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# X-ray analysis of spontaneous lateral modulation in $(InAs)_n/(AlAs)_m$ short-period superlattices

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## Abstract

The lateral composition modulation in $(InAs)_n/(AlAs)_m$ short-period superlattices was studied by means of synchrotron x-ray diffraction. By choosing specific diffraction vectors having a large component closely parallel to the modulation direction, we are able to observe a number of lateral satellite peaks around the zero-order short-period superlattice peak. A model, incorporating both composition and strain, is used to simulate the intensities of these satellites. Our results provide a quantitative fit and permit the evaluation of the composition amplitude.

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Spontaneous lateral composition modulation (LCM) in III-V semiconductor alloy films introduces significant modifications to the opto-electronic properties of semiconductor materials which are of interest for producing quantum-wire lasers and photodetectors. Recent studies show that LCM can be manipulated by growing short-period superlattices (SPS) consisting of two lattice-mismatched components, such as $(\mathrm{InAs})_n/(\mathrm{AlAs})_m$, by molecular beam epitaxy (MBE).[1] Growth studies have shown that the modulation is controlled by the global strain of the SPS layers and the substrate miscut.[2,3] The morphology of the modulated structure has been demonstrated in several transmission electron microscopy (TEM) and atomic force microscopy (AFM) analyses,[2–4] which suggested that the LCM is accompanied by a strain modulation that perforce follow the composition profile. In evidence of this modulation, lateral satellites around Bragg reflections in x-ray reciprocal space maps indicate the formation of LCM on a macroscopic scale. However, a quantitative measure of the modulation in terms of either strain or composition has so far not been addressed. The purpose of this work is to present a quantitative determination of the amplitude and wavelength of the LCM by means of x-ray diffraction together with a theoretical consideration of the effect of strain.

The LCM in the $(\mathrm{InAs})_n/(\mathrm{AlAs})_m$ SPS can have different orientations and more than one variant in a single sample. For simplicity, the particular sample studied here was $(\mathrm{InAs})_{1.99}/(\mathrm{AlAs})_{1.43}$ SPS grown on an InP (001) substrate by MBE which is known to exhibit a single variant.[2–4] The InP substrate is miscut by about 2° towards the [100] direction, which leads to a single modulation direction roughly along the [100] direction.

Details of the growth and morphology of the LCM structures as well as some preliminary x-ray studies can be found in Refs. 2-4. Conventional coplanar 224 diffraction indicates that the SPS structure was grown pseudomorphically on the InP substrate.

In order to improve the sensitivity of x-ray scattering to the LCM, we have chosen 402 and 602 peaks which have the largest accessible components of the diffraction vector **h** parallel to the modulation direction, given our experimental conditions (see below). However, these reflections are not achievable in a coplanar geometry and we have used an inclined arrangement where the scattering plane defined by the wave vectors of the primary and incident beams is not perpendicular to the sample surface. This is accomplished by keeping the incident and diffracted beams symmetric with respect to the sample surface, while rotating the $\chi$-angle in a standard four-circle diffractometer (as shown in Fig. 1). Measurements were done on beamline X14A at National Synchrotron Light Source at the Brookhaven National Laboratory with an energy of 8.0478 keV.

Figure 2a shows the measured 402 and 602 reciprocal space maps in the (010) reciprocal lattice plane (normal to the K-axis in Fig. 1). In both maps, the substrate peaks are not completely visible. This is because the LCM lies not exactly along [100], but is slightly tilted away, as can be seen in the reciprocal space maps lying in the (001) plane (Fig. 2b), in which the satellite distribution is neither symmetrical with respect to the Bragg point nor lying directly parallel to the [100] axis. Clearly, more lateral satellite peaks are presented in the 602 map, as expected if strain is a major contribution to the satellite pattern. This is because the x-ray scattering from strain depends on the value

$\mathbf{h}\cdot\mathbf{u}$, where $\mathbf{u}$ is the displacement due to startin. From the spacing between the neighboring satellites, we determine an average LCM wavelength of $L = (328 \pm 5)$ Å. The vertical periodicity of the sample gives rise to vertical (superlattice) satellites. In this paper, however, we report only on the zero-order superlattice satellite, which is fully sufficient for determining the modulation wavelength and amplitude and is thereby insensitive to the vertical structure of the SPS.

In order to obtain the modulation amplitude from the x-ray data, we have calculated the intensity distribution in reciprocal space. Since we have considered only the zero-order superlattice satellite, for the sake of simplicity we replace the actual sample superlattice structure by a vertically homogeneous layer $\mathrm{In}_p\mathrm{Al}_{1-p}\mathrm{As}$, whose chemical composition is only a function of the $x$-coordinate in the modulation direction. In so doing, we do not address the origin of the LCM, but rather assess its amplitude and strain. The composition function $p\,(x)$ is given as:

$$p(x) = p_0 + A\cos(Gx),\ \ G = 2\pi/L, \tag{1}$$

where $p_0$ is the average indium concentration, $A$ is the composition amplitude, and $G$ is the distance of the lateral satellites in reciprocal space. This modulation gives rise to a periodic intrinsic mismatch with respect to the InP substrate,

$$\delta(x) = \frac{p_0 a_{\mathrm{InAs}} + (1-p_0)\,a_{\mathrm{AlAs}}}{a_{\mathrm{InP}}} - 1 + A\cos(Gx)\frac{a_{\mathrm{InAs}} - a_{\mathrm{AlAs}}}{a_{\mathrm{InP}}}, \tag{2}$$

and a periodic modulation of x-ray scattering amplitude, or susceptibility, $\chi_{\mathbf{h}}(x)$,

$$\chi_{\mathbf{h}}(x) = p_0\chi_{\mathbf{h},\mathrm{InAs}} + (1-p_0)\,\chi_{\mathbf{h},\mathrm{AlAs}} + A\cos(Gx)\,(\chi_{\mathbf{h},\mathrm{InAs}} - \chi_{\mathbf{h},\mathrm{AlAs}})\,. \tag{3}$$

The calculation of the x-ray scattering consists of two steps. In the first step, we calculate the displacement field $\mathbf{u}(\mathbf{r})$ on the basis of the mismatch (??) employing the elastic Green function.[5] In this method we make the (initial) assumption that the layer is elastically isotropic and its elastic constants do not depend on the chemical composition of the layer. The method takes into account the relaxation of internal stresses at the free surface of the layer. Since we assume an ideally periodic LCM along the $x$-axis, the displacement vector $\mathbf{u}$ has only two components $(u_x, u_z)$, where $z$-axis is parallel to the outward surface normal. Then

$$u_j(x,z) = \int_{-\infty}^{\infty} \mathrm{d}x' \int_{-T}^{0} \mathrm{d}z' \delta(x') g_j(x-x', z, z'),\ j = x, z, \qquad (4)$$

where $g_j(x-x', z, z')$ is the elastic Green function defined in Ref. 5, and $T$ is the entire layer thickness. As an example, in Fig. 3 we show the calculated displacements in one lateral period $x \in [-L/2, L/2]$.

Using the displacements and the lateral profile of the scattering density (??), we compute the scattering intensity using kinematical scattering theory,

$$I(\mathbf{q}) = |F(\mathbf{q})|^2,\ F(q_x, q_z) = \int_{-\infty}^{\infty} \mathrm{d}x \int_{-T}^{0} \mathrm{d}z \chi_{\mathbf{h}}(x) \mathrm{e}^{-\mathrm{i}(q_x x + q_z z)} \mathrm{e}^{-\mathrm{i}\mathbf{h}.\mathbf{u}(x,z)}, \qquad (5)$$

where $\mathbf{q} = \mathbf{K}_s - \mathbf{K}_i - \mathbf{h}$ is the reduced scattering vector, $\mathbf{K}_{i,s}$ are the wave vectors of the incident and diffracted beams, respectively, $\mathbf{h}$ is (as before) the diffraction vector, and $F$ is the structure factor of the layer. Since both the displacement field and the scattering amplitude are periodic along the $x$-axis, the structure factor can be expressed as a periodic sequence of narrow $\delta$-like peaks centered on the points of the one-dimensional reciprocal lattice of the LCM:

$$F(q_x, q_z) = \sum_m \delta(q_x - mG) F_m(q_z). \tag{6}$$

The intensity of the satellite $m$ is simply given by $I_m(q_z) = |F_m(q_z)|^2$. Fig. 4 shows the calculated integrated intensities $\Phi_m = \int \mathrm{d}q_z I_m(q_z)$ for several satellites and several composition amplitudes $A$. It follows that the maximum of the envelope curve of the integrated intensities shifts to higher satellites with increasing $A$. This behavior is analogous to the shift of satellite envelope maximum to higher m as described in earlier literature using Bessel functions.[6] This fact allows us to determine the value of $A$ from the measured data.

In Fig. 5, we plot the measured and simulated integrated intensities of the lateral satellites (in (010) plane) for both 402 and 602 reflections. The theoretical data have been normalized to the same height of the maximum of the envelope curve. From this figure it follows that $A = 0.12 \pm 0.01$ in our particular sample.

A direct comparison of measured and simulated reciprocal space maps is complicated by the resolution function of the diffractometer. Since the diffraction geometry is not coplanar, the resolution function has a shape of a stretched inclined parallelogram. This is the reason for the inclination of the lateral satellites measured in plane (010) (see Fig. 2a).

In summary, we have presented a method to evaluate quantitatively the lateral composition modulation in $(\mathrm{InAs})_n/(\mathrm{AlAs})_m$ short-period superlattices. Specific reflections having the largest accessible component of diffraction vector parallel to the sample surface, were chosen in order to obtain a maximum possible signal from the LCM structure. The amplitude of the LCM was obtained, via a strain analysis, from the distribution of x-ray satellite intensities. Further experiments are in progress both to map out the entire satellite distribution and to use grazing incidence diffraction to explore the depth dependence in from the surface.

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## Figure captions

Fig.1 Schematic diagram of the diffraction geometry. The inset shows the reciprocal lattice points we are interested in.

Fig.2 (a) Reciprocal space maps measured about the 402 (left panel) and 602 (right panel) reflections in the reciprocal lattice plane (010). The H and L coordinates are parallel and perpendicular to the sample surface, respectively; (b) The same situation as in (a), but taken in the reciprocal plane (010). "S" indicates where the substrate peak should be. The intensity contours are in logarithmic scale with a step of 0.17. Note that the substrate peaks are not completely visible in the (010) plane, but in the (001) plane, due to the tilt.

Fig.3 Components $u_x$ (left) and $u_z$ (right) of the displacement field calculated for a layer thickness $T = 1000$ Å, modulation period $L = 300$ Å and modulation amplitude $A = 0.2$. The step of the contours is $\Delta u = 0.25$ Å. The plus and minus signs indicate where the strain is positive and negative.

Fig.4 Integrated intensities of the satellites calculated for various amplitudes $A$ about the 402 and 602 reflections.

Fig.5 Comparison of the measured and simulated integrated intensities of the satellites (in (010) plane) about the 402 and 602 reflections.