A thermally removable SiO$_x$ surface protecting layer on Si (100) for molecular beam epitaxy

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Ultra-thin SiO_x (with $x \leq 2$) layer plays a key role in Si technology especially for the CMOS foundry processes approaching nm-level. Besides various functions of SiO_x by only manipulating x value and thickness, [1-3] it becomes a favourable material as surface protecting layer for Si-molecular beam epitaxy (Si MBE), especially important for the growth on patterned Si substrates after a series of fabrication processes. This is because SiO_x can be thermally decomposed to generate an atomically flat surface, without introducing any reducing agent (e.g., H_2) to affect the growth.[4] Moreover, recent MBE growth indicates that surface reconstructions with bi-atomic terraces can form by thermally removing an oxide layer, which is critical to supress antiphase boundary defects towards high quality III-V materials monolithic grown on Si.[5] However, there has been insufficient knowledge in preparing a reliable thin SiO_x protecting layer for MBE growth so far, and consistent confusions of the concepts have been used in literatures regarding the fabrication methods.

In this work, we systematically studied the oxidation and deoxidation mechanisms of ultra-thin SiO_x layers fabricated on Si (100) for MBE growth. From several growth approaches, a chemically synthesized SiO_x thin layer is developed for reproducible thermal deoxidation in a Si MBE chamber. From transmission electron microscopy (TEM) observations, the SiO_x thickness is ~2 nm with a clear Si/SiO_x boundary to stop further oxidation in air (**Fig.a**), working well as a surface protection layer. An atomically flat surface is realized after thermal deoxidation process, examined by atomic force microscopy (AFM). The subsequent epitaxial growth is performed with the same MBE by depositing a thin Ge epitaxial layer, as it is not only broadly applied for all group IV integrations but also a good buffer layer for III-V on Si growth. [6,7] The epitaxial layer exhibits a reduced thread dislocation defect density (down to 3×10^8/cm^{-2}) compared with its counterpart grown on a thermally removed natural oxide layer. In the meantime, a reduced tensile strain from 0.29% to 0.24% were confirmed by x-ray diffraction (XRD) and Raman spectroscopy measurements, corresponding to a variation of Ge-Γ_1 transition energy from 0.772 to 0.783 eV confirmed by absorption spectroscopy measurements (**Fig.b**). Our work introduces a SiO_x surface protecting layer for high quality MBE growth on Si substrates, opening a way for both all-group IV and III-V on Si integrations.

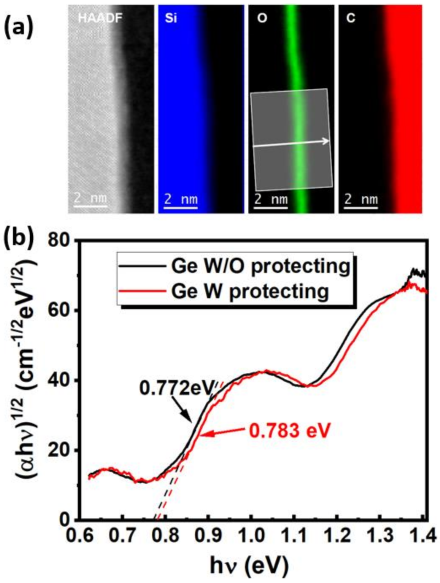

Fig. a TEM image and EELS element distribution of the SiO_x layer. **Fig. b** Absorption spectra of Ge epitaxial film on Si (100).

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