

## Project: I. 3: FRONT-END PROCESSES FOR MICRO- AND NANODEVICES

**Project Leader:** C. Tsamis

**Key Researchers:** V. Ioannou–Sougleridis, P. Dimitrakis, D. Tsoukalas, C. Tsamis

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### Objectives

- Study of dopant diffusion/activation and point/extended defect kinetics in Group-IV semiconductors (Silicon, Strained Silicon, Germanium) for CMOS applications
- Thermal processes for ultra-thin gate dielectrics (oxides, oxynitrides) in Group-IV semiconductors for CMOS applications
- Process optimization for Nanodevices (Fabrication, Electrical Characterization)
- Continuum and atomistic simulation of processes and devices

### Research activities and main results within 2010

#### **Task I: Influence of thermal oxidation on the interfacial properties of ultrathin strained silicon layers\***

**N. Kelaidis, V. Ioannou-Sougleridis, P. Dimitrakis and C. Tsamis**

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The formation of a reliable dielectric layer on strain-Si substrates is a key point in achieving enhanced device performance, taking advantage of the beneficial effect of strain to carrier mobility. Therefore, the study of the oxidation of strained Silicon is a necessary step in understanding the physical phenomena involved in dielectric formation and electrical performance of the MOS device, as well as the limitations in s-Si processing. Additionally, the well-established method of nitridation of SiO<sub>2</sub>, was extended to strained-Silicon substrates in order to address a number of phenomena related with reliability problems when performing standard oxidation on s-Si.

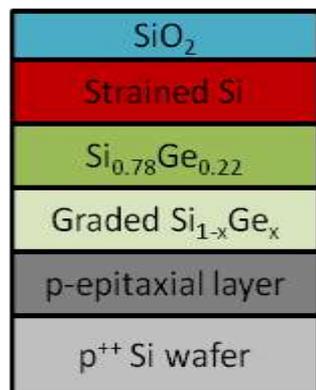
During this year we examined the influence of thermal oxidation on the electrical characteristics of ultra-thin strained silicon layers grown on relaxed Si<sub>0.78</sub>Ge<sub>0.22</sub> substrates under moderate to high thermal budget conditions in N<sub>2</sub>O ambient at 800 °C. The strained-Si / relaxed Si<sub>x</sub>Ge<sub>1-x</sub> heterostructure substrate used is schematically shown in Fig. 1. Epitaxial p-type silicon layer, with resistivity 1 Ωcm and thickness 2.75 μm, was grown on top of a 5 mΩcm p<sup>++</sup> boron doped wafer, followed by a graded Si<sub>x</sub>Ge<sub>1-x</sub> layer in which the Ge content increases linearly from 0 to 22 %. On top of the graded Si<sub>x</sub>Ge<sub>1-x</sub> a constant composition Si<sub>0.78</sub>Ge<sub>0.22</sub> layer and a s-Si layer 13 nm thick, were grown successively. The Si<sub>x</sub>Ge<sub>1-x</sub> and the s-Si layers were not intentionally doped with boron. However, a residual doping in the low range of 10<sup>14</sup> cm<sup>-3</sup> is expected due to the deposited system auto-doping effects. Figure 2 shows a bright field cross-section HRTEM image from the as-grown sample along the [110] axis. The image indicates the good quality of the epitaxial s-Si layer of 13 nm thickness.

Figure 3 and 4 are typical electrical characteristics of the samples. The experimental results of the oxidation of ultra-thin s-Si layers on relaxed SiGe virtual substrates, under moderate to high thermal budget conditions indicate the following:

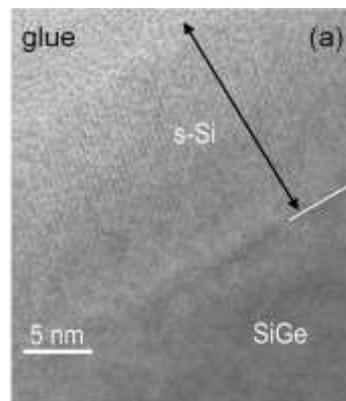
- a) The interface trap density increases with the oxidation time, as long as the s-Si layer remains between the growing thermal oxide and the underlying SiGe substrate.
- b) The density of interface traps across the bandgap, as extracted from the high-low C-V method, indicates a rather featureless and constant D<sub>it</sub> profile within the energy range E<sub>v</sub>+0.35 to E<sub>v</sub> +0.6 eV. Below E<sub>v</sub>+0.35 eV the D<sub>it</sub> show a rapid decrease, while the increase above E<sub>v</sub>+0.6 eV is attributed to generation effects.

c) The analysis of the  $G_p/\omega$ - $f$  characteristics as a function of temperature indicates that the energy location of the interfacial traps lies within the energy range of  $E_v+0.37$  to  $E_v+0.4$  eV..

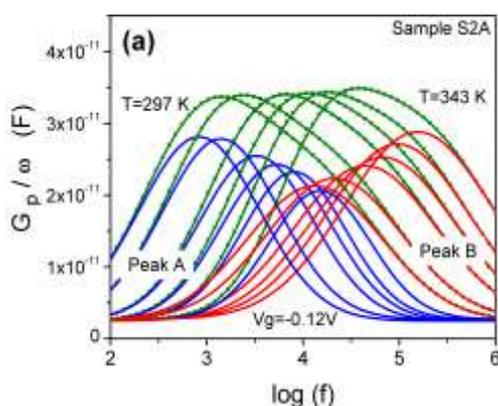
d) The conductance analysis revealed very clearly that generation effects dominate the capacitor behaviour at the weak inversion and depletion regions which in turn impose restrictions to the extraction of a correct interface density profile. Detailed analysis can be found in reference [2].



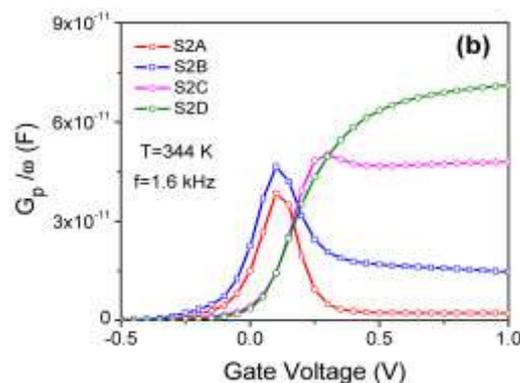
**Figure 1.** Schematic diagram indicating the ordering of the several layers of the strained-silicon structure.



**Figure 2.** Cross-sectional HRTEM image showing the as-grown S2R sample along the  $[110]$  zone axis. The 13 nm thick s-Si layer is visible while the s-Si/SiGe interface is indicated by the white line.



**Figure 3.** Evolution of the conductance vs. frequency characteristics with temperature at the depletion region of samples S2A.. The characteristics were assumed to arise from two different loss mechanisms, and they were deconvoluted into two Gaussian contributions.



**Figure 4.** Conductance-Voltage characteristics of all oxidized samples recorded at 344 K. It is evident that the increase of the oxidation time creates significant amounts of bulk traps which dominate the  $G$ - $V$  at the highest temperatures.

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## Task II: Gallium diffusion in Germanium\*

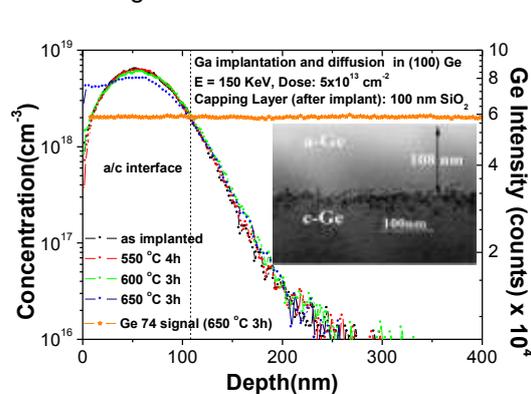
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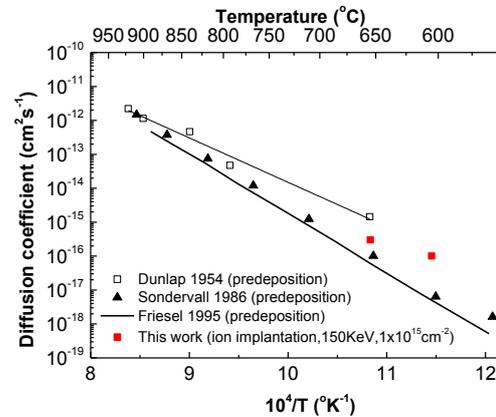
During this year we continued our investigation on the diffusion of Ga in Ge substrates, for high as well low implantation doses, using furnace annealing in the temperature range 550-650°C and for times up to 240min. Moreover, following previous studies, the possible influence of Ge surface passivation on Ga diffusion was also investigated. Figure 5 shows Ga ToF-SIMS profiles in the case of low dose Ga implantation and annealing for samples covered with SiO<sub>2</sub>. The maximum concentration of the as-implanted profile is  $C_p = 6.3 \times 10^{18} \text{ cm}^{-3}$  at a projected range  $R_p \sim 56 \text{ nm}$ . Representative TEM image of the as-implanted substrate is shown as an inset. The amorphous layer extends to 108 nm from the surface. We observe also the absence of a honeycomb subsurface structure reported in the literature for the case of high dose implants of heavy ions in Ge. No significant Ga diffusion has been

observed at 550°C. Negligible diffusion has been observed also at 600°C. By increasing the temperature at 650°C a trend of Ga diffusion (in particular out-diffusion towards the SiO<sub>2</sub>/Ge interface) is clearly observed, which leads to a change of the profile shape and height in the near - peak (now  $C_p \approx 5 \times 10^{18} \text{ cm}^{-3}$ ) region. Selected SIMS measurements have been performed also in samples covered with 100 nm Si<sub>3</sub>N<sub>4</sub>. The overall picture remained the same. This means that the change of the capping layer did not affect, in any way, the point defect kinetics in the substrate and consequently the dopant diffusion under the present experimental conditions.

Simulations were performed using Synopsys Sentaurus process simulator. A constant diffusivity model has been used in order to simulate the diffusion of the tail regions of the profiles, keeping the high concentration regions immobile in order to represent the possible clustering phenomenon. The best fitting of the tail regions has been obtained using a diffusivity value of  $1 \times 10^{-16} \text{ cm}^2 \text{ s}^{-1}$  for 550 and 600°C and a value of  $3 \times 10^{-16} \text{ cm}^2 \text{ s}^{-1}$  for 650°C. A surprisingly high Ga diffusivity has been estimated at 550°C, which is equal to the corresponding at 600°C. This could have its origin to the small differences between the corresponding profiles, which are below the SIMS resolution limit. However a possible physical origin, being under investigation, cannot be excluded. Figure 6 shows the diffusivity values obtained at 600 and 650°C compared to literature data. The obtained values are in good agreement with previously reported results taking into account the different experimental methodologies used.



**Figure 5.** Ga profiles in Ge, after low dose – high energy implantation and annealing at 550-650°C. A TEM image of the as-implanted sample is also shown as inset.



**Figure 6.** Ga diffusion coefficients obtained at 600°C and 650°C in the case of 150KeV,  $1 \times 10^{15} \text{ cm}^{-2}$  implantation.

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### Task III: Arsenic and Phosphorus diffusion in Germanium\*

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We have performed arsenic and phosphorus diffusion experiments and activation related phenomena in co-doped germanium substrates utilizing conventional thermal annealing. Chemical profiles were obtained by Secondary Ion Mass Spectroscopy (SIMS), sheet resistance was estimated by the Van der Pauw method. Our study covers the temperature range from 600 to 750°C. We accurately described the dopant profiles with a quadratic dependence of the dopants diffusion coefficient on the free electron concentration. In our simulations we considered the dopant pile-up near the surface and dopant loss owing to outdiffusion during the annealing. Although the double donor co-doping technique exhibited no advantage over mono-doping with P concerning the level of activation and junction depth, it was interesting to observe the different diffusion behavior of the two dopants. Whereas the diffusion of As indicates a retardation under co-doping the diffusion of P remains either unaffected or is slightly enhanced by co-doping. The activation level of the co-doped samples remains lower compared to the respective mono-doped samples, except for the highest annealing temperature.

## Laser Annealing for diffusionless dopant activation in Silicon using nanosecond to millisecond pulses

A. Implementation of Plasma Doping and **nanosecond laser annealing** in the non-melt regime has shown to hold great promise for the realization of Ultra Shallow Junctions, designed for the sub 45nm node. This work includes extensive simulation of these two emerging techniques using the Synopsys Sentaurus Process software tool, in direct comparison with experimental data for each step involved in the process. Analytical calculations were performed in order to investigate the interaction of the KrF Excimer laser annealing and silicon regarding the temperature gradients induced into silicon and the boron diffusion kinetics. On the other hand, analytically obtained surface temperature profiles of each annealing condition, were used as input to KMC calculations of the boron diffusion and activation behaviour. Simulation predictions, in accordance with SIMS measurements revealed very limited dopant profile movement (maximum 2.5nm), combined with high levels of electrical activation close to the maximum theoretically predicted ones. As the results obtained by calculations are in consistency with the experimental, it is evident that the combination of both analytical and Kinetic Monte Carlo tools, allows for sufficient physical understanding of the underlying mechanisms for these advanced process steps.

B. We investigate **CO<sub>2</sub> laser annealing at millisecond time** scale for the fabrication of Ultra Shallow Junctions, able to fulfill the requirements imposed for sub-45nm CMOS nodes. Silicon samples doped with Boron using BF<sub>3</sub> plasma implantation technique at low energy (0.4 and 0.6keV) were used to ensure ultra shallow as implanted boron concentration profiles. Our aim is to achieve high electrical activation level of the dopant, while maintaining the Boron concentration profile as immobile as possible. Samples have been irradiated at a variety of annealing conditions regarding the duration of the irradiation and the power density; however, in every case the peak surface temperature was kept in the 1150-1250°C. Sheet resistance measurements indicate significant enhancement in the activation levels, while chemical characterization by means of SIMS, shows very limited movement of the dopant concentration profile, especially for short pulse duration conditions.

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## PROJECT OUTPUT IN 2010

### Publications in International Journals and Reviews

1. "Gallium Implantation and Diffusion in Crystalline Germanium", N. Ioannou, D. Skarlatos, N. Z. Vouroutzis, S. N. Georga, C. A. Krontiras and C. Tsamis, *Electrochemical and Solid-State Letters*, 13 (3) H70-H72
2. "Influence of thermal oxidation on the interfacial properties of ultrathin strained silicon layers", Ioannou-Sougleridis V, Kelaidis N, Skarlato, D. Tsamis C, Georga S.N., Krontiras, C.A., Kominou Ph., Speliotis Th., Dimitrakis P., Kellerman, B., Seacrist, M., To appear in *Thin Solid Films*
3. "Experiments and simulation on diffusion and activation of codoped with arsenic and phosphorous germanium", Author(s): Tsouroutas P, Tsoukalas D, Bracht H, *J. of Appl. Phys.* Volume: 108 Issue: 2 Article Number: 024903 Published: JUL 15 2010
4. "Formation of silicon ultra shallow junction by non-melt excimer laser treatment", Florakis A., Papadimitriou A, Chatzipanagiotis N, et al., *SOLID-STATE ELECTRONICS* Volume: 54 Issue: 9 Pages: 903-908 Published: SEP 2010
5. "Non-melting annealing of silicon by CO<sub>2</sub> laser", Florakis A, Verrelli E, Giubertoni D, et al. Source: *Thin Solid Films* Volume: 518 Issue: 9 Special Issue: Sp. Iss. SI Pages: 2551-2554 Published: FEB 26 2010