HIGH RESOLUTION X-RAY DIFFRACTION AND PHOTOLUMINESCENCE CORRELATION AS AN ACCURATE AND NONDESTRUCTIVE EVALUATION TECHNIQUE FOR PHEMT STRUCTURES

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ABSTRACT
Nondestructive and accurate evaluation of epitaxial layers is of critical importance to the semiconductor industry. High Resolution X-ray diffraction (HRXRD) is an ideal method for evaluating quantum wells and heterostructures. However, HRXRD assessment of thin epilayers (~100Å) requires signal integration times of several hours. On the other hand, room temperature photoluminescence (RTPL), which is also a noninvasive technique, provides a quick and qualitative evaluation scheme and is particularly well suited for thin epilayer heterostructures. We have combined these two techniques and developed a precise, accurate and rapid scheme for evaluation of AlGaAs/InGaAs/AlGaAs pseudomorphic high electron mobility transistor (pHEMT) structures.

INTRODUCTION
Exact determination of epitaxial layer thickness and composition is of vital importance to semiconductor device manufacturing. Since pHEMTs are the dominant power transistors at microwave and millimeter wave frequencies and since their device performance is critically influenced by thickness and composition variation in the channel layer, these parameters must be controlled and monitored to a high degree of precision prior to any wafer processing. Therefore, a sensitive wafer characterization technique is highly desirable for complete wafer evaluation. In addition to accuracy, the characterization method must be noninvasive and fast.

HRXRD is a powerful tool used in evaluation of epitaxially grown wafers, which, due to its sensitivity to both composition and thickness, has previously been exploited to assess pHEMT structures 1-3. When HRXRD is combined with a dynamical diffraction model, it leads to a highly accurate quantitative diffraction profile simulation technique, which can provide accurate quantitative information about the epitaxial layers. However, HRXRD on thin layers is time consuming and not readily compatible with the fast turn around required in an epitaxy growth environment. We have extended HRXRD by combining it with RTPL to characterize pHEMT wafers rapidly.

Photoluminescence can in principle be used for the determination of thickness and composition of thin quantum wells such as the InGaAs channel of a pHEMT structure by relating the energy position of various emission lines to the epitaxial parameters. Relating these energy levels to
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actual epilayer thickness and In mole fraction from first principles is quite challenging. In the absence of such a formulation, we have correlated the HRXRD data with RTPL subband energy levels, and the result is a scheme that evaluates pHEMT structures quantitatively with the accuracy of HRXRD, but in less than ten minutes. Such a scheme has been employed successfully for:

1. screening of incoming wafers prior to processing
2. optimizing the growth process by fast turn around determination of thickness and In mole fraction on calibration runs.

EXPERIMENTAL
For these experiments, two sets of pHEMT samples were grown in two different MBE systems with In\textsubscript{1-x}Ga\textsubscript{x}As channel layer thicknesses from 100-150 Å and In mole fractions x\textsubscript{i} from 12-25%. The first set of samples were grown in a Riber 32 solid source MBE system. Arsenic was evaporated as As\textsubscript{4} from a valved source. The GaAs growth rate was 0.5 µm/hr as verified by depth measurements above an AlAs etch-stop layer in N-GaAs calibration runs. Substrate temperature was measured by optical pyrometry with emissivity calibrated against the melting point of aluminum. AlGaAs compositions were measured in dedicated calibration runs by both RTPL and HRXRD. The second set of samples was grown in a Riber 49 production MBE system with similar, but not identical pHEMT structures. The pHEMT structures were standard double pulse doped pHEMTs with AlGaAs barriers and an InGaAs channel and a thick n\textsuperscript{+} GaAs cap layer.

The rocking curve profiles were obtained using a Philips MRD-4 system. The incident x-ray beam was produced at 35 mA and 45 kV settings (1.6 kW) of the generator and passed through a four-crystal Bartel monochromator in symmetric Ge (220) mode to collimate the beam, filter out various Cu emission lines, and produce the CuK\textalpha\textsubscript{1} line. Since the InGaAs layer is pseudomorphic and the lattice constant varies perpendicular to the surface direction only, we have used (0 0 4) diffraction with an Ω–2θ scan. In this mode of operation, we obtain a very high signal intensity of 8 x 10\textsuperscript{6} cps. Since the InGaAs layer is thin, the diffraction signal intensity from it is very weak, thus requiring high incident beam intensities to obtain good signal to noise ratios. Additionally, we have used a long count time of 30 seconds per step, in order to improve the signal to noise ratio further and exactly identify the Pendellosung oscillations. The resulting profiles exhibit various diffraction features far more clearly than previously published data\textsuperscript{1-3}.

The RTPL is performed on a J-Y U1000 1-meter double monochromator. The samples are excited using an Ar\textsuperscript{+} laser, and the emission is passed through the spectrometer and detected by a cooled Ge detector using phase sensitive detection. The spectra are corrected for system response and then analytically fitted to an equation\textsuperscript{7} containing E\textsubscript{1}, E\textsubscript{2}, the electron energy levels in the InGaAs channel quantum well, E\textsubscript{F}, the conduction band Fermi level, and amplitudes of emissions along with E\textsubscript{fh}, the hole Fermi level, as parameters.
RESULTS AND DISCUSSIONS

Figure 1 shows a typical HRXRD of a pHEMT structure along with a simulation for it. There are four main features in the scanned profiles; the substrate signal, which is narrow and has the highest intensity and appears at 33.08 degrees; the InGaAs layer signal, to the far left of the substrate peak, which is very broad and has low intensity; the peak labeled A, which is to the immediate left of the substrate peak, is due to the combined influence of the InGaAs channel, the AlGaAs Schottky layer, and the GaAs cap layer thickness; and the high frequency, low intensity Pendellosung oscillations. The frequency of these oscillations are inversely proportional to the total layer thickness of the layers from GaAs cap layer down to the InGaAs channel layer. The scan profiles were interpreted using a simulation software program based on the dynamical model developed by Fewster and Curlings, which is based on Takagi-Taupin equations.

Using this model, we note that the signal from InGaAs channel layer is weak and broad, since this layer is thin, of the order of 150 Å. However, a small change in its layer thickness substantially alters the scan profile everywhere except in the vicinity of the GaAs substrate peak. As the thickness of the InGaAs layer is increased, the broad InGaAs peak becomes narrower and its intensity increases. Also, peak A is altered as it moves to lower angles and away from the substrate peak, which is due to the increase of the superposition of scattered waves from the InGaAs layer and the layers above it. As the In mole fraction in the InGaAs layer is increased, the broad peak moves farther to the left i.e. to lower Ω values. The InGaAs channel layer
parameters influence the diffraction profile more significantly than any other layer, since InGaAs has the largest lattice constant difference from GaAs. It is this InGaAs peak that must be matched by simulation very closely to produce accurate results. The AlGaAs Schottky layer thickness alters the high frequency oscillations and moves peak A, and the Al mole fraction also induces changes in the scan profile. The GaAs cap layer thickness variation has the same effect as the Schottky layer variation. Small variation in the parameters of layers under the channel produce no significant effect on the scan profile.

Thus, the simulation proceeded by first matching the GaAs substrate peak intensity and position, followed by adjustments to the InGaAs layer, In mole fraction and thickness, to obtain the best fit, and then the Schottky layer thickness and the GaAs cap layer thickness variation to optimize the fit. In some scans, it was necessary to alter parameters of the buffer superlattice to obtain an acceptable fit. Using this scheme, the InGaAs channel layers thickness and ternary mole fractions were determined to ± 3Å and ± 0.2%. Variations larger than these values produced simulations that were visually judged to be substantially different than the actual scans.

Two additional notes need to be made here. First, the simulation program does not take into account the diffuse background scatter, which appears on both sides of the main substrate peak. This signal is due to imperfection in the substrate and can be measured on a bare substrate and subtracted out from the scan profile, and the resulting profile is then comparable to simulated profiles. However, since it is not critical to our work, this is not considered here. Secondly, the agreement between the simulation and the scanned profile is based on a visual, subjective judgment and not on a numerical fitting routine, such as a chi-square minimization program. Thus as stated above, a clear, noise free diffraction profile is needed to produce visually accurate results.

A typical RTPL spectrum along with the calculated fit is shown in Figure 2. It is noted that the spectrum is broad with several features that are not very well defined or readily quantifiable as compared to low temperature PL spectra. However, a line shape fitting routine has been developed, which can identify the subband energy positions $E_l$.

Figure 2. RTPL spectrum of a pHEMT structure (solid line) and line shape fit (dashed line).
and $E_2$ as well as Fermi energy position $E_F$ in the conduction band from such spectra. The details of this procedure are published separately\textsuperscript{7-8}.

Briefly, the $E_1$ and $E_2$ obtained from RTPL can be used to calculate the effective InGaAs channel band gap $E_g$, using an adjustable parameter which weighs the influence of the energy separation ($E_2-E_1$). $E_g$ is then plotted vs. In mole fraction as obtained from HRXRD and this parameter is adjusted to obtain the best linear fit. This plot is shown in figure 3.

Similarly, the InGaAs channel layer thickness as obtained from HRXRD is plotted vs. $\beta(E_1-E_2)^{\gamma}$ with $\beta$ and $\gamma$ as adjustable constants. The result is two algebraic relationships between actual layer parameters and readily obtainable RTPL fitting routine data. Figure 4 presents this plot for two sets of samples. It is clear that RTPL results are closely related to the actual material parameters. However, this relationship is not unique and is dependent on the layer structure details.

The errors in this evaluation consist of errors in HRXRD simulation as described earlier and the errors in $E_1$ and $E_2$ determination by RTPL. The RTPL errors are $\Delta E_1=\pm1$ meV and $\Delta E_2=\pm2$ meV, which when related to material parameters through the above procedure
produce Δ [In]=±0.0015 and Δt=±1.3Å depending on the thickness of the channel. Since these two sources of error are independent of one another, the overall errors are calculated to be Δ [In]=±0.0025 and Δt=±3.4.5Å.

The HRXRD and RTPL correlation technique can then deduce pHEMT channel parameters, exploiting the high precision of the x-ray diffraction and the relative ease and speed of RTPL technique. In our present set up this process takes less than ten minutes, and with additional improvements in the data acquisition scheme it is expected that this time will be reduced to 1-2 minutes.

**SUMMARY**

We have extended the x-ray diffraction technique for pHEMT layer evaluation by combining RTPL and HRXRD, and have developed a scheme that can characterize such structures to a very high degree of accuracy within a few minutes. We have correlated the RTPL data to HRXRD results of pHEMT structures, and subsequently have used RTPL routinely to quickly and precisely evaluate pHEMT channel parameters. The upper limits for the In mole fraction and channel thickness precision are 0.25% and 3-4.5Å respectively.

**REFERENCES**