Impact of Germanium Concentration on the Ultraviolet Nanosecond Laser Annealing of Intrinsic Si_{1-x}Ge_x Epitaxial Layers

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Abstract:

Variations in chemical composition and crystalline quality of pseudomorphic $Si_{1-x}Ge_x$ layers were studied after annealing with a nanosecond UV laser. Several regimes were highlighted, from sub-melt to full SiGe layer melt. High Ge concentrations (above 55% for x=0.2 in the as-grown layer and above 80% for x=0.4) were obtained close to the surface for melted samples. A low relaxation level was correlated with a smooth liquid/solid interface at the end of the partial melt regime and in the full melt regime.

1. Introduction

Driven by the need for higher dopant concentrations and lower diffusion lengths, annealing processes continuously evolve towards shorter timescales. Nowadays, they are reaching the nanosecond scale, resulting in very limited thermal budgets. In the case of silicon, the energy of a nanosecond laser with an ultraviolet wavelength is absorbed in the very first nanometers, typically less than 30 nm. As a result, the surface can reach very high temperatures, eventually their melting points, while maintaining the underlying layers at much lower temperatures. On Si and Ge, this technique has already proven its ability to reach dopant activation above the solid solubility limit, or to crystallize amorphous layers [1]. However, there is far less information on the nanosecond laser annealing of SiGe layers, even though it could be beneficial for contact performances [2]. This study aims to gain insight on the composition and strain modification after UV nanosecond laser annealing (UV-NLA) of undoped strained Si_{1-x}Ge_x layers with x varying from 0 to 0.4.

2. Experimental

30 nm-thick undoped pseudomorphic Si_{1-x}Ge_x layers were grown at 550°C on n-type Si (100) substrates, with x varying from 0 to 0.4. The epitaxial growth was performed in a 300 mm Reduced - Pressure Chemical Vapor Deposition tool. Samples were then subjected to UV-NLA in a SCREEN-LT3100 system, operating at 308 nm wavelength with a 145 ns FWHM pulse. Energy densities were chosen to study regimes ranging from sub-melt to full SiGe layer melt. Melt threshold was detected using in-situ Time-Resolved Reflectivity (TRR) at 635 nm, and surface quality was evaluated by AFM and SP2 Haze measurements. Germanium profiles after annealing were obtained with Time of Flight Secondary Ion Mass Spectrometry (ToF-SIMS). Corrections on the profiles were performed with Ref. [3] protocol. Reciprocal space maps (RSM) around the (224) reflection were used to calculate relaxation levels. Additional information on crystalline quality was obtained thanks to cross-sectional Transmission Electron Microscopy.

3. Results and discussion

Energy density thresholds for surface melt were measured by TRR, and confirmed by SP2 Haze. For TRR, the melt threshold is considered to be the first energy density at which a sharp reflectivity increase occurs. An abrupt SP2 Haze increase is also the signature of the onset of melt. As shown in Fig.1, both metrics yield the same trend, with an almost linear decrease of the melt threshold as the Ge content increases. SP2 melt thresholds are consistently at lower energy densities than TRR thresholds. This is likely due to the higher Haze sensitivity.



Fig.1 Surface melt thresholds from SP2 Haze and TRR functions of Ge content in the SiGe layers. The inset shows $1 \times 1 \ \mu m^2$ AFM images just above the melt threshold for *(i)* Si, *(ii)* Si_{0.8}Ge_{0.2} and *(iii)* Si_{0.6}Ge_{0.4} annealed at 1.82, 155 and 1.35 J/cm²

SIMS measurements were performed on $Si_{0.8}Ge_{0.2}$ and $Si_{0.6}Ge_{0.4}$ to obtain the Ge depth profiles shown in Fig.2 (a) and (b), respectively. They enable to identify additional annealing regimes, by showing the energy densities for which the Si substrate starts to melt. In both cases, this occurs between 2.00 J/cm² and 2.20 J/cm². For samples in the partial melt regime, i.e. for energy densities between the surface melt threshold and ~2.00 J/cm², a peculiar profile is observed: just above the SiGe/Si interface, the Ge concentration is close to that of the original SiGe layer, while it decreases in the middle

of the layer. The concentration increases again near the surface and reaches high values. For samples in the full melt regime, the increase is visible through the whole layer and becomes sharper near the surface. This is due to Ge segregation: during solidification, only a fraction of the Ge atoms are incorporated. The rest is pushed towards the surface. Profiles are similar for both series, with much higher Ge contents close to the surface for Si_{0.6}Ge_{0.4} samples. Relaxation values in the different regimes were extracted from (224) RSMs. As shown in Fig.3, strain relaxation varies with the Ge concentration: no relaxation is observed for Si_{0.9}Ge_{0.1} layers, while a relaxation close to 30% occurs at the beginning of the partial melt regime for Si_{0.8}Ge_{0.2} layers.



Fig.2 Germanium depth profiles after nanosecond laser annealing of (a) $Si_{0.8}Ge_{0.2}$ and (b) $Si_{0.6}Ge_{0.4}$ layers.

A return to a pseudomorphic state is observed at the end of partial melt (2.00 J/cm²) for these layers. Similar results are observed for Si_{0.7}Ge_{0.3}, but the annealing leads to low relaxation levels only in the full melt regime. Finally, for Si_{0.6}Ge_{0.4}, the relaxation range is wider, with higher strain relaxation values. In that case, the full melt regime leads to the formation of a complex layer, as evidenced by the RSM in the inset of Fig. 3. The main SiGe peak indicates that the layer is strained, but a wide diffused contribution is also observed around it. This is consistent with the presence of defects in a 10 nm thick layer near the surface as confirmed by TEM, while the remainder of the layer is defect-free.



Fig. 3 Relaxation levels from (224) RSM after laser annealing of SiGe layers with 10, 20, 30 or 40 % at.Ge. The inset shows the (224) RSM of a $Si_{0.6}Ge_{0.4}$ sample annealed at 2.20 J/cm².

Rough liquid/solid (l/s) interfaces were observed for process conditions yielding relaxed samples. Fig. 4 shows STEM-HAADF micrographs of Si_{0.8}Ge_{0.2} and Si_{0.6}Ge_{0.4} samples in the partial melt regime. The chemical contrast of such images enables to identify the deepest position of the l/s interface (red arrows). Indeed, the bright layer at the bottom corresponds to the un-melted layer. In both cases, the interface depth fluctuates over several nanometers, while HR-TEM images show defects crossing through the whole layers. Those samples were near 25% and 95% relaxed, respectively.



Fig.4 STEM-HAADF micrographs of (a) $Si_{0.8}Ge_{0.2}$ annealed at 1.80 J/cm² and (b) $Si_{0.6}Ge_{0.4}$ annealed at 1.81 J/cm², showing the interface between the liquid and solid layers.

Higher energy densities that led to smoother l/s interfaces (at 2.00 J/cm² and above for both series) had lower relaxation values. For Si_{0.8}Ge_{0.2}, the sample annealed at 2.00 J/cm² was pseudomorphic, while the Si_{0.6}Ge_{0.4} one exhibited a pseudomorphic bottom layer (~20nm) and defects in the near surface layer. This is coherent with the corresponding RSM, shown in Fig 3, where the double spot indicates a strained layer and a relaxed layer. Thus, a smooth l/s interface seems to be required to obtain a pseudomorphic SiGe layer. The Ge content also has to be taken into account: a higher content results in the formation of defects in the near surface layer, and a wider range of laser energies leading to relaxation.

3. Conclusions

Different regimes were identified for the nanosecond UV laser annealing of 30 nm-thick $Si_{1-x}Ge_x$ layers, with x varying from 0 to 0.4. Similar evolutions were observed, with a melt threshold at lower energy densities for higher Ge contents. The transition from partial melt to full melt occurred between 2.00 and 2.20 J/cm² for all concentrations. Relaxation was observed on a wider range of energy densities for higher Ge contents, and returned to low values if the liquid/solid interface was smooth.

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