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AN X-RAY DIFFRACTION STUDY OF DISORDER IN GaAlAs-GaAs SUPERLATTICES

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Abstract

An intentional disorder has been introduced in MBE grown GaAlAs-GaAs superlattices by varying, following a gaussian law, the thicknesses of the GaAs wells. The experimental X-ray diffraction diagrams given by these structures show in the vicinity of non-zero order satellite reflections, unusual effects (extra-peaks) increasing with disorder. A mathematical model based on the kinematical theory was established: it allows the computing of the detailed shape of the diffraction profiles, provided the growth sequence is known.

1 - INTRODUCTION

X-ray diffraction experiments are at the present time in current use to determine the characteristic structural parameters of well-ordered artificial semiconductor based superlattices [1-5]. They can also provide useful information in the case of non regular structures since the diffraction profiles are affected by random fluctuations in composition and in layer thicknesses [6,7].

A series of 6 intentionally disordered GaAlAs-GaAs superlattices was grown by MBE in order to study by photoluminescence the carrier localization and the inhibition of carrier transport along the growth axis as a function of an increasing disorder [8]. Their diffraction diagrams show subsidiary peaks (out of Bragg positions) which cannot be explained by statistical models based on the homogeneity of the disordered structures [9,10]: however as the growth sequence is known the contribution of each layer to the scattered intensity can be taken separately into account, no attempt being made to separate the disorder term and the average structure term in the expression of the scattered amplitude.

2 - EXPERIMENTAL

The samples were grown by MBE on Si doped "laser quality" GaAs wafers following a procedure described elsewhere [11]. Their particular configuration is shown in fig.1: SL1 and SL2 are identical and symmetrical with regard to W0. Six samples were investigated: in the first one (reference sample) SL1 (and SL2) is strictly periodic with expected

Fig. 1: Schematic diagram of the samples structure.
values of 0.3 for the Al content of 30 Å for the thicknesses of the GaAs or GaAlAs sublayers. In the others, the thickness of the GaAlAs barriers is constant whereas those of the GaAs wells vary randomly following a gaussian law with a mean expected value of 30 Å and a standard deviation $S$. $S$ characterises the disorder intentionally introduced and varies from 0 to 11.76 Å. The main observed characteristics of the investigated samples are gathered in table 1.

<table>
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<th>$S$(Å)</th>
<th>$T_e$(Å)</th>
<th>$W_e$(Å)</th>
<th>C(Å)</th>
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<th>$x$</th>
<th>$n_B$</th>
<th>$\bar{n}_w$</th>
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<td>12.08</td>
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Table 1: $S$, standard deviation of the well thicknesses. $T_e$, total thickness of the epitaxy. $W_e$, enlarged well thickness. C, mean value of the superperiod. $\bar{x}$, mean Al-content in the epitaxy. $x$, Al-content in the barriers. $n_B$, number of molecular planes in the barriers. $\bar{n}_w$, average number of molecular planes in the wells.

A cross sectionnal dark field TEM image (fig. 2) of the most disordered sample illustrates one of the growth sequences.

Figure 3a shows that non-zero order satellite peaks which reveal the SL modulation, are affected by disorder whereas the mean 001 peaks remain unchanged (fig. 4). These satellites are not much broadened but they split into smaller peaks and as disorder increases so does the angular range covered by each group of peaks around the satellite positions of the non-disordered SL. It is however possible to define, in each satellite group, a mean peak position at the center of gravity of the group. Thus the $\pm 1$ mean satellite peak positions and the mean 001 SL peak were used in the usual manner to determine the SL period C, and the mean Al-content value $\bar{x}$ in each sample.

**Fig. 2:** (002) dark field TEM image of sample $S = 11.76$ Å.

**Fig. 3:** X-ray diffraction diagrams close to the 002 GaAs substrate reflection a) observed b) calculated. Only the first order satellite peaks are shown because they are intense and always visible even when disorder is high.
Fig. 4: Typical DDX profiles close to the 004 GaAs substrate reflection showing the similarity of the zero order satellite peaks of samples S = 0 and S = 11.76 Å.

Fig. 5: Model for the calculation of 001 scattered intensity.

Fig. 6: Magnified diffraction profiles corresponding to the -1 order satellite of the highest disordered sample (S = 11.76 Å).

3 - THEORY

The theoretical profiles were calculated considering that the layer thicknesses are proportional to the opening times of the ovens and that the steps at the interfaces are only one molecular plane high [12, 13]. Figure 5 shows the model for the scattered intensity calculations for this type of structures. The expression for the scattered amplitude at angle θ was directly derived from the basic kinematical expression:

$$F(θ) = \sum_{j=1}^{M} f_j \exp(ikz_j)$$

where $k = 4\pi \sin θ/λ$, $M$ is the number of molecular planes in the structure, $f_j$ is the complex scattering factor of the $J$-th molecular layer and $z_j$ its z-coordinate.

In the model of figure 5 only one step of one monolayer is drawn at each interface since the real steps positions do not matter when one views the reciprocal space along the 001 direction. Only the proportion $p_j$ of each material at each interface molecular plane is important. A full mathematical development of expression (1) is to be published [14].

The $x$ value in GaAlAs layers was taken to be equal to $x_{obs} (1 + n_W/n_B)$ where $n_W$ and $n_B$ are the mean numbers of molecular planes in the wells and in the barriers respectively, calculated assuming their ratio is as intended. The results are shown in fig. 3b facing the observed diagrams.

4 - DISCUSSION

As long as the disorder is low ($S < 1$ Å) the experimental diagrams and the calculated ones display a decrease of the maximum intensity of the satellite peaks and also an increase of their width at half maximum. Above $S = 1.25$ Å satellite peaks become sharper and a fine structure begins to appear on each side of their base. The corresponding calculated diagrams all show a splitting of the $±1$ order satellite peaks, together with an increasing difference of intensity of the two components of the main peak. This non-equilibrium is reflected in the observed diagrams and explains for instance why the observed $-1$ order peak is narrower for sample $S = 1.25$ Å than for sample $S = 0$. For higher values of $S (≥ 3.14$ Å) extra peaks become visible outside the Bragg positions practically without interruption in the investigated angular range in agreement with the theoretical expectations. Inhomogeneities such as in-plane gradients of period and Al content were not taken into account in the calculations. In spite of this, there is a good agreement between observed and calculated patterns. This is particularly obvious for sample $S = 11.76$ Å which has the highest well thickness standard deviation (fig. 6). But, although the disturbance due to disorder in the observed diagrams is less striking for values of $S < 3.14$ Å,
it can still be detected (with the help of theoretical diagrams) even in the least disordered samples. This means that the residual disorder inherent in the MBE technique is less than 0.57 Å in standard deviation for the reference sample.

5 - CONCLUSION
This study of a series of intentionally disordered samples has enabled us to show experimentally the effect of disorder on the diffraction patterns. A theoretical model which takes into account every layer of the stacking was worked out and calculations based on this model led to an excellent agreement between observed and calculated diagrams. When disorder is low the experimental diagrams are weakly disturbed and an analytical averaging expression only depending on the mean structure and the standard deviation of the varying parameter ought to be satisfactory. On the contrary in the case of very disordered samples, the basic scattering expression (1) has to be used, at least when the number of deposited layers is low, as in this study. As a matter of fact, we verified that when this number increases, keeping the standard deviation constant, the complex satellite peak structures smooth out to broadened peaks.

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