EXPERIMENTAL REPORT
RAPPORT D'EXPERIENCE

Programme Committee Proposal Number
N° Projet Comité de Programme

PROJECT TITLE : *TITRE DU PROJET :*

DAFS (Diffraction Anomalous Fine Structure) STUDY OF STRAINED III-V EPITAXIAL SEMICONDUCTORS

LIGNE : **D2AM** **IF**

INSTRUMENT :	PETITS ANGLES	☐	EXAFS	☐
	7 CERCLES	X	G M	☐
	BIO-CRISTALLOGRAPHIE	☐	S U V	☐

NUMBER OF RUNS USED
NOMBRE DE SESSIONS EFFECTUEES : 15 / HS13

STARTING DATE
DATE DE DEMARRAGE : *Septembre 96*

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Strained pseudobinary III-V semiconductors are of great interest for their important applications in the field of electronic and optoelectronic devices : the presence of strain reduces the symmetry of the crystal and modifies the electronic band structure. On the other hand it has been shown that the performances of the epitaxially grown heterostructures are affected by the composition gradient at the interfaces. Therefore much efforts are made to determine the local strain thru the whole heterostructures as well as the atomic structure at the interfaces.

XAFS (X-ray Absorption Fine Structure) spectroscopy would be the most suitable technique to get information about the short-range structure of these compounds but it cannot be applied in a straightforward way due to the peculiar nature of the epitaxial samples : too much thin to be measured in transmission and often grown on a substrate having some of the atomic components in common with the epilayer. Glancing-angle EXAFS or SEXAFS, have been used but they solve the problem only in part, since the signal collection is restricted to a few monolayers below the surface, allowing a quasi-surface measurements of very thin layers. The aim of our collaboration was to study the structural properties of different strained III-V semiconductors samples by using the alternative approach given by the DAFS spectroscopy. DAFS combines the local structural sensitivity of XAFS with the long range crystallographic sensitivity of X-ray diffraction by measuring Bragg peak intensities as a continuous function of energy through an absorption edge. The energy dependent modulation of the peak intensity contains local structural information similar to that of XAFS. The advantage of DAFS for studying this kind of systems, is to give structural information about the whole heterostructure by choosing the Bragg peaks (site-selective Bragg peak) of the strained phase.

In the first part of the paper [1], we present the general formalism for analysing EDAFS oscillations. The procedure is valid for any type of crystallographic structure, i.e. centrosymmetric or otherwise. The first-order EDAFS oscillations may be expressed with a formula very similar to the EXAFS one. For the one-anomalous-site analysis, the structure is not *a priori* necessary, and a standard EXAFS analysis may be performed. As a general trend, the DAFS spectra are very sensitive to the crystallographic Debye Waller (DW) factors. The measurements at different edges are a way to decorrelate the DW and the occupation factors of the anomalous atoms.

It has been shown with the weak 006 reflection of GaAsP which has a large anomalous effect, that a very small variation of the structural parameters may be detected. For the weak 006 reflection of GaAsP, an atomic displacement as low as one hundredth of an angström leads to crystallographic phase shift of about 60°, which has been clearly evidenced by the DAFS spectra. This small variation is comparable with the variation predicted by the elastic theory, as we can deduce from the values of the lattice parameters reported in the previous section for the bulk alloy and the pseudomorphic epilayer (a_0= 5.608 Å and $a_\perp$ = 5.566 Å respectively). If we assume that the contraction of $a_\perp$ is linear with the strain content, the difference in $a_\perp$ between sample G29 (ε= 0.4%) and sample G33 (ε =0.7%) should be equal to (5.566-5.608)*(0.3/0.8) Å = -0.015 Å, which would be consistent with the small contraction of 0.0096(3) Å detected by the DAFS analysis.

Using DAFS we have studied two different kinds of strained semiconductor compounds, in a different strain regime: a Strained Layer Superlattice of $(GaP)_2(InP)_3$ and three single epilayers of $GaAs_{1-x}P_x$ (x=0.23-0.20) grown on a GaAs (001) substrate. In the first case, the strain is accommodated by plastic deformation of the lattice ; in the second case the strain it is partially relaxed by dislocation generation leaving a certain amount of residual strain in the lattice.

We can draw three main results about the local microscopic structure of the two systems. First, we measure an elongation of 0.04 Å of the Ga-P bondlength in the SLS sample. Since this elongation agrees with elastic theory, the theory still holds for very thin epilayers (2 ML) with a high strain content (3.6%). In this sense, the results reported in literature are not yet very clear ; deviations have been observed for buried single layers of InAs [32] and for InGaAs epilayers with a thickness lower than 10 Å [33], whereas elastic deformation has been observed on a 2ML InAs/GaAs sample [13]. Our results have added information on a real SLS system in which the short-range order could not be studied by any other EXAFS-like approach.

Second, concerning the $GaAs_{1-x}P_x$ samples, the Ga-As and Ga-P bond distances (r_{Ga-As}=2.44±0.01Å and r_{Ga-P}=2.37±0.02 Å) do not vary, within the standard deviation, as a function of residual strain, remaining very close to the correspondent bulk value of the starting binary compounds as was observed for the relaxed pseudobinary alloy. The next-nearest-neighbor distances obtained by a multishell analysis of the raw EDAFS data compare well with the values predicted for the relaxed and pseudomorphic alloy.

Third, we compare EDAFS spectra of two $GaAs_{1-x}P_x$ samples recorded with two different orientations of the X-ray polarisation vector. The most strained and thinnest sample shows a difference in the low k-region of the spectrum (which is more sensitive to the presence of P atoms) when switching the X-ray polarisation from [110] to [1-10] direction. The multishell fit analysis indicates that for the [1-10] direction, the number of P atoms seen by the Ga absorber is much lower, as deduced qualitatively by comparing the two spectra with the GaP and GaAs bulk measurements. That result may be understood in terms of a partial P ordering mechanism. It is quite surprising to observe a change in the Next Nearest environment of Ga, when turning the polarization in the polar plane, i.e. the growth plane, that should be in this sense, supposedly isotropic. However the EDAFS shape could also depend, in a more subtle way, on anisotropies of the atomic scattering factor related to ordered deviations from the cubic symmetry, of the absorber atomic environment. Further experiments are needed to give a definite answer.

[1] M. G. Proietti, H. Renevier, J. L. Hodeau, J. Garcia, J. F. Bérar, P. Wolfers, "The Diffraction Anomalous Fine Structure (DAFS) spectroscopy applied to the study of III-V strained semiconductors", Phys Rev. B ~~accepted~~ 7479 (1999)