EUROPEAN SYNCHROTRON RADIATION FACILITY

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Experiment Report Form

	Experiment title: *Local Atomic struture in SiGeSn epitaxial thin films*	**Experiment number**: **MA-5463**
Beamline: BM08	**Date of experiment**: from: 02.02.2023 to: 07.02.2023	**Date of report**:
Shifts: 15	**Local contact(s)**: Alessandro Puri	*Received at ESRF:*

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Report:

The proposal is aimed at obtaining a systematic description of Sn local structure in $Ge_{1-x}Sn_x$ thin films grown in $Ge_{1-y}Si_y$ virtual substrates.

We measured the Sn K edge XAFS spectra on 15 thin film samples as a function of film thickness (30-700 nm), Sn content (x = 5% - 26%), deposition method (CVD, MBE) and substrate temperature. Some sample has been measured with the x-ray polarization oriented nearly parallel (about 10°) and nearly perpendicular (about 80°) to the film plane (Fig. 1).

Sn K-edge x-ray absorption spectra were collected in fluorescence geometry keeping the samples at the LN temperature. Total fluorescence yield was collected using ultrapure-Ge multidetector (8 detectors), the substrate Ge fluorescence was attenuated using 3mm Al filter in front of the detector, the total counts per diode was kept less than 9×10^4 cps to keep the detector deadtime less than 5% and reduce not linearity effects. The Sn K_α fluorescence was selected using the MCA electronics. The **major limitation to the signal statistics was the intense anelastic signal from the background representing about 90% of the total fluorescence** on the detectors.

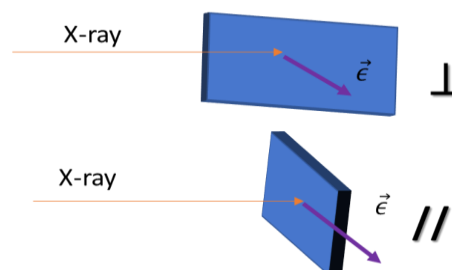

Fig. 1 Geometry for polarization dependent measurements

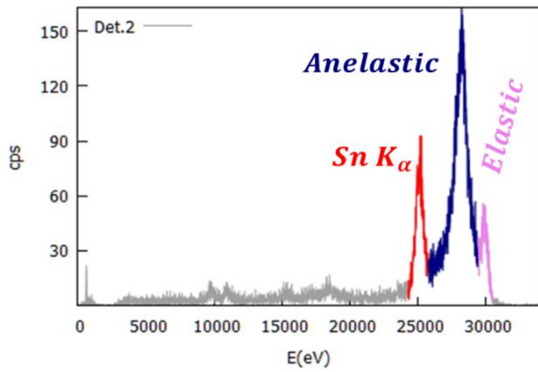

Fig. 2: MCA output from one of the Ge detectors, the **Elastic** (cyan), **Compton** (blue) and **Sn K$_a$** (red) contributions are highlighted.

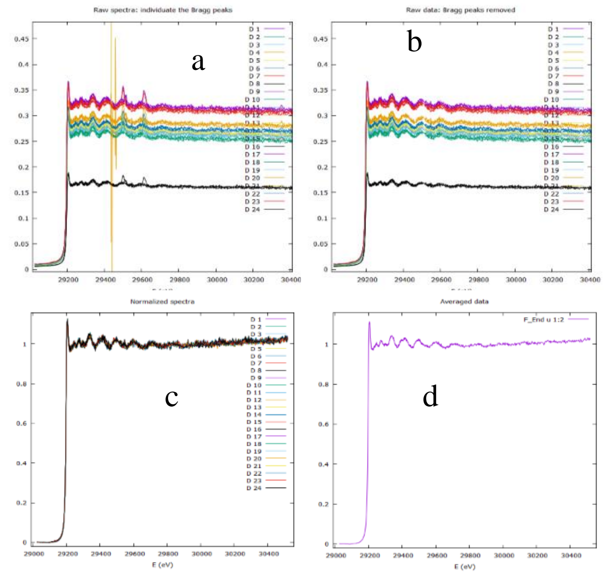

Fig. 3: Procedure for data treatment: **a**. the raw Sn K edge XAS spectra:3 scans, 8 detectors/scan, measured rotating the sample by 0.5 deg. each, **b**. raw data from which the regions of the Bragg peaks are removed, **c**. the raw data are normalized, and **d**. averaged.

To improve the data statistics and remove the Bragg peaks from the substrate each scan was repeated 3-4 times tilting the sample by some 10^{-1} deg. This allows to individuate and remove the Bagg peaks as shown in fig. 3 with a procedure we implemented via Python script. Data collection required in average 6-7 hours per sample/polarization.

We obtained good quality spectra (estimated noise on the averaged spectra is around 5×10^{-3} of the Jump discontinuity) up to k= 14-15A^{-1}.

The preliminary analysis on the thicker (700 nm) CVD deposited sample (x=0.11) has been carried out assuming Sn atoms isolated in Ge lattice, considering two single scattering shells, Ge_1 and Ge_2 plus the multiple scattering contribution Sn-Ge_1-Ge_2 as shown in fig. 4. The Sn-Ge_1 bond length around 2.6Å indicates about 6% dilated Sn-Ge bond respect to pure Ge (being the Ge-Ge bond length 2.45Å). The Sn-Ge_2 distance is found around 4.1Å, 2.5% longer than Ge-Ge_2 distance in pure Ge.

The best fit also points out a structural residue evident in the low k region but masked by the statistical noise above k~8 Å^{-1}. The preliminary analysis suggests this residue related to Sn-Sn contribution originating from not random Sn distribution in the Ge network. We must stress here that the data statistics here obtained is the best obtainable with the setup used at BM08 in a reasonable acquisition time (6-7 hours per averaged spectrum). To improve the data quality keeping a reasonable collection time, a detection set-up based on crystal analysers would be suitable.

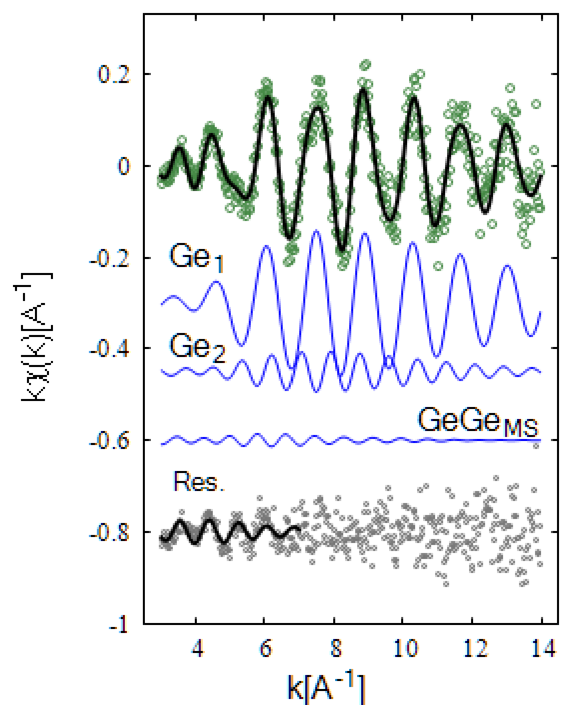

Fig. 4: Sn K edge multi-shell EXAFS data analysis in k space (left panel): the experimental (green dots) data and best fit (black line) are presented at the top, partial contributions (blue) are shown below, shifted for clarity. The residual (exp-best fit) is presented at the bottom. In black is evident a structured residue indicating a structural contribution different from that Sn impurity in Ge phase.