ESRF	**Experiment title:** Single crystal diffuse scattering measurement of atomic disorder in semiconductor alloys.	**Experiment number:** 01-02-619
Beamline: BM1A	**Date of experiment:** from: 14/09/02 and 17/03/03 to: 17/09/02 and 19/03/03	**Date of report:** 2/28/04
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Report:

Ternary semiconductor alloys, in particular $Ga_{1-x}In_xAs$, have technological importance because they allow important properties, such as band-gaps, to be tuned continuously between the two end-points by varying the composition x. Surprisingly, there is no complete experimental determination of the microscopically strained structure of these alloys. Both theory [1] and extended x-ray absorption fine structure (XAFS) experiments [2] have shown that Ga-As and In-As bonds do not take some average value but remain close to their natural lengths of $L_{Ga-As} = 2.437$ Åand $L_{In-As} = 2.610$ Åin the alloy. Recently we extended these results using the atomic pair distribution function (PDF) analysis of x-ray powder diffraction data. This allowed the local and intermediate range structure to be determined with much greater precision. The distinct near-neighbour In-As and Ga-As bonds could be resolved in the high real-space resolution PDF. The data across the entire alloy series were successfully modeled using a supercell model based on a simple two-parameter Kirkwood potential resulting in the most complete understanding of the local structure to date [4].

The problem is that the orientational averaging that occurs in measurements from powders removes directional information from the data and lowers the information content of the measurement making it hard to distinguish competing potential models. Also, the powder measurements are rather insensitive to chemical short-range order that is a very important determinant of the semiconductor properties. Single crystal diffuse scattering is much more sensitive to chemical short-range order. It also retains directional information about long-range strain and short-range atomic displacements and is a much more severe test of the models. We therefore carried out a

single-crystal diffuse scattering measurement at the Swiss Norwegian Beamline, BM1A in collaboration with Thomas Weber. Single crystals of the 50% doped sample $x = 0.5$, were obtained from Marin Gospodinov, at U. Sophia. Data were collected using the rotation method in transmission with a MAR345 image plate detector. Data-sets were collected every 0.2° over a range of 120°. Arbitrary slices of reciprocal-space were reconstructed using the program XCAVATE [5].
The results are interesting. We observe size-effect scattering as expected and Huang-scattering butterflies around $h00$ and $k00$ points reproduce the shapes of the calculated diffuse intensities. However, the diffuse scattering around the $hh0$ peaks are highly symmetric in the data whereas the models, calculated using the Kirkwood-Keating model, indicate that these peaks also should have butterfly shaped Huang scattering. This is not currently understood and we are working on an interpretation. We also would like to repeat the measurements with better crystals but currently do not have a reliable source. A comparison of the measured and calculated intensities are shown in Fig. 1.

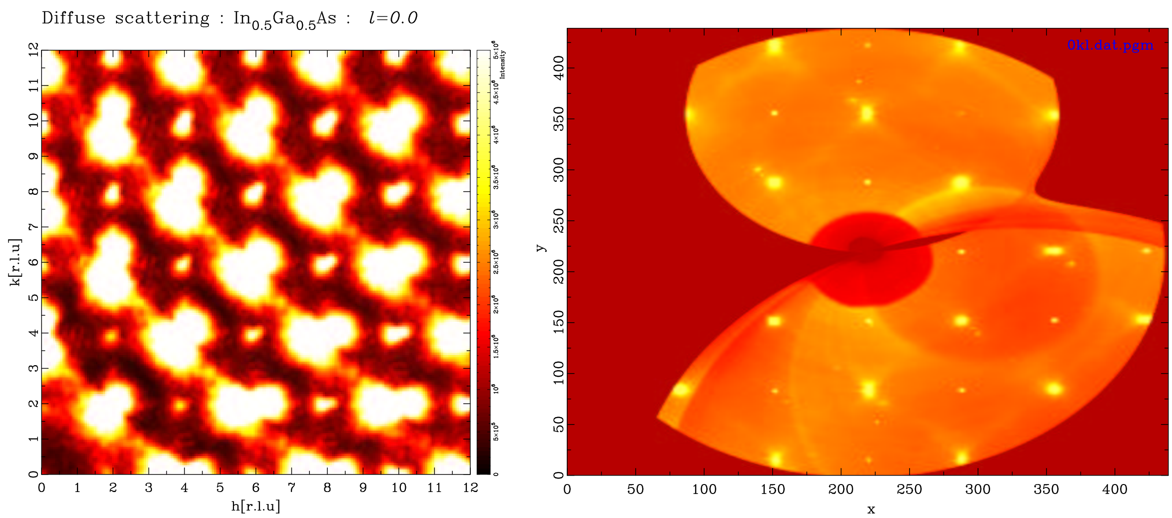

Figure 1: False-color contour plots of diffuse scattering signals from $In_{0.5}Ga_{0.5}As$. In each case the $hk0$ plane of reciprocal space is shown. The left panel shows the calculated scattering from a model based on the Kirkwood-Keating potential. The right hand panel is the measured scattering. The color scales and the range or reciprocal space that are presented are different but the general features are well reproduced: Huang scattering butterflies pointing towards the origin of reciprocal space at the Bragg-points and extended size-effect scattering along $hk0$ directions.

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