Modeling of Optical Constants of III-V Semiconductors

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Abstract - Accurate *in situ* measurement of temperature and composition is of great importance to the development of real-time controllers for MBE growth of III-V compound semiconductors. Spectroscopic Ellipsometry (SE) has proved to be an accurate, non-invasive tool to determine these variables through the experimental measurement of Optical Constants (OC) that are sensitive to temperature and composition changes of the sample.
A general procedure to model OC databases as a function of frequency, temperature, and composition was developed. Furthermore, a simple algorithm can invert the model to estimate temperature and composition of a sample from measured OCs. The method was applied to model OC databases of AlGaAs and near-lattice-matched InAlAs and InGaAs that were collected at ASU in the past. Experimental results show that the method achieves the level of accuracy required for temperature and composition control during MBE growth.

1. The OC model.

The optical properties were fit using an 8th order transfer function (TF) model with temperature (T) and composition (X) dependent coefficients. The model can be expressed as:

$$\hat{\varepsilon}(s,T,X;\theta)=\frac{b_8 s^8+\cdots+b_1 s+b_0}{a_8 s^8+\cdots+a_1 s+1}=\frac{B(\theta)}{A(\theta)}$$

where, $s=j\hbar\omega$ (j=√-1, $\hbar\omega$=Energy in eV). The coefficients $a_1\cdots a_8$, $b_0\cdots b_8$, are real valued polynomials of the form $\theta_1+\theta_2 T+\theta_3 T^2+\theta_4 X+\theta_5 X^2$. For better numerical properties, Legendre polynomials are used instead of powers of T and X.

The coefficients θ are adjusted to minimize the mean square error between the model $\hat{\varepsilon}$ and the experimental values ε, i.e., $e=\varepsilon-\hat{\varepsilon}=\varepsilon-\frac{B}{A}$.

While A and B in the above expression are linear in θ, the error function e is not. To avoid the numerical problems associated with nonlinear parameter fitting, we use the linear equation error $e'=\varepsilon A(\theta)-B(\theta)$. This can be solved by conventional linear least squares, but represents a weighted version of the original error e. To minimize the original error (i.e., to undo the weighting effect) the following linear recursive algorithm initialized with $A_0=1$:

- at step k (k=1,2,...) find θ to minimize $e'_k=\varepsilon\frac{A_k(\theta)}{A_{k-1}}-\frac{B_k(\theta)}{A_{k-1}}$ by linear least squares, so that the polynomials A_k, B_k are determined.

This algorithm shows in practice fast convergence to a near optimal solution, which is then refined by Levenberg-Marquard (nonlinear optimization) algorithm.

2. T and X Determination.

The temperature and composition of a sample can be estimated from measured OC's. Unknown temperature and composition (T_x, X_x) are estimated by Least Square (LS) regression:

$$(\hat{T}_x,\hat{X}_x)=\arg\left(\min_{T,X}\sum_i\left|\varepsilon(s_i,T_x,X_x)-\hat{\varepsilon}(s_i,T,X;\theta_*)\right|^2\right)$$

3. Results and Conclusions.

The complex index of refraction of $Al_xGa_{x-1}As$ at 600°C was modeled for X between 0-1, and energy of 1.3-4.5 eV, with a resulting RMS modeling error of 0.52%. The model was used to predict X on the same database used in the fitting, resulting in RMS error of 0.0025 Al. The results for $In_xGa_{x-1}As$ and $In_xAl_{x-1}As$ complex dielectric constant are presented in the following tables. The model was obtained for T in the range of 425-550°C, and X between 0.49-0.54 In.

MODELING	InGaAs	InAlAs
RMS error	0.32%	0.34%
Max. error	2.0%	1.5%

T and X Prediction	InGaAs		InAlAs	
	T(C)	X(%)	T(C)	X(%)
RMS error	1.7	0.58	1.4	0.14
Max. error	4.7	1.5	3.2	0.42

Recent testing of the model with experimental data obtained from other runs showed that these errors roughly duplicate. This is still a satisfactory level of accuracy.

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