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# Determination of indium and nitrogen content in four-component epitaxial layers of $In_xGa_{1-x}As_{1-y}N_y$ deposited on GaAs substrate

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The paper presents a new method of determination of the percentage content of indium ($x$) and nitrogen ($y$) in four-component epitaxial layers of $In_xGa_{1-x}As_{1-y}N_y$, based on a distance between a layer and a substrate reflection for rocking curves obtained from high resolution X-ray diffraction. In the method, a symmetrical (004) and at least two asymmetrical (e.g., (224) and (115)) reflections are taken into consideration. For the investigated ranges of the values of the $x$, $y$ parameters of the four components, we have described the dependences of distances between reflections $\Delta\omega_{(004)} = f_1(x,y)$, $\Delta\omega_{(224)} = f_2(x,y)$, $\Delta\omega_{(115)} = f_3(x,y)$ based on the rocking curve simulation software HRS (High Resolution Simulation – Philips). Based on the result, we present a procedure which allows us to characterize parameters of the epitaxial layers. The properties of the proposed procedure have been verified on experimental examples.

Key words: *X-ray; epitaxial layer; InGaAsN*

## 1. Introduction

One of the commonly applied methods of structural characterization of epitaxial layers is rocking curve simulation based on numerical solution of Takagi-Taupin's equations [1–3]. Rocking curves simulation software, e.g. HRS (High Resolution Simulation, Philips) [4, 5] allows one to determine precisely composition of multilayers what is very useful in characterization of various types of three-component layers. The distance between the reflection of the layer and reflection of the substrate characterizes the content of individual components of the layer. Unfortunately, application of this method to four-component layers like $In_xGa_{1-x}As_{1-y}N_y$ is limited. The limitation is connected with independent influence of the individual contents of components of the layer on the reflection location with reference to the substrate layer.

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Therefore, determination of the contents of elements in four-component layers is possible only in combination with other methods such as, e.g., photoreflectance [6]. This results from the fact that the same distances between reflection from the layer and reflection from the substrate for different contents of In and N may be obtained (Fig. 1). Thus, an additional method is needed that would allow us to determine the content of one of the components of the layer.

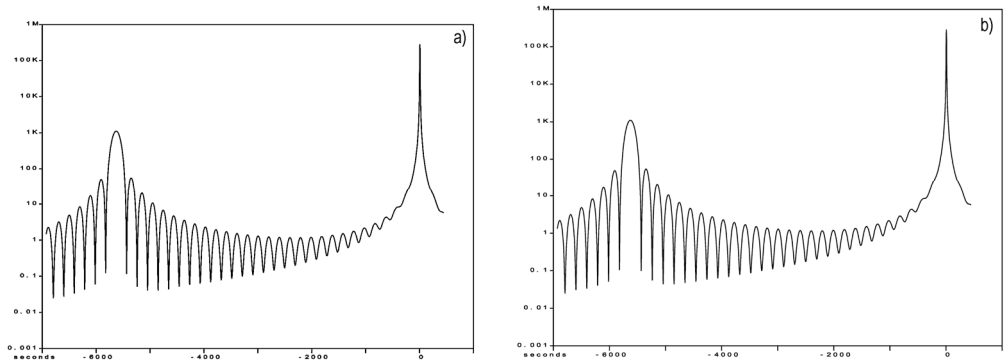


Fig. 1. Rocking curves (004) for $In_xGa_{1-x}As_{1-y}N_y/GaAs$ layer: a) $x = 27.5\%$, $y = 2\%$, b) $x = 22.5\%$, $y = 0.75$

In the paper, we describe a new method for determination of the contents of individual components of the layer based on XRD measurements and rocking curves simulation software.

## 2. Determination of indium and nitrogen contents in four-component epitaxial layers

The first step of the method is to determine (using simulation software) the matrix of distances between layer and substrate reflections for the assumed range of contents of In and N in the investigated layer. Such simulation has been carried out for a few reflections, e.g. (004), (224), (115). As a result, the matrix with distances between reflections $\Delta\omega$ can be obtained (Fig. 2).

| N | In | | |
|---|---|---|---|
| | 10% | … | 35 % |
| 0.5% | … | … | … |
| … | … | $\Delta\omega$ | … |
| 2.5% | … | … | … |

Fig. 2. Matrix of distances between peaks and the contents of In and N in the layers

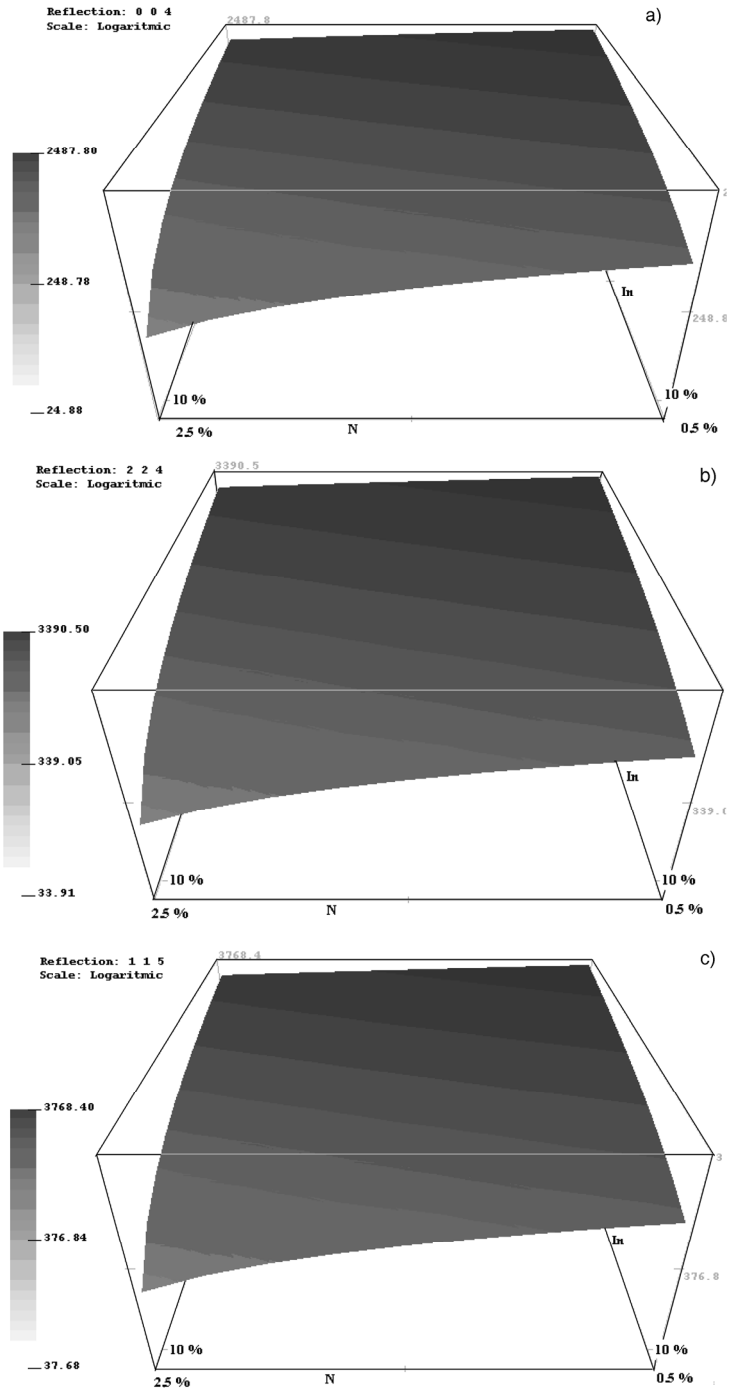


Fig. 3. Three-dimensional presentation of the relationship between In and N contents of a layer and distances between reflections: a) $\Delta\omega_{(004)} = f_1(x, y)$, b) $\Delta\omega_{(224)} = f_2(x, y)$, c) $\Delta\omega_{(115)} = f_3(x, y)$ for InGaAsN layers

The matrix is three-dimensional, where $X$ and $Y$ axes are the In and N contents in the layer for a given reflection, and Z axis is the distance between reflections of the simulated curve (Fig. 3). It is possible to describe each individual reflection by analytical equations (based on the matrix) determining three-dimensional spaces. Such spaces for each InGaAsN layer are well described by the formula

$$Z = AX^2 + BX + CY + D$$

For all considered spaces, the equations are as follows:

$$\Delta\omega_{(004)} = -2.666X^2 + 8.318X - 27.79Y + 0.03652 \quad (1)$$

$$\Delta\omega_{(224)} = -3.94\ X^2 + 11.46X - 37.82Y + 0.0449 \quad (2)$$

$$\Delta\omega_{(115)} = -4.532\ X^2 + 12.80X - 42.01Y + 0.04856 \quad (3)$$

The derived functions are shown in the form of three-dimensional charts in Fig. 3. In the next step, a system of equations for two reflections has been solved. Instead of $Z$, we have taken a real value of the distance between reflections from the rocking curve of InGaAsN layer. If the solution of such an equation equation exists, the values of $X$ and $Y$ will be directly obtained, being the searched values of In and N contents in the layer. Unfortunately, for the considered InGaAsN layers, an unequivocal solution of such a system of equations does not exist. Thus, for the matrices $\Delta\omega_{(hkl)} = f_1(x,y)$, an algorithm determining the value of $\Delta\omega$ and related contents of In and N has been designed. The algorithm is based on a comparison of the points of the matrix with distances between reflections taken from the measurement. Because the matrix contains discrete values of $\Delta\omega$, the value that is provided to the algorithm must be specified in the range of $\Delta\omega \pm \delta\omega$, where $\delta\omega$ is given as ± 0.5% of $\Delta\omega$.

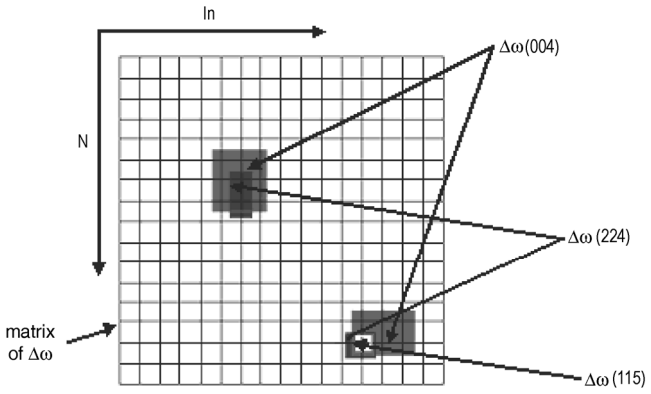


Fig. 4. General idea of the process of finding a solution

For a single reflection, a few In and N contents may be comparable with measured $\Delta\omega$. Therefore, the algorithm operates on a number of reflections, decreasing the prob-

ability of occurrence of the same value of $\Delta\omega$ for different pairs of In and N (Fig. 4). Common values obtained for three reflections were assumed as a solution.

## 3. Conclusions

The distances between reflections from a layer and a substrate have been calculated in four-component $In_xGa_{1-x}As_{1-y}N_y$ epitaxial layers. A new algorithm was designed allowing determination In and N content in InGaAsN layers. The algorithm is versatile for all four-component layers, if only the Takagi–Taupin equations are applicable. As an example, calculations have been performed for a layer containing 35% of In and and 2.5% of N. The distances between reflections (Fig. 5) have been obtained as follows: $\Delta\omega_{(004)}$ = 6904 arcsec, $\Delta\omega_{(224)}$ = 9432 arcsec, $\Delta\omega_{(115)}$ = 10498 arcsec.

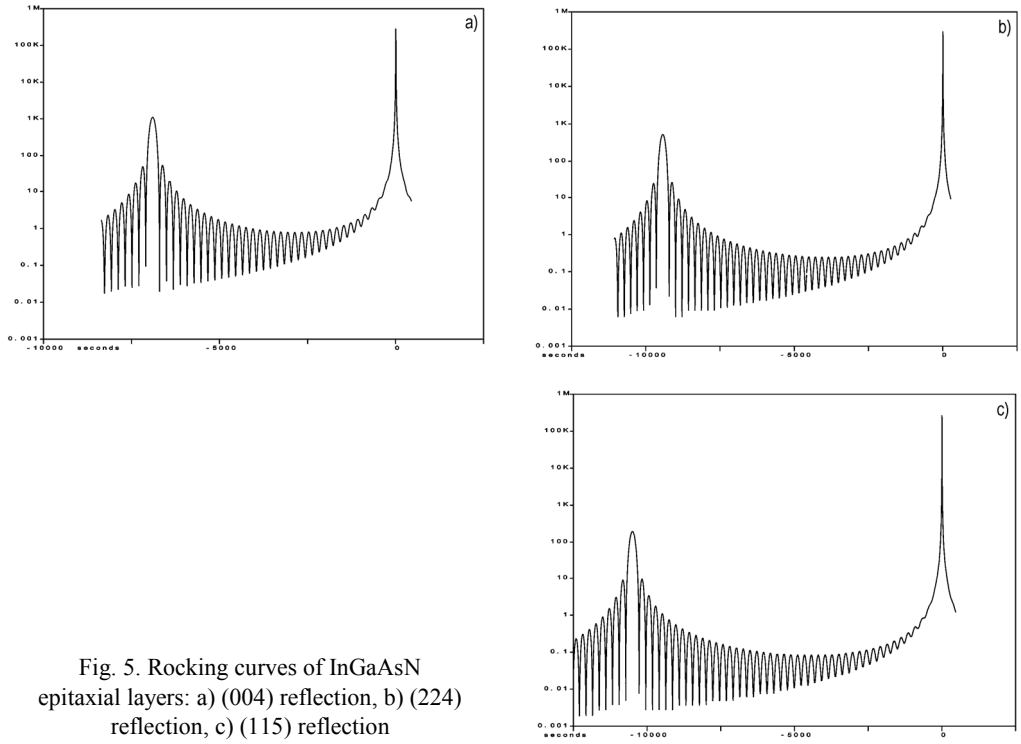


Fig. 5. Rocking curves of InGaAsN epitaxial layers: a) (004) reflection, b) (224) reflection, c) (115) reflection

Based on the applied algorithm, the following contents of In and N have been found:

reflection (004): In = 35% , N = 2.5% and In = 27.5% , N = 0.75%,

reflection (224): In = 35% , N = 2.5% and In = 27.5% , N = 0.75%,

reflection (115): In = 35% , N = 2.5%.

The correct values have been obtained for all three reflections. Moreover, the structure with a distance between reflections in the range of ±0.5% of $\Delta\omega$ was found.

This result confirms that upon increasing the number of reflections, the probability of choosing an incorrect pair of solutions decreases.

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