the surface oxide is fully removed. It is demonstrated that the surface roughening is associated with surface oxygen removal. In order to prevent surface roughening, a small amount of oxygen atoms ($>5\times10^{12}/\text{cm}^2$) need to remain on the surface. The interfacial oxygen leads to stacking fault defects in the subsequent epitaxial Si, with a density in the range of 1×10^{6}-$1\times10^{8}/\text{cm}^2$.

Alternatively, a hydrogen pre-bake process in a chlorine containing environment is developed to fully remove the surface oxide on SiGe. By adding chlorine containing gases, the SiGe surface is stabilized against roughening which allows surface oxide to be fully removed. At the same time, the chlorine atoms on the surface don’t incorporate in the film during Si epitaxy, so that a clean interface is obtained. Si grown on SiGe with this new pre-bake process shows a reduction of defect density by more than two orders of magnitude. Significant reduction of defect density for strained Si grown on thermally mixed SiGe on insulator (TMSGOI) is also observed. An optimized pre-bake process includes a mixture of DCS and HCl in the hydrogen gas, with the ratio of DCS and HCl chosen to have zero growth rate of Si.