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Local structure in semiconductor superlattices and epilayers

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We report XAFS studies of two related strained semiconductor systems: nominally matched short period InGaAs/InP(001) superlattices and strained epilayers of $In_xGa_{1-x}As$ on InP(001). In InGaAs/InP superlattices coordination numbers deviate significantly from the abrupt interface case, demonstrating the presence of strained interface layers. This provides a local structural explanation for the non-negligible average lattice mismatch measured by diffraction. The analysis of strained epilayers of $In_xGa_{1-x}As$/InP(001) allows us to study in detail bond lengths in strained semiconductors. We demonstrate that, notwithstanding the rigidity of semiconductor bonds, strain induces variations of nearest neighbor distances: bond lengths can be stretched or compressed. A model which reproduces strain-induced variations is presented

Keywords: semiconductor alloys, strain, heterostructures, superlattices

1. Introduction

Advanced semiconductor growth techniques are able to deposit semiconductor samples with high biaxial strain. From the point of view of local structure this adds a new dimension to XAFS studies: the effect of biaxial strain on local structure can now be studied, thus providing information on the *real* (not average) atomic structure in strained semiconductor layers. Also of interest is the characterization by XAFS of thin semiconductor layers and interfaces as atomic selectivity and local sensitivity provide information not accessible with other techniques.
The $In_xGa_{1-x}As$/InP(001) system is one of the most important heterostructures in optoelectronics. We describe XAFS studies of two sets of samples containing $In_xGa_{1-x}As$ and InP layers which illustrate the capabilities of XAFS in the study of strained semicondutors. In nominally matched, short period superlattices (SPSLs) of InGaAs/InP (we use InGaAs for $In_xGa_{1-x}As$ with x=0.53) we identify and quantify the presence of bonding configurations not expected in a superlattice (SL) with abrupt interfaces. The study of $In_xGa_{1-x}As$ epilayers on InP(001) as a function of concentration demonstrates the presence of variations in bond length induced by strain in a very clear way.

2. XAFS experiments

XAFS measurements were performed in the fluorescence mode at the Ga and As K-edges at the "GILDA" (BM8) beamline of the ESRF using a dynamically sagittally focussing monochromator (Pascarelli *et. al.*, 1996) with Si(311) crystals. Harmonics were rejected with two grazing incidence mirrors and fluorescence detection was accomplished with either a single element or a seven element hyper-pure Ge detector. In order to avoid deadtime corrections the total count rate on the detector was limited to 20 000 c/s and a shaping time of 0.25 μsec was used on the amplifier. Data analysis was performed using standard procedures using experimental standards of InAs, GaP and GaAs. More detailed information can be found in Boscherini *et. al.*, (1998) for the SPSLs and in Romanato *et. al.* (1998) for the epilayers, and in the electronic archive of these proceedings.

3. InGaAs/InP short period superlattices

Five InGaAs/InP superlattices deposited on InP(001) were grown by Metal-Organic Chemical Beam Epitaxy or Chemical Beam Epitaxy. The periodicity of the structures ranges from 30 to 60 Å. The most important aspect of the growth procedure in the present context is the use of the "growth interruption" technique: just-grown InP layers are exposed for a few seconds to AsH_3 flux before depositing the InGaAs layer and an exposure to PH_3 is used at the reverse interface. This procedure optimizes the optoelectronic response of the structures.
At the In composition employed these samples are nominally lattice matched. However, high resolution X-ray diffraction (D2AM beamline, ESRF) indicates the presence of a non-negligible average lattice mismatch with the substrate, which ranges from -0.14 % to 0.87 % as measured at the (004) reflection. The origin of the lattice mismatch is explained by the XAFS measurements. In fact, at the Ga edge a clear Ga-P nearest neighbour contribution is present.

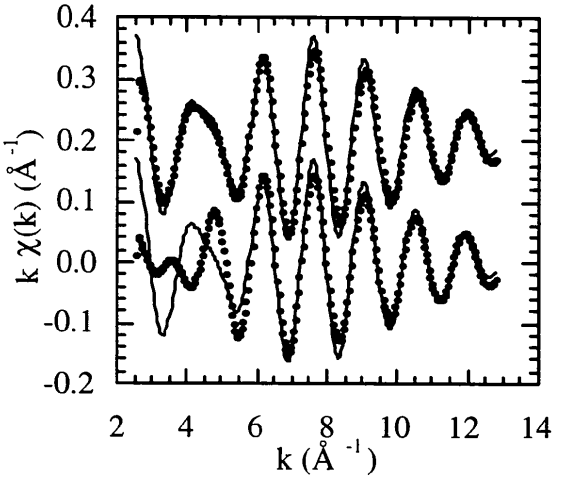

Figure 1
Comparison of first shell fits for the Ga edge spectra of one of the SPSL samples without (bottom) and with (top) Ga-P contribution.

This is demonstrated in Fig. 1 where we show for one sample the inverse FT of the first shell peak fitted with only Ga-As contributions (bottom) and with a combination of Ga-As *and* Ga-P contributions (top). In a SL with abrupt interfaces Ga-P bonds are expected only at the interface; it is possible to demonstrate that the Ga-P coordination numbers (CNs) we measure are always significantly higher than expected in such ideal SLs with periods equal to the ones of our samples. At the As edge we detect As-In and As-Ga contributions; however a significant excess of As-In contributions is measured with respect the abrupt interface case, even if interface bonds are taken into account.

This evidence demonstrates the presence of interface layers between InGaAs and InP. Based on the growth sequence employed and on indications from other techniques it is possible to model the SLs as composed of the two nominal layers plus two *strained* interface layers of $InAs_xP_{1-x}$ (under compressive strain) and $In_{0.53}Ga_{0.47}As_{1-y}P_y$ (under tensile strain). The CNs measured are related to thickness and concentrations of the interface layers and quantitatively justify the average lattice mismatch measured by diffraction.

4. $In_xGa_{1-x}As$ epilayers on InP(001)

The study of InGaAs/InP has revealed the presence of strained interface layers. In a previous publication (Pascarelli *et. al.*, 1997) we have presented a detailed study of the local structure in one of the strained layers at the InGaAs/InP heterostructure, i.e. strained $InAs_xP_{1-x}$. Here, we concentrate on $In_xGa_{1-x}As/InP$ in which it has been possible to detect the bond length variations due to strain extremely well. Previously, Kuwahara *et. al.* (1994) and Tabuchi *et. al.* (1994) had reported bond length relaxations at the critical thickness for semiconductor epilayers. Similar results to ours for a $In_{0.22}Ga_{0.78}As$ layer on GaAs(001) have been reported by Woicik *et . al.* (1997) and for the same system here studied by Woicik *et. al.* (1999).

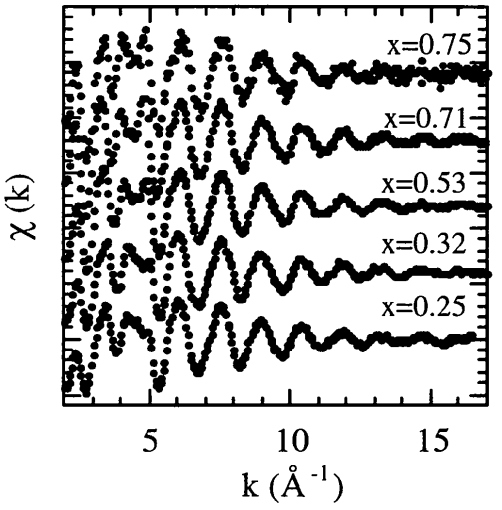

Figure 2
Raw Ga-edge XAFS signals for $In_xGa_{1-x}As/InP(001)$ epilayers over the full thickness and concentration range.

Seven pseudomorphic $In_xGa_{1-x}As$ epilayers were deposited by metal-organic vapor phase epitaxy, with x in the range 0.25 to 0.74; this concentration range corresponds to strain values ranging between 2 and -1.4 %. Sample thicknesses range between 8 and 460 nm. Extracted XAFS signals in the entire thickness and composition range are shown in Fig. 2 for the Ga edge, illustrating the high signal-to-noise ratio obtained.

The Ga-As and As-In bond lengths are plotted as a function of x in Fig. 3. Also shown are data points for two relaxed samples (i.e. samples whose thickness is above the critical thickness for strain relaxation), a linear fit of the data of Mikkelsen & Boyce (1983) for the bulk alloy and the predictions of the model described in detail in Romanato *et. al.* (1998) for the strained alloy. Thanks to the number of experimental points measured over the wide concentration range this plot clearly demonstrates that the *slope* of the distance-concentration relation is inverted in the strained alloy with respect to the unstrained case. The main elements of the model which reproduces the data very well are: a first-order expansion of the atomic coordinates in the unit cell under tetragonal distortion for the binary-on-binary case which yields a relation between the variation of the bond length and strain followed by an extension to the pseudobinary case. Macroscopic elastic constants are used to describe the variation of the lattice parameters.

This study is of general interest since it addresses the relation between elasticity theory and local structure. We believe it significantly expands our understanding of local structural distortions in semiconductor alloys, complementing the earlier work on bulk alloys (Mikkelsen & Boyce, 1983; Balzarotti *et. al.*, 1984).

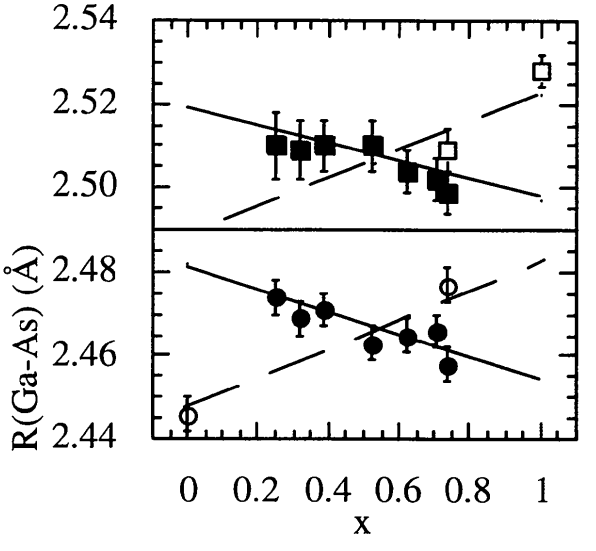

Figure 3
Ga-As and As-In bond lengths for $In_xGa_{1-x}As/InP(001)$: strained samples are reported as filled symbols, relaxed samples as empty ones. Also shown is a linear fit to the data published by Mikkelsen and Boyce (1983) for bulk $In_xGa_{1-x}As$ (dashed line) and the predictions of our model (continuous line).

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