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Report:

To achieve the proposal aims we have collected a series of X-ray absorption spectra of unmodified and hydrogen modified ($T_{red} = 350^o$C, $t_{red} = 1,\ 3,\ 17$h) bismuth-silicate and bismuth-germanate glasses at Bi $L_3$-edge and Ge K-edge. XAS data-analysis have been performed using the GNXAS method. XANES analysis, in which we have represented the signal from the reduced glasses, $\alpha_{redu}(E)$, as a linear combinations from unreduced glass, $\alpha_{unredu}(E)$, and from pure crystalline Bi, $\alpha_{Bi}(E)$, has been used to estimate the fraction, (1-$p$), of bismuth atoms which have local neighborhoods as in metallic bismuth.

The XAFS data are of excellent quality and we are able to observe the structural evolution of the local (short-range) order as a function of the reduction time and glass composition.

The comparison of the obtained experimental results with the results of molecular dynamics (MD) simulations allowed to verify the interaction models and their parameterisations used in MD calculations. Satisfactory agreement between experimental and theoretical data has been obtained (see Figure 1) for the short range structure. Encouraged with this agreement we performed also a thorough analysis of the medium range ordering in MD-simulated structures.

We also performed several X-ray absorption temperature scans at fixed photon energy (SEXAD - Single Energy X-Ray Absorption Detection), in order to recognise the sensibility of this method to phase transitions in the metallic nano-granules present in the reduced glasses. Preliminary data collected during this experiment prove, that the simultaneous usage of SEXAD, EXAFS and XRD methods is a very effective way

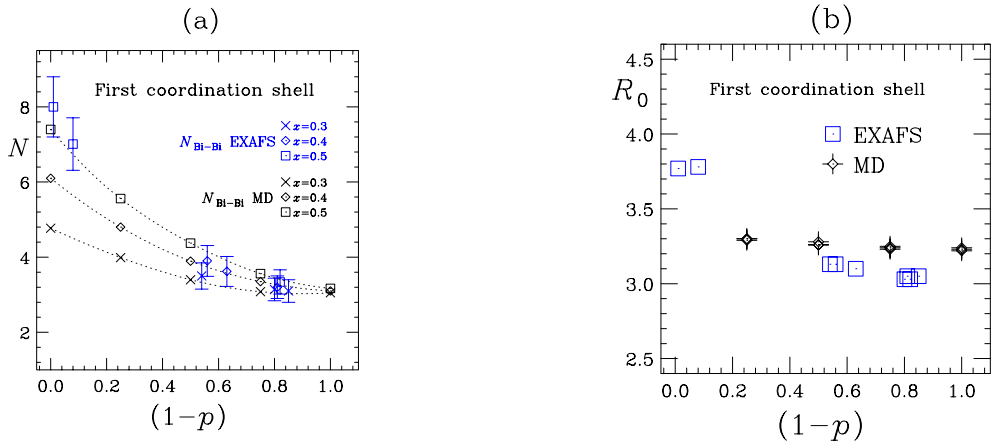


**Fig.1.** Comparision of the EXAFS and MD results, reduced $x\mathrm{Bi_2O_3}$ $(1-x)\mathrm{SiO_2}$ glasses: (a) Bi-Bi coordination number, (b) the most probable Bi-Bi distance

to get detailed insight into the granular structure present in the glass matrix on a given stage of the modification process. This measurement, together with the GNXAS determination of the short-range structure parameters, the tempeartures of a phase transitions, and the mean granule radius, makes possible the reconstruction of the size distribution of the metallic nano-granules confined in the glass matrix.
Preliminary results presented in this report and in [1-5] are very promising for structural investigations of the reduced silicate glasses containing Pb and Bi atoms. Other data recorded during HS-1663 experiment are currently being analysed, and several other papers are in preparation [6,7].

## References

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