ESRF	**Experiment title:** XAFS investigation of the electronic and structural properties of Ga dopant in SiGe and pure Ge epitaxial layers for MOSFET applications	**Experiment number**: HC-5047
Beamline:	**Date of experiment**: from: 08/11/2022 to: 14/11/2022	**Date of report**: 14/03/2023
Shifts:	**Local contact(s)**: Francesco d'Acapito, Alessandro Puri	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

Didier Grandjean*, QSP, KU Leuven, Celestijnenlaan 200D, 3001 Leuven, Belgium

Gianluca Rengo*, KU Leuven, Celestijnenlaan 200D, 3001 Leuven, Belgium

Clement Porret*, IMEC, Kapeldreef 75, 3001 Leuven, Belgium

Report:

We collected X-ray Absorption Spectroscopy (XAS) spectra at the Ge and Ga K-absorption edges on a series of Ga-doped $Si_{0.35}Ge_{0.65}$ or Ge monocrystalline epitaxial layers prepared via chemical vapour deposition (CVD) by co-flowing in a reaction chamber the Si, Ge, and Ga precursor gasses on a 300 mm Si substrate.
A total of 78 spectra were collected, with 8 acquired at low temperature using a liquid nitrogen setup. The measurements were performed in fluorescence mode with grazing incidence to maximize the fluorescent emission.

The acquired spectra showed good quality, even for the samples with the lowest Ga loading ([Ga] = 6×10^{19} at./cm^3 corresponding to a 0.12% dilution). For the latter samples six spectra acquisitions were collected, in order to enhance the signal-to-noise ratio, while two acquisitions were sufficient for the samples with the highest [Ga]. The main measurement problems encountered were: (i) instability of samples at LN temperature, due to difficulty in fixing the sample to the holder and the presence of grease contaminants in the chamber affecting the spectra quality (only at low temperature), and (ii) presence of a few glitches in the end part of the spectra measured at the Ga k-edge. However, these minor issues did not affect the successful completion of the planned measurements.

In this study, we investigated the influence of two parameters on the local structures of Ga and Ge in (Si)Ge: (i) the Ga concentration, and (ii) the effect of different annealing processes at different temperatures. Currently, only the data from the first parameter have been analysed and the main results are reported below. Data reduction and fitting were performed using the softwares "Athena" and "Artemis" from the DEMETER package.

The sample names reflect the flow of Ga precursor used during their deposition. F5 was grown with the lowest Ga-flow and F40 with the highest, with a 8 fold flow increase. Figure 1 shows the best fits of the Fourier transform of the k^2-weighted EXAFS acquired at the Ga and Ge K-edges of sample F20 up 4 Å before phase correction. All the results of the fitting of the first shell are reported in Table I.

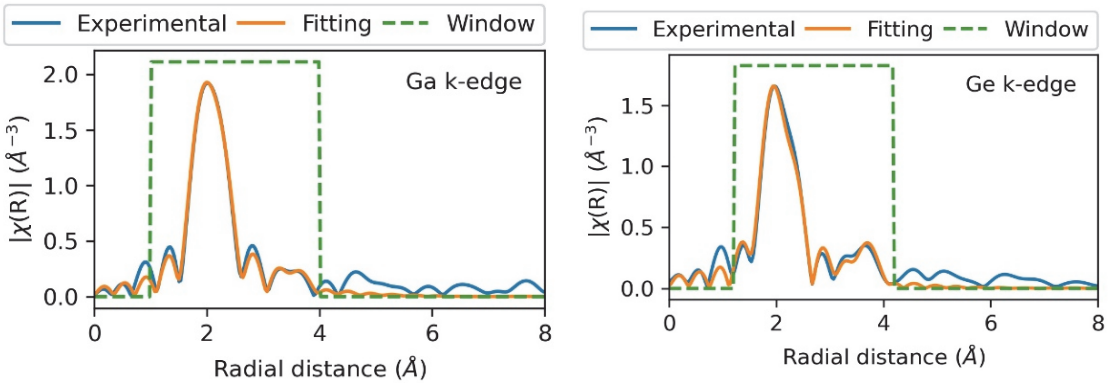

Figure 1: Fourier transforms of the k^2-weighted EXAFS signals acquired at the Ga (left) and Ge (right) K-edges of a SiGe:Ga layer (sample F20).

Table I Summary of EXAFS fitting results for the 1st coordination shell of $Si_{0.36}Ge_{0.64}$:Ga samples.

Sample (abs. atom)	Atom-shell.	R (Å)	N	σ^2 ($Å^2$)
F5	Si-1st	2.37±0.04	0.7 ± 0.3	0.003
(Ga)	Ge-1st	2.42±0.01	3.3 ± 0.3	0.003
F10	Si-1st	2.37±0.02	1.0 ± 0.2	0.003
(Ga)	Ge-1st	2.40±0.01	3.1 ± 0.5	0.003
F20	Si-1st	2.36±0.03	1.0 ± 0.3	0.003
(Ga)	Ge-1st	2.40±0.01	2.9 ± 0.5	0.003
F20	Si-1st	2.40±0.01	1.7 ± 0.2	0.005
(Ge)	Ge-1st	2.43±0.01	3.2 ± 0.4	0.005
F40	Si-1st	2.37±0.02	1.2 ± 0.2	0.005
(Ga)	Ge-1st	2.40±0.01	3.7 ± 0.3	0.004

The possibility to measure both the Ga and the Ge spectra on same samples enabled a direct comparison of the local atomic environments of these two elements. The primary finding of this study is that the average Ge coordination number around Ga dopants is higher than the concentration determined via Secondary Ion Mass Spectrometry (SIMS). Specifically, the first coordination shell of Ga having Ge concentrations of ~ 75%, which is 10% higher than the alloy's stoichiometry. Conversely, [Ge]% in the first shell of Ge for sample F20 amounts to 65%, which is in line with the composition of the host alloy. This indicates that Ge atoms are preferentially incorporated as Ga nearest-neighbours during the epitaxy process. Although no clear trend emerged when varying the [Ga], sample F5 had a remarkably high average [Ge]% in the first coordination shell. This observation implies that the Ge-enrichment around the Ga dopants may be stronger if a lower Ga concentration is present in the epilayer.

These results will be presented as a poster titled: "Influence of Ga concentration on the local atomic structure and material properties of Ga-doped $Si_{0.35}Ge_{0.65}$ epitaxial layers" at the ISTDM/ICSI 2023 conference that will be held in May 2023. Furthermore, the fitting results of the complete dataset will be combined with *ab initio* theoretical simulations of the Ga local environment in $Si_{0.35}Ge_{0.65}$ and expected defect configuration for this dopant-matrix system and published as an extended journal paper.