ESRF	**Experiment title:** Structural properties of solid and molten Ge-Si alloys in the dilute limit	**Experiment number:** HS-1806
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Report:

Accurate EXAFS (*Extended X-ray Absorption Fine Structure*) at the Ge K-edge, ESXD (*Energy-Scanning X-ray Diffraction*) and SEXAD (*Single-Energy X-ray Absorption Detection*) temperature scans of solid (RT) and molten ($950 < T < 1500$ °C) GeSi alloys have been collected exploiting the highly automated experimental setup available at BM29. The measurements were performed in a high vacuum furnace ("L' Aquila Camerino" oven) which allows for the collection of high-temperature x-ray absorption and diffraction data.

The GeSi samples have been realized *in situ*, heating up to about 1500 °C (for some minutes) several mixtures of the two constituent semiconductors (confined in inert BN matrices) and than quenching the melts. Following this method a wide range of Ge_xSi_{1-x} concentrations have been easily obtained: x = 0.01, 0.05, 0.10, 0.25, 0.50, 0.75, 1.00. In figure 1 the whole process of formation of the $Ge_{10}Si_{90}$ alloy is shown. ESXD and SEXAD have been used to monitor sample changes, melting temperature and homogeneity. These additional investigations have made in evidence that good solid random solutions have been obtained for the alloys with x = 0.05, 0.01, 0.10. On the contrary not perfectly homogeneous solid solutions have been created at the other concentrations. This could be caused by the low quenching rate achievable with our oven, which does not allow a rapid cooling of the homogeneous melt. The slow cooling at intermediate concentrations (x = 0.25, 0.50, 0.75) makes possible the nucleation of regions characterized by slightly different alloy compositions, generating not homogeneous solid solutions.

In the second part of the experiment a set of Ge_xSi_{1-x} (x = 0.005, 0.01, 0.1) alloys deposed onto cold substrate by MBE have been measured at RT with the EXAFS fluorescence set-up available at BM29. In spite of the high counting 13 channels Ge detector and the low concentration of photoabsorbing atoms, the XAS data collected in the fluorescence configuration are characterized by a worse signal to noise ratio than in the transmission set-up.

A preliminary data analysis has been performed for the liquid GeSi alloys using the GNXAS package. The extracted high quality EXAFS signals are shown in figure 2. The analysis confirms that these signals are the weighted sum of two single scattering signals associated with two different bondlength distributions (Ge-Ge and Ge-Si). To our knowledge these are the first experimental EXAFS data of liquid GeSi covering the whole range of concentrations. The fitting procedure has been realized taking into account the double electron excitation features (1s3d, 1s3p and 1s3s) affecting the absorption background near the Ge K-edge. The raw data analysis results suggest that the Ge-Ge and the Ge-Si bondlength distributions are well-defined and constant along all the concentrations. Now efforts have to be devoted to analyze accurately these data and to obtain precise structural results.

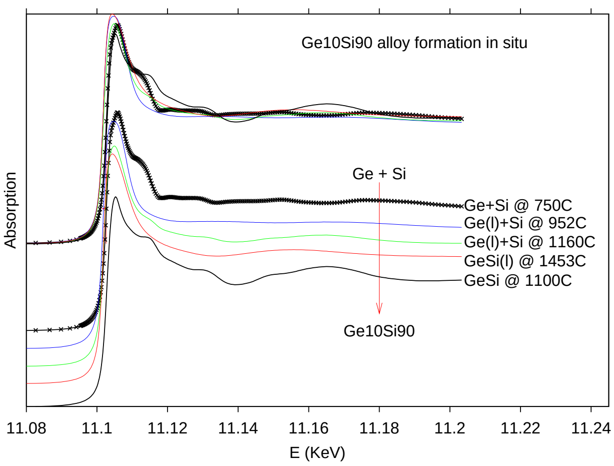

fig. 1

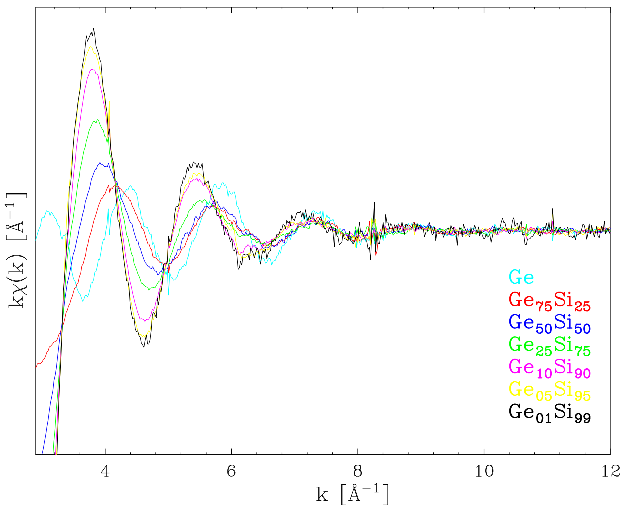

fig. 2

fig. 1: Sequence of the $Ge_{10}Si_{90}$ alloy formation *in situ* starting from weighted quantities of Ge and Si. Increasing the temperature the melting of Ge occurs (at 937 °C), then at 1414 °C also Si melts and the liquid GeSi appears. At 1100 °C the cooled alloy is solid.

fig. 2: The extracted EXAFS experimental signals are shown for all the measured concentrations. The GNXAS analysis confirms that these signals are the weighted sum of two single scattering signals associated with two different bondlength distributions (Ge-Ge and Ge-Si).