Preproduction prediction of the optical normalized reflectance transient of MOVPE-grown AlGaAs films using transfer matrix method

Jianwei Zhang [a,b], Yongqiang Ning [a,*]

[a] State Key Laboratory of Luminescence and Application, Changchun Institute of Optics, Fine Mechanics and Physics, Chinese Academy of Sciences, 3888 Southeast Lake Road, Changchun 130033, China
[b] Graduate University of the Chinese Academy of Sciences, Beijing 100049, China

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ABSTRACT

This paper reported on the prediction and analysis of the optical normalized reflectance (NR) transient of AlGaAs multi layers and Distributed Bragg Reflector (DBR) using transfer matrix method (TMM). The simulation result correlated well with the measured NR transient of grown samples. Deviations of $Al_xGa_{1-x}As$ composition between the expected and real grown sample were predicted successfully. Smaller optical oscillation amplitude in the first DBR layer was predicted and could be used as an indication of Al composition. Special characteristics of NR transient within the first three pairs of DBR were also clarified using the calculated transmissivity changing with the growth thickness. TMM simulation of NR transient was thus shown to be a convenient and reliable pre-production technique, also not restricted to the AlGaAs material.

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1. Introduction

With the development of metal organic vapor phase epitaxy (MOVPE), many complex multilayer devices such as VCSELs had been grown successfully [1,2]. Non-destructive in situ monitoring of normalized reflectance [3] and reflectance anisotropy spectroscopy (RAS) [4] was incorporated into the MOVPE to improve the growth technique. Many such reports appeared recently aiming at the in situ monitoring of growth rate, temperature and composition of epitaxial layer based on the reflection spectroscopy [5–8]. Parameters of grown layers gained from the NR transient were even as accurate as ex situ measurements such as SEM and TEM [9]. Thus it would be reliable if used as the pre-production technique for evaluating the information of growing layer. However, such applications had not been reported before. To apply the NR transient as the pre-production technique, simulation of the time resolved NR data of expected structure was needed to be carried out first before the costly fabrication process.

In this work, the numerical calculation of the NR transient of multilayer structures was carried out based on the transfer matrix method (TMM). Comparison between the simulated and monitored reflectance data proved that it was efficient in assessing the growth equality and calibrating the parameters during the growth process.

The physical origin of some special peculiarities in the NR transient of DBR was also clarified.

2. Modeling and experimental

2.1. Modeling

Detailed description about TMM had been presented in Refs. [10,11]. The main principle of TMM was shown below.

As shown in Fig. 1, parameters n and d were the real part of the refractive index and thickness of each layer, and the subscript character indicated different layers. Signals of a, b, c, d... indicated the interfaces between these layers. Normal incidence of linearly polarized plane electromagnetic wave on the structure was assumed.

When the electromagnetic wave transmitted through the structure consisting of m layers, then the following transfer matrix could be obtained:

$$\begin{bmatrix} B \\ C \end{bmatrix} = \prod_{i=1}^{m} \begin{bmatrix} \cos\delta_i & i\sin\delta_i/n_i \\ in_i\delta_i & \cos\delta_i \end{bmatrix} \cdot \begin{bmatrix} 1 \\ n_{sub} \end{bmatrix} \qquad (1)$$

Refractive index and phase change of the ith layer were expressed by n_i and δ_i. We defined $Y = C/B$ from Eq. (1). Reflectance R and transmissivity T were then calculated:

$$R = \left(\frac{n_0 - Y}{n_0 + Y} \right) \cdot \left(\frac{n_0 - Y}{n_0 + Y} \right)^* \qquad (2)$$
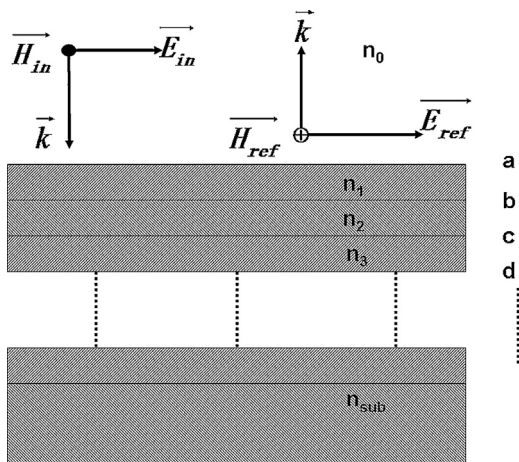
Fig. 1. Normal incidence of plane electromagnetic wave on a multilayer structure consisting of layers on an infinite thick substrate.

$$T = \frac{4 - n_0 n_{sub}}{(n_0 B + C) - (n_0 B + C)^*} \qquad (3)$$

To carry out the TMM simulation of the growth process, each layer was divided into many homogeneous sub-layers, then the reflectance of grown structure after increasing by a sub-layer could represent the reflectance at corresponding growth time in the time resolved NR data. The thickness and refractive index of these layers were utilized in the simulation. Also the transmissivity of grown layers at different growth time could be obtained following this method. And it could be used for explaining the oscillation characteristics of NR transient.

2.2. Experimental

Epilayers were grown on undoped (0 0 1) GaAs substrate in a 3×2 planetary MOVPE reactor. The source materials included trimethylgallium (TMGa), trimethylaluminium (TMAl), and arsine (AsH$_3$). A pressure of 100 mbar and a growth temperature of 970 K were used to realize mirror-like surface quality. In situ measurements were performed with LayTec EpiRAS 200 spectrometer mounted above the viewport of reactor. To reduce the sensitivity of NR to the surface roughness, the monitoring photon energy $E < 3$ eV for the optical measurement was chosen.

Two samples were grown, with their SEM images shown in Fig. 2. The expected grown layers of sample 1 were GaAs buffer, Al$_{0.25}$Ga$_{0.75}$As, GaAs, Al$_{0.4}$Ga$_{0.6}$As, GaAs in turn. Sample 2 was the Distributed Bragg Reflector (DBR) mirrors, consisting of 23 pairs of Al$_{0.12}$Ga$_{0.88}$As/Al$_{0.9}$Ga$_{0.1}$As layers. The designed central wavelength of DBR structure was 980 nm.

The normalized reflectance is the reflectance of grown layers divided by the reflectance of a reference sample. The reflectance of GaAs substrate R_{GaAs} was measured prior to each growth process and used thereafter as reference R_{ref}, then the NR can be defined as:

$$NR = \frac{R}{R_{ref}} = \frac{R}{R_{GaAs}} \qquad (8)$$

3. Results and discussion

3.1. Simulated and monitored NR transient of sample 1 at the monitoring photon energy of 2.3 eV (539.1 nm)

In Fig. 3, the simulated and measured NR transients were shown with the refractive index profile shown to identify each layer.
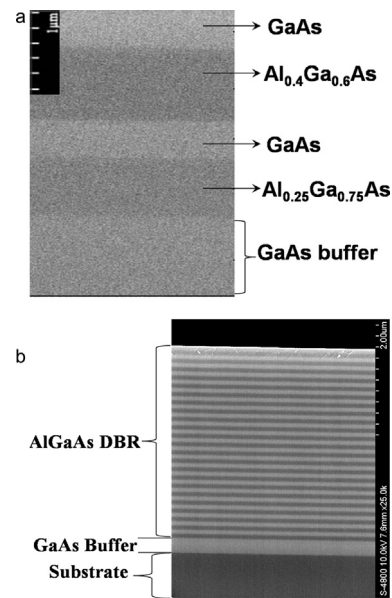

Fig. 2. SEM images of grown samples: (a) sample 1 and (b) sample 2.

FP oscillations of NR transient were observed due to the optical interference. The amplitude of FP oscillation was damped for each layer due to the optical absorption. The converged value of this FP oscillation was determined only by the optical constants (refractive index n and extinction coefficient k) and could be used for distinguishing the Al composition of each layer [12].

The relationship between the compositions and converged values of simulated NR were gained, as shown in Fig. 4. Also the compositions and converged values of real grown layers were shown. The composition of real grown sample was calibrated by XRD. The Al compositions for each layer were 0, 0.255, 0, 0.352, 0, while the expected one were 0, 0.25, 0, 0.4, 0. We could see from Fig. 4 that the simulated result was accurate in predicting the composition deviation. Thus it would be useful in predicting the compositions of grown layers during the growth process. In fact, the growth parameters such as the source flow etc. could be changed in real time when the average value of NR was found to be deviant during the above process.
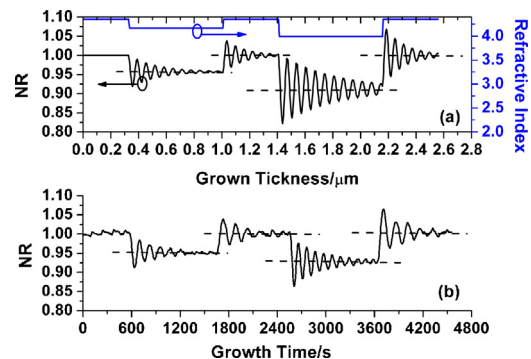

Fig. 3. (a) Simulated NR transient of sample 1, with the refractive index shown to identify different layers, corresponding layers was GaAs/Al$_{0.25}$Ga$_{0.75}$As/GaAs/Al$_{0.4}$Ga$_{0.6}$As/GaAs and (b) monitored NR transient during the growth process of sample 1.