ESRF	**Experiment title:** Examination of the intermediate length scale of amorphous SiO by inelastic X-ray scattering	**Experiment number**: HS-2242
Beamline: ID 28	**Date of experiment**: from: 18.02.2004 to: 26.02.2004	**Date of report**: 01.03.2005
Shifts: 21	**Local contact(s)**: A. Beraud	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

T. Wieder*, A. Hohl*, A. Skomorokhov*, H. Fuess,
Institute for Materials Science, Darmstadt University of Technology, Petersenstraße 23, D-64287 Darmstadt, Germany

Report:

Amorphous silicon monoxide (SiO) is a suitable material for the study of structure on the intermediate length scale (around 5 nm) because of its particular morphology. Recently, we developed a new structural model for this material of commercial relevance [1]. SiO it consists of amorphous SiO_2 clusters, amorphous nano-sized Si clusters, and a sub-oxidic interface (ca. 10 at.%) between the clusters. In as-deposited samples the cluster sizes are in the range of 1 - 2 nm. By annealing the clusters grow at the expense of the interface and partial crystallization begins in the pure Si region. Using *ex situ* samples at different annealing stages, one can investigate clusters of different diameters in the intermediate length scale.

In order to find correlations between the stage of disproportionation within SiO samples and the dependence of inelastic scattering intensity on energy E and momentum transfer Q we performed the inelastic X-ray scattering (IXS) experiment HS-2242 at the beamline ID28. Due to the morphology of material with disproportionation clusters strong elastic intensity from small angle scattering covers the inelastic contribution of E scans (constant-Q cuts) in the low-Q region.

Very soon we will obtain inelastic neutron scattering (INS) data and present combined INS and IXS results (from E scans at high Q) on the phonon density of states and the Debye temperature and sound velocity. Here we present results from Q scans (constant-E cuts) at low and high Q for three different treated SiO samples.

From E scans it could be shown that at a lower Q values only elastic contribution was significantly detected. The spectra of SiO, that has been annealed at 950 °C, which is just at

the onset of crystallisation (Fig. 1) show a distinct double peak feature at Q values of about 15 nm^{-1} and 20 nm^{-1}, which can be related to SiO_2 and Si clusters, respectively. However, in the static structure factor (pure elastic) of SiO obtained from X-ray diffraction only one broad peak appears for the amorphous sample volume just below the crystallization onset, and a nearly similar broad peak plus a narrow (Bragg) peak appear for the partly crystallized sample volume just above the crystallization onset. This different behavior will be subject of further studies.

The Q scans in the high-Q region show a certain similarity to the static structure factor, but also clearly resolved inelastic contribution with different ratio of inelastic to elastic scattering for the samples, which has been derived from E scans. The sample annealed at 950 °C shows the highest ratio of 1.06 (probably related to a high degree of disorder at the onset of crystallization), a sample annealed at 1150 °C shows a lower ratio of 0.46 (probably due to a higher degree of order due to larger cluster sizes and crystallinity), and the as-deposited sample (with more homogeneous morphology) shows a medium ratio of 0.73.

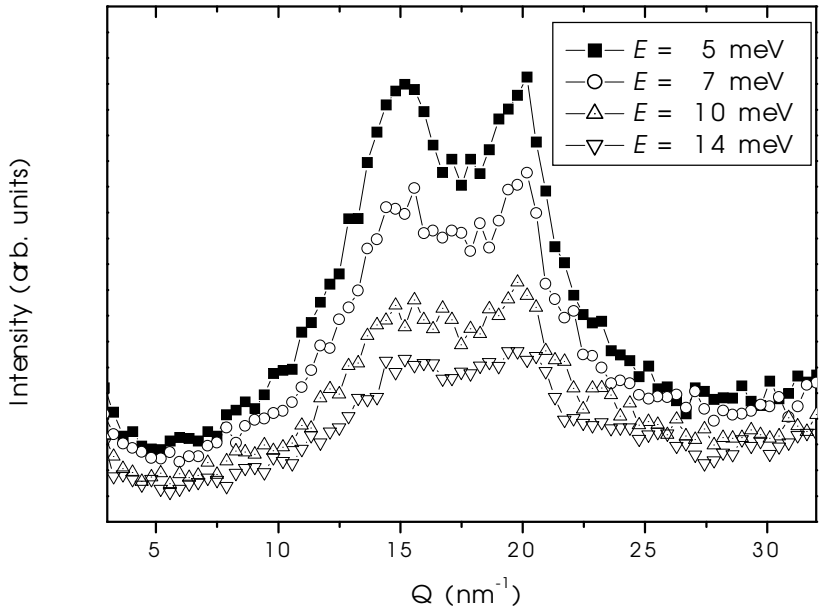

Figure 1. Constant-E cuts for SiO annealed at 950 °C. The points are connected by a line as guide to the eye.

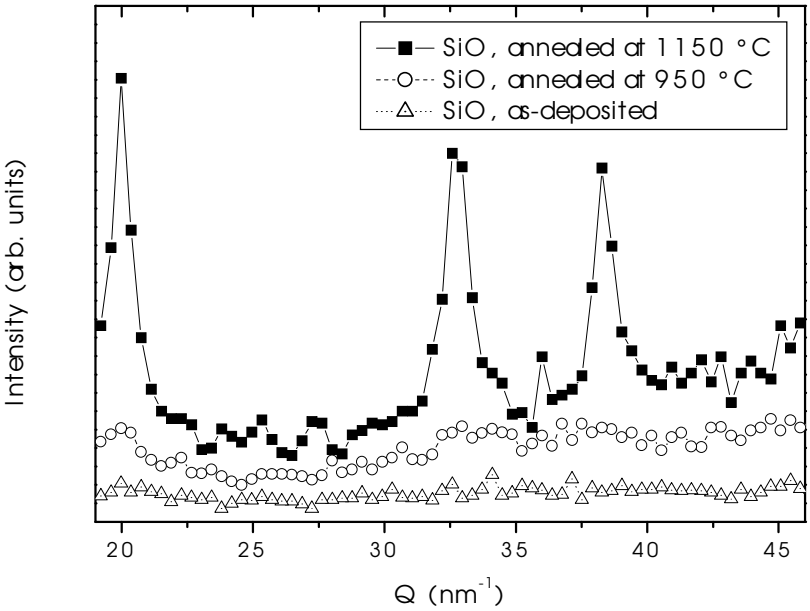

Figure 2. Q scans at fixed energy transfer E = 10 meV. The points are connected by a line as guide to the eye.