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Report:

GeSn materials are attracting growing interest as promising flexible group IV alloys thanks to a sizable improvement of the charge transport properties and to the advantages offered by strain, lattice constant and bandgap engineering [1]. We have recently synthetized metastable GeSn alloys (with Sn concentrations up to 12.6%) on Ge buffered Si(001) substrates through a novel low temperature Chemical Vapor Deposition technique (CVD) using Ge_2H_6 and $SnCl_4$ as precursors [2]. Although high resolution X-ray diffraction reciprocal space mapping (HR-XRD RSM) in combination with electron microscopy allowed an extensive study the crystal structure and surface morphology of GeSn layers as a function of Sn content and film thickness, the Sn local environment and its variation as a function of the lattice strain remains largely unknown. Recent atom probe tomography results suggest a clustering of the Sn atoms [3] with strain relaxation. However, atom probe tomography does not allow to determine if the Sn atoms are located substitutionally and moreover, the algorithm used to visualize the Sn atom location can lead to artefacts.
The goal of this experiment was to probe the local order around Sn atoms (i.e. lattice location and bond lengths to neighboring atoms) in monocrystalline GeSn layers deposited on Ge/Si(001) substrates using the EXAFS technique at Sn K-edge. This should allow determining how the Sn atoms are incorporated in strained GeSn lattice and, possibly, how they are rearranged during strain relaxation.

Experimental

EXAFS data have been collected in fluorescence mode using the 9-element Ge fluorescence detector at Sn K-edge (29200 eV). Mesurements were carried out in ambient conditions and under grazing incidence to minimize influence from the substrate and increase the Sn fluorescent signal. Ionization chambers were filled with Ar/He gas mixture. Data were collected up to k= 15 $Å^{-2}$ with typical acquisition times of 45 min (1 to 20 s/point). Due to limitations of the Si (111) monochromator, the energy resolution at Sn K-edge did not exceed

ca. 1.5 eV in the XANES regions. 3 spectra were averaged to improve the signal to noise ratio to an optimal level. A total of 19 GeSn samples with different Sn% and strain relaxation degree have been measured, as listed in the table:

Sn %	GeSn strain relaxation degree (%)							
	0		15-30		40-50		65-75	
	sample ID	thickness(nm)	sample ID	thickness(nm)	sample ID	thickness(nm)	sample ID	thickness(nm)
2.9	E121097D11	300						
6.4	E110684d14	27	E120580D11	144			E113591D03	530
7.1	E110684d22	68	E110684D21	113	E120580D09	210	E120227D20	500
8.1	E110684d08	42	E110684D16	105	E100198D12	240	E112374D13	420
9.1	E110684D07	58	E110684D17	116	E120580D10	210	E120580D04	300
10.2	E110686D02	45	E120750D07	126			E113591d02	466

The quality of the data varied dramatically from a very good signal to noise ratio for the samples with the highest GeSn tickness to a poor quality for the samples with the thinnest layer. Moreover a significant number of glitches appeared systematically in the EXAFS signals probably due to parasitic diffraction originating from the high cristallinity and the strong expitaxial character of the deposited layer. We have tried to minimize these effects by carefully rotating the samples in the X-ray beam but a large number of spectra will need to be manually corrected.

Preliminary EXAFS analysis

Due to a combination of low Sn content and reduced thickness resulting in an increasing tendency for glitches and noise in the experimental data, fully strained samples with lower Sn% (left column of the table) could not be fitted unambiguously.
Preliminary results (Fig. 1a & 1b) on the other samples have shown that Sn atoms were clearly incorporated into the Ge crystalline lattice with a tendency for local Sn enrichment during strain relaxation, as suggested by previous APT findings on the same samples. Detailed EXAFS analysis is still underway to identify more quantitative trends.

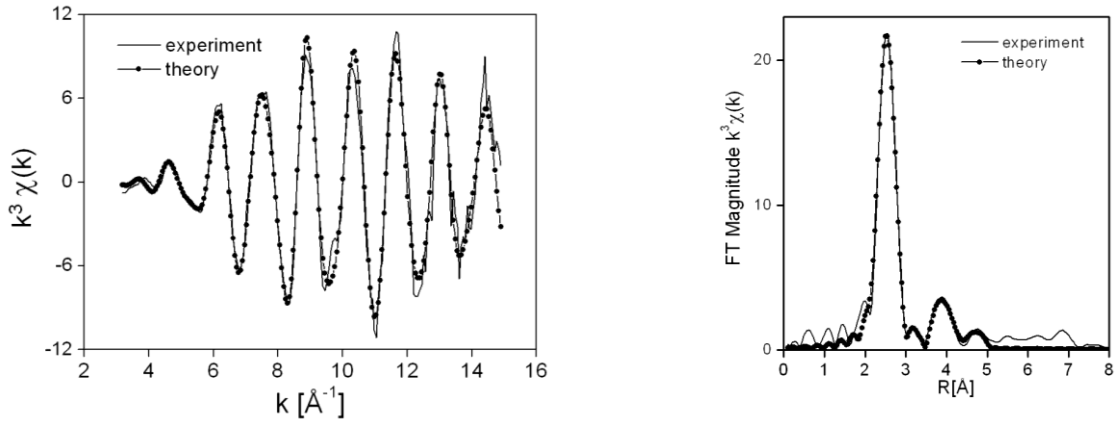

Figure 1: (a) k^3-weighted EXAFS (left) and **(b)** corresponding phase-corrected Fourier Transform (right) of sample E112374D13.

References

[1] J. Kouvetakis et al., Annu. Rev. Mater. Res. 36, 497 (2006)
*[2] B. Vincent et. al, APL **99**, 152103-1 (2011)*
[3] A. Kumar et al., submitted to IFES 2012