EUROPEAN **S**YNCHROTRON **R**ADIATION **F**ACILITY

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ESRF

ESRF	**Experiment title:** Study of Bi clustering and Bi-N dimers formation in GaAsBi and GaAsBiN alloys	**Experiment number**: MA-436
Beamline: BM29	**Date of experiment**: from: 29 August 2007 to: 1 September 2007	**Date of report**: 12/08/08
Shifts: 9	**Local contact(s)**: M. Vaccari	*Received at ESRF:*

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Report:

This was a continuation of proposal MA-237. The experiment was successfully carried out and we completed the scheduled dataset. The new Bi L-edge EXAFS spectra have the same quality as in the previous report.
A paper reporting results of the two experiments has been very recently published in Physical Review B.

We used X-ray absorption spectroscopy to investigate the local structure around Bi atoms in $GaAs_{1-x}Bi_x$ layers grown on GaAs, as a function of Bi concentration, in order to detect short range order. We found that static disorder in the Bi next nearest neighbors interatomic distances dramatically increases when the Bi concentration is increased.
At 1.2 % Bi concentration (sample A), the Bi atoms are randomly distributed whereas at 1.9 % (sample B), they tend to form next nearest neighbor pairs. When the Bi concentration rises to 2.4 % (sample C), our results suggest that some of the Bi atoms form small Bi clusters. Such strong deviations from a random distribution are likely to play an important role in the occurrence of the giant optical bowing recently measured in this alloy.

Fig. 1 shows the Fourier Transforms of the EXAFS signal for three samples with increasing Bi concentration (going from A to C). Comparing the FT of samples A and B, the first evident difference is that, despite an almost identical amplitude of the first and third main peaks, the second peak is strongly damped in sample B. The three main peaks correspond to the different atomic coordination shells around Bi, so that the damping affects the mixed Bi-As shell.

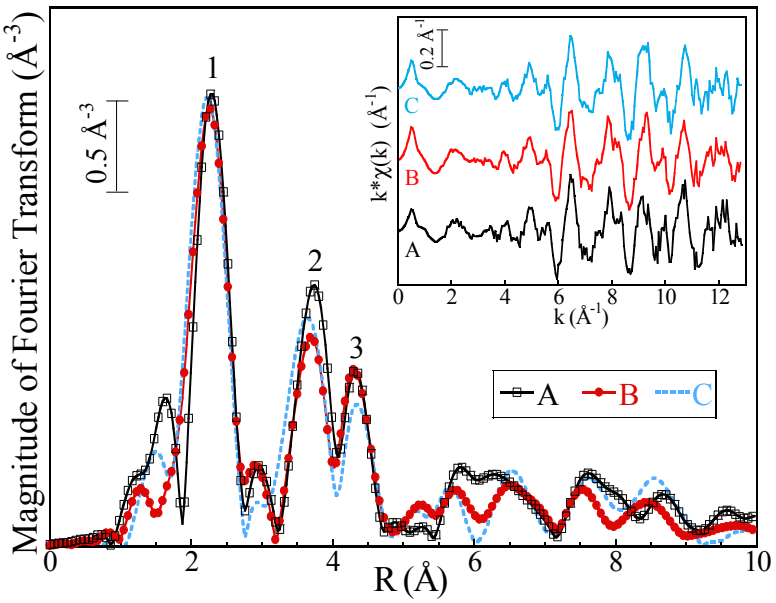

Fig. 1: EXAFS Fourier trannsform for te three samples, in the inset raw

Fig. 2 reports the fits performed on the FT of samples A and B. The spectrum from sample A (bottom) is well fitted with a random distribution of anions. As for sample B (top), if we fix the Debye-Waller values to those determined for sample A, it is evident that the 2nd shell peak cannot be reproduced by a random model (red open circles) due to the amplitude damping. The spectrum for sample B can be very well fitted by assuming the formation of a Bi pair (i.e. presence of a second Bi atom in the first anionic shell around the central Bi) and calculating the relative broadening of the distances distribution via a valence force field (VFF) method. Such broadening is at the origin of the FT amplitude damping reported in Fig. 1, which is perfectly accounted by our structural model without the need of fitting or modifying "ad hoc" the DW factor. In the case of the sample with highest concentration (C) the situation is more complex with formation of a fraction of Ga-centered Bi tetramers (see published paper for more details).

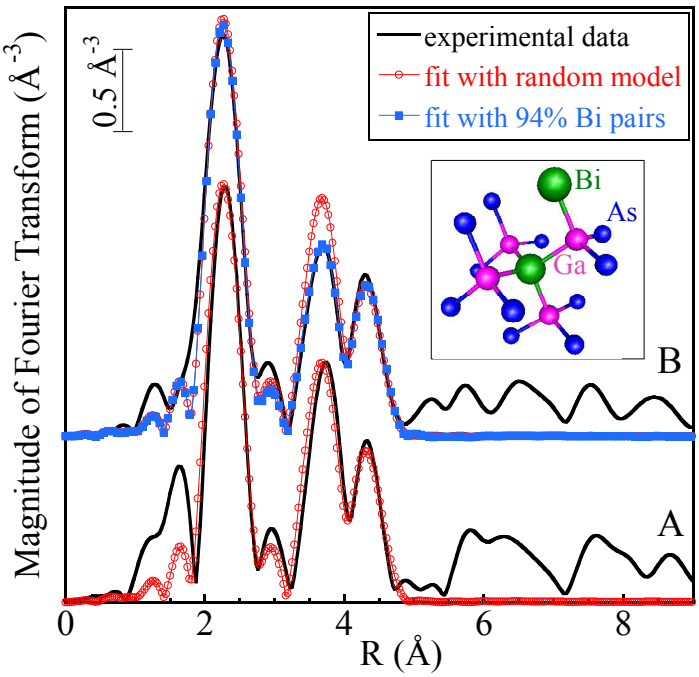

Fig. 2: Fits on the FT for samples A and B using random and pair structural models, the latter one is sketched in the inset

Publications:

G. Ciatto, E. C. Young, F. Glas, J. Chen, R. Alonso Mori, and T. Tiedje, "Spatial correlation between Bi atoms in dilute $GaAs_{1-x}Bi_x$: From random distribution to Bi pairing and clustering", **Phys. Rev. B** 78, 035325 (2008)