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Standing Waves Investigation of InAsP/InP Superlattices

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Abstract. X-ray standing waves measurements have been performed on a set of six InAsP/InP superlattices exhibiting a wide range of lattice strain values and on both the (002) and (004) reflections. The objective was to assess the XSW technique as a structural probe in superlattices. For samples with perpendicular lattice misfit less than 1.5% we find clear XSW modulations in the As fluorescence; this signal is well reproduced by simulations performed by solving the Takagi-Taupin equations. For samples with higher misfit a negligible XSW signal is found, indicating considerable lattice disorder.

1. INTRODUCTION

The X-ray standing waves technique (XSW) [1] is commonly used to determine the structure of an impurity with respect to a perfect crystal, be it on the surface or in the bulk. In the most usual version, the standing wave field is set-up by the diffracting planes of choice and perfect crystal dynamical theory is used to obtain the reflectivity and phase vs. angle functions needed to interpret the data. In this paper we report on an attempt to extend the technique to semiconductor superlattices (SL), the objective being to assess the ability of XSW to obtain structural information in these systems, and in particular on thin interface layers. The behaviour of the XSW field in distorted epi-layers has been studied theoretically [2]; there have also been two recent experimental reports of the application of XSW in SL's; in one case, one Si/Ge SL was studied [3], while in the other [4] two InAs/GaAs SL's were investigated; in both cases the (004) reflection was used. In the present paper we report on XSW measurements on six InAsP/InP SL's exhibiting a wide range of misfit values using both (004) and (002) reflections; the same samples have also been studied by XAFS [5] in a parallel investigation.

A detailed, microscopic, characterization of SL's is of great importance in the field of semiconductor materials science. The particular system studied here, a set of InP/InAsP SL's, is of two-fold importance. First of all, it is a model for the InP-InGaAs interface in unstrained InGaAs/InP SL's. It is well known that the performance of these devices is strongly influenced by the microscopic structure of the buried interfaces[6]; as an example, imperfections of the crystal lattice cause scattering processes yielding a reduction of the exciton decay time, a limitation in the electron mobility and an increase of the non radiative recombination. Secondly, InAsP is the active, strained, layer in InAsP/InGaP strain compensated lasers.

2. SAMPLES AND EXPERIMENTAL

Six InAsP/InP SL structures were grown in the CSELT laboratories on InP(001) [7]. The main sample characteristics are described in Tab. 1; samples 1 - 5 were grown by LP-MOCVD while sample 6 was grown by CBE. Notice that the perpendicular lattice misfit ranges from 0.34 to 2.7 %. The sample characteristics have been determined by high-resolution x-ray diffraction (HRXRD)[8,9] and confirmed by TEM. In particular the former technique, which is directly related to the XSW technique developed here, is able to measure the SL period, P , and the average As concentration of the SL, $\langle x \rangle$. A typical HRXRD spectrum is composed of a peak originating from the substrate, a 0-order SL peak, and higher order SL replicas. Under the assumption that the SL can be described as a two-component system, an InP layer of thickness $P-t$ and a ternary layer of thickness t , with perfect reproducibility and negligible interface roughness, a model which we will call the Ideal Uniform Abrupt SL (IUASL), the As concentration in the ternary layer may be deduced: $x = \langle x \rangle t/P$.

XSW measurements were performed at the ID 32 beamline of the ESRF. The radiation from the undulator was

Table 1: Nominal sample characteristics as deduced by HRXRD: P : period; t : thickness of ternary layer; x : As concentration in ternary layer; N : number of periods; $\epsilon_{\perp} = (a_{\perp} - a_0)/a_0$, perpendicular lattice misfit.

Sample No.	Growth Code	P (Å)	t (Å)	x	N	$\epsilon_{\perp}$ (%)
1	32	77	10	0.05	100	0.34
2	114	61	10	0.17	1000	1.2
3	157	93	15	0.20	50	1.4
4	137	90	10	0.33	50	2.3
5	183	63	13	0.24	300	1.6
6	205	97	12	0.40	62	2.7

Fig. 1 As K_{α} fluorescence yield XSW signals for all samples.

field set-up here has a periodicity equal to the average SL (002) or (004) planes we conclude that we are observing XSW signals which give us information on the position of the As atoms with respect to these planes. For samples 4 - 6, which have a higher As concentration, the XSW signal is extremely small if not absent.

4. SIMULATION OF XSW SPECTRA

In order to analyze spectra such as those presented in Fig. 1 and 2 it is not possible to use standard dynamical theory. In fact, we are dealing with a wave field set-up by a crystal with two components, one of which under strain. The Takagi-Taupin [8] equations have therefore been solved using the recursion formula by assuming a model structure for each sample. In particular, the aforementioned IUASL model was assumed for the samples.

As an example, we show in Fig. 3 the depth and angle dependence of the electric field intensity for sample 1. The origin of the depth scale is the SL-air interface; the SL is approximately 8000 Å thick. At the origin of the angular scale is the substrate peak; its intensity undergoes characteristic beating due to the small difference in lattice spacing between substrate and overlayer. At negative angles, the characteristic derivative-like signal associated with the SL average diffracting planes grows with distance from the substrate.

Fig. 2: Fluorescence yield and reflectivity for (002) and (004) reflections for sample 3.

monochromatized at 12.5 keV with a 10^{-4} bandpass by a cryogenically cooled Si(111) double crystal monochromator. The nominal vertical divergence of the beam on the sample was 20 μ rad. Samples were positioned on a multi-circle diffractometer with a vertical scattering geometry. As K_{α} fluorescence was monitored as a function of incidence angle for the 002 and 004 reflections with a high-purity Ge detector positioned $\sim 5^{\circ}$ above the horizontal in the vertical plane containing the electric vector of the incoming beam; this choice guarantees good surface sensitivity and minimizes the elastically scattered radiation. Along with the fluorescence yield, the diffracted intensity (the reflectivity, in XSW terminology) was measured with a NaI(Tl) detector.

3. RESULTS

The XSW spectra are shown for all samples in Fig. 1. In Fig. 2 we show fluorescence and reflectivity for the (002) and (004) reflections of sample 3. The angular scale is referred to the substrate reflectivity peak; at this angular position a symmetrical peak is observed in the XSW yield. This observation is compatible with the negligible coherent fraction expected for the As atoms, which are embedded in the SL structure, with respect to the XSW field set-up by the substrate (which has a different lattice parameter with respect to the SL). At negative angles, and at roughly the same position as the 0-order SL reflectivity peak, a clear XSW signal is observed for samples 1 - 3. Assuming that the XSW

Fig. 3: Intensity of the electric field for sample 1

The result on the first three samples indicates that our method and underlying hypotheses are fundamentally correct. A detailed comparison indicates that the coherent position used is not perfectly adequate to reproduce the data; this is not surprising given the crudeness of the VCA. In these samples XSW can therefore give useful structural information.

The very small or absent signal on samples 4 - 6 indicates that coherent fraction of As in these samples is very small; these samples have a rather high misfit and therefore our result indicates the presence of interdiffusion, roughness or lattice disorder due to the high accumulated strain.

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Fig. 4: Comparison of experimental spectra (dots) with simulations, as described in the text.

In order to simulate a XSW signal for the As some assumption must be made regarding the local structure in the ternary alloy. As a starting point we have chosen the Virtual Crystal Approximation (VCA): each atom is positioned in its ideal crystallographic position, i.e. that determined by elementary geometry by its two relevant lattice parameters ($a_{\perp}$ and $a_{\parallel}$).

It must be pointed out that it is well known that this approximation is not strictly valid for bulk ternary alloys; moreover, As XAFS measurements on the same sample here presented have shown that the VCA is not valid locally [5]. Therefore the VCA must be considered a starting point for further structural refinement.

Using the two cited approximations, IUASL and VCA, we have simulated the As XSW signal for samples 1 - 3. Examples of the comparison between data and simulation for sample 1 are shown in Fig. 4.

5. DISCUSSION

The results presented can be summarized in the following way: for samples 1 - 3 the simulation using the VCA and IUASL models reproduces very well the experimental lineshapes while samples 4 - 6, which exhibit a higher lattice misfit, have a very small signal and consequently a very low coherent fraction.