



	Experiment title: Study of Bi clustering and Bi-N dimers formation in GaAsBi and GaAsBiN alloys	Experiment number: MA-237
Beamline: BM29	Date of experiment: from: 15/11/2006 to: 20/11/2006	Date of report: 12/08/2008
Shifts: 18	Local contact(s): Gianluca CIATTO	<i>Received at ESRF:</i>
Names and affiliations of applicants (* indicates experimentalists): Dr. Gianluca CIATTO* Mr. Roberto Alonso MORI* Prof. Tom TIEDJE Mr. Arvin YAZDI Dr. Erin YOUNG*		

Report:

The experiment was successfully performed and, thanks also to the data recorded during its continuation MA436, we were able to complete the analysis of bismides epilayers in the 1.2-2.4 % Bi concentration range. The quality of all Bi L2-edge EXAFS spectra recorded in fluorescence detection mode with a 13-element hyperpure Ge detector was very satisfying, however more energy resolution and flux would have been useful for a detailed study of the XANES line shapes.

A paper reporting the results of the experiment 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.

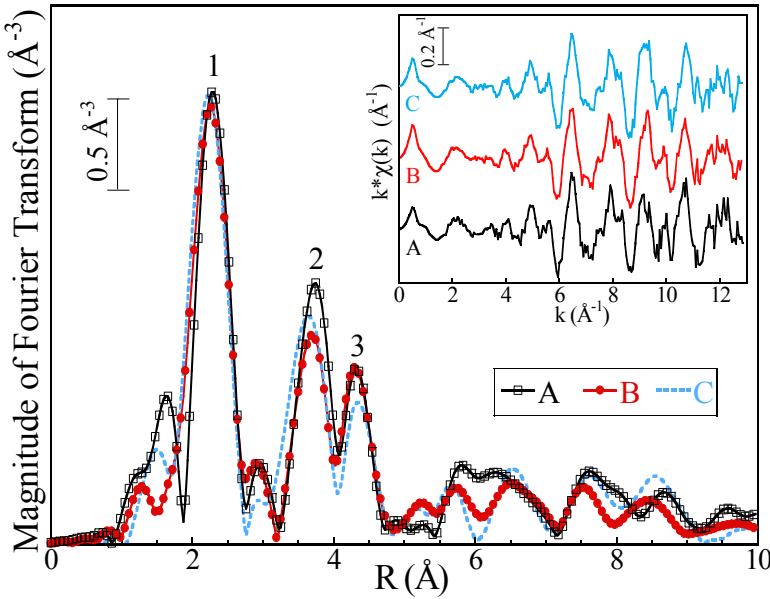


Fig. 1: EXAFS Fourier transform for three samples, in the inset raw

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).

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)

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

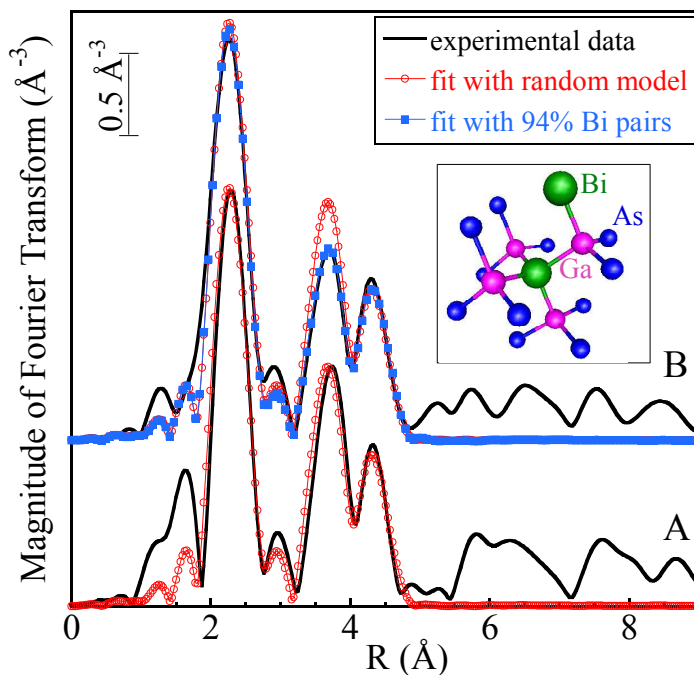


Fig. 2: Fits on the FT for samples A and B using random and pair structural models, the latter one is sketched in the inset