

Design of Thin Film Stacks for Non-Destructive Electro-Optical Characterizations by Spectroscopic Ellipsometry

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Spectroscopic ellipsometry (SE) is a general and non-destructive tool to characterize the optical properties of thin films. However, most commercial SE do not provide an additional signal amplifier, making it very challenging to investigate minor but crucial changes in thin-film layers such as those induced by the electro-optical effect (EO). Therefore, in this work, we develop a transfer matrix method (TMM) to design the transparent electrode in terms of material choice and thickness to achieve an EO measurement by SE with high resolution of index change (δn). Based on our models, a δn resolution of $5e-5$ for the EO-effect in BaTiO₃ grown on Si(001) using molecular-beam-epitaxy has been successfully demonstrated.

Introduction

Nowadays, advance thin film technology drives a wide spectrum of electro-optical (EO) device applications such as optical modulator, display and thin film transistor...etc [1-2]. However, EO characterizations for thin films remains challenging due to tiny volume of thin film material and its minor index change (δn) after applying bias (typically from $e-3$ to $e-5$). Therefore, several EO characterization techniques were relying on the lock-in amplifier to obtain detectable signals [3-4]. Even though spectroscopic ellipsometry (SE) is a general tool to study the optical properties of thin films, most commercial SE don't provide an additional signal amplifier, making it very difficult to investigate EO in thin films.

In this work, despite the lack of lock-in amplifier for commercial SE, we can achieve an EO characterization with δn resolution of $5e-5$ by designing top transparent electrode and optimization of measurement condition for BaTiO₃ (BTO) grown on Si(001) using molecular-beam-epitaxy.

Top Electrode Design & AOI Optimization For EO Measurement

$$\frac{r_{TM}}{r_{TE}} = \tan(\Psi)e^{i\Delta} \quad (1)$$

SE spectrum $\tan(\Psi)$ and $\cos(\Delta)$ in the formula (1) describe the reflection coefficient ratios of layer stacks for TM (r_{TM}) and TE (r_{TE}) polarizations. With known angle of incidence (AOI) for measurement, thickness as well as refractive indices of each layer in the stack, the spectrum can be computed based on transfer matrix method (TMM). In order to obtain the optimal EO measurement for 100nm BTO on 10nm SrTiO₃ (STO) on Si, we are going to use TMM to optimize spectrum response with respect to BTO index difference (δn_{BTO}) by investigating transparent electrode in terms of material choice, thickness and AOI, respectively. The optimization process and calculation are based on the assumption that only BTO index change will be induced by external electric field.

Figure 1 shows the calculated $\text{Tan}(\Psi)$ and $\text{Cos}(\Delta)$ using 15nm gold as a top electrode at $\text{AOI}=75^\circ$. Since $\text{Cos}(\Delta)$ shows the phase terms of the signal, its EO sensitivity is more than amplitude term $\text{Tan}(\Psi)$. For the reason, the following discussion will be only based on the behaviour of $\text{Cos}(\Delta)$ spectrum. Starting from the top electrode candidates, we are comparing the $\text{Cos}(\Delta)$ spectrum response at 75° with respect to BTO index change $\delta n = 0$ and 0.2 by using a top electrode, (a) 15nm Au, (b) 50nm ITO and (c) 200nm ITO. From calculation model, bias-induced δn_{BTO} leads to spectrum shift ($\delta\lambda$). One can be noticed is that the larger intensity variation within the spectrum, the more spectrum difference will be obtained, making easier to observe signal from EO effect. For the reason, in the figure 2, 200nm ITO is a better candidate for EO measurements than 15nm gold and 50nm ITO as a top transparent electrode. Then, we are optimizing AOI from 55° to 75° for 200nm ITO/100nm BTO/10nm STO/Si, as described in the figure 3. Within whole spectrum from 350nm to 850nm, $\text{AOI}=65^\circ$ shows a broadband better response with respect to δn_{BTO} . Hence, based on our TMM model, taking 200nm ITO as a top transparent electrode on 100nm BTO/10nm STO/Si and measuring $\text{Cos}(\Delta)$ at $\text{AOI } 65^\circ$ can achieve high resolution δn_{BTO} for EO characterizations. Figure 4 presents the full mapping of $\text{Cos}(\Delta)$ response with δn_{BTO} from -0.2 to 0.2 under the optimal condition.

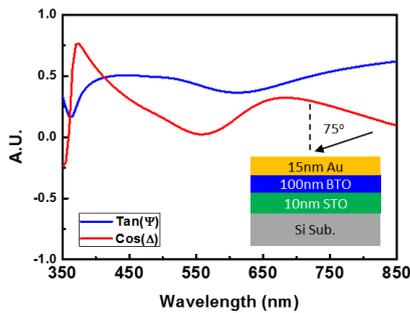


Figure 1. The calculated spectrum of $\text{Tan}(\Psi)$ and $\text{Cos}(\Delta)$ at 75° based on transfer matrix method (TMM) for 100nm BTO on 10nm STO on Si using 15nm Au as a top transparent electrode.

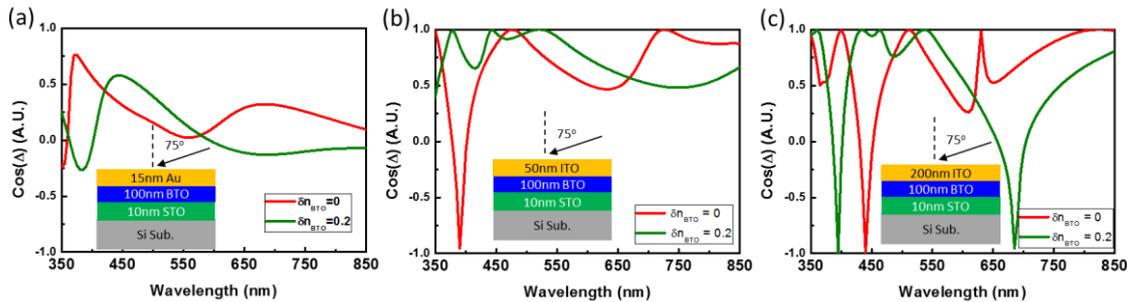


Figure 2. The calculated spectrum response for $\text{Cos}(\Delta)$ at 75° with respect to BTO index change $\delta n = 0$ and 0.2 for 100nm BTO on 10nm STO on Si using (a) 15nm Au, (b) 50nm ITO and (c) 200nm ITO as a top electrode.

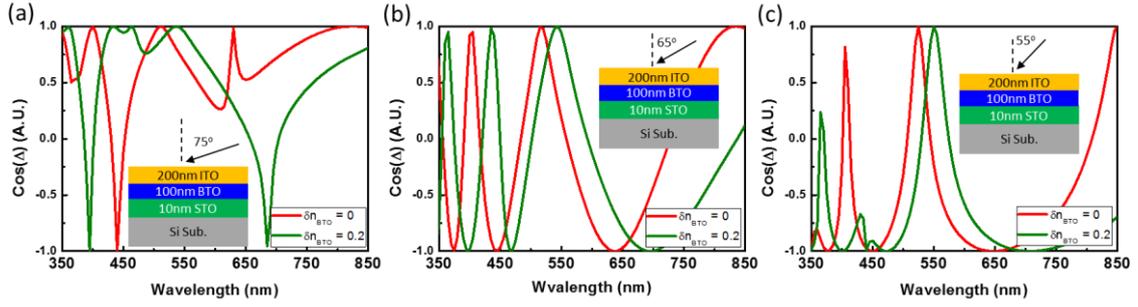


Figure 3. The calculated spectrum response for $\text{Cos}(\Delta)$ at (a) 75° , (b) 65° and (c) 55° with respect to BTO index change $\delta n = 0$ and 0.2 for 100nm BTO on 10nm STO on Si using 200nm ITO as a top electrode.

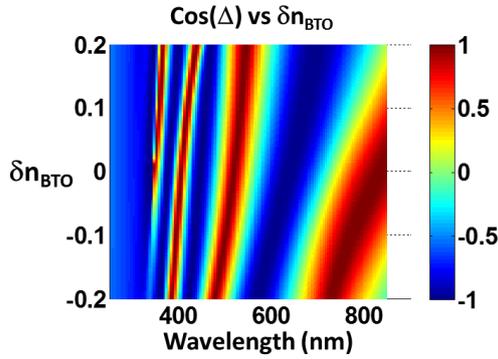


Figure 4. The calculated mapping of $\text{Cos}(\Delta)$ response with respect to different BTO index change (δn_{BTO})

Electro-Optical Measurement And Calculation

$$\delta\lambda(V) = \frac{\frac{d\text{Cos}(\Delta(\lambda(V)))}{dV}}{\frac{d\text{Cos}(\Delta(\lambda(V)))}{d\lambda}} \delta V \quad (2)$$

$$\delta n(\lambda(V)) = \frac{dn(\lambda(V))}{d\lambda} \delta\lambda \quad (3)$$

$$r_{eff} = \frac{2\delta n_{\text{BTO}}}{n_{\text{BTO}}^3 E} \quad (4)$$

In fact, any EO phenomena induced by the bias such as δn_{BTO} and $\delta\lambda$ are so minor that the approximation analysis via increment differentiation is valid. During the characterization, the given applied bias alters the $\text{Cos}(\Delta)$ intensity. Such amounts of spectrum variation resulted by external bias can be attributed to corresponding effect of wavelength shift ($\delta\lambda$), which is also the function of voltage. Then, according to the increment differentiation in the formula (2), the $\text{Cos}(\Delta)$ derivative in function of voltage and wavelength in the figure 5(a) can compute the $\delta\lambda$, as shown in the figure 5(b).

Besides, in order to convert $\delta\lambda$ into δn_{BTO} , the fitted BTO index dispersion in the figure 6(a) needs to be taken into account. Since the $\delta\lambda$ in figure 5(b) is small compared with the whole spectrum, the similar increment analysis in the formula (3) can be implemented to evaluate the corresponding δn_{BTO} by $dn/d\lambda$, as presented in the figure 6(a). The figure

6(b) shows the δn_{BTO} result with high resolution around $5\text{E-}5$. In addition, by the formula (4), the effective pockels coefficient can be evaluated with known electric field (E) as well as BTO index (n_{BTO}). Because the domain orientations in the BTO layer here are in-plane and random, the measured r_{eff} is comparatively smaller than reported values [3]. However, the in-plane poling procedure is expected to align orientations and improve the EO phenomenon.

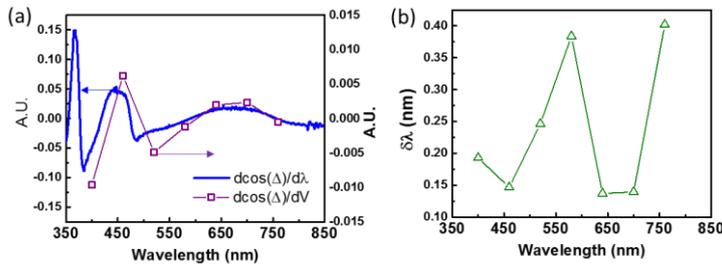


Figure 5. (a) The measured spectrum of $\text{Cos}(\Delta)$ derivative in terms of λ and voltage. (b) The computed corresponding $\delta\lambda$ based on formula (2).

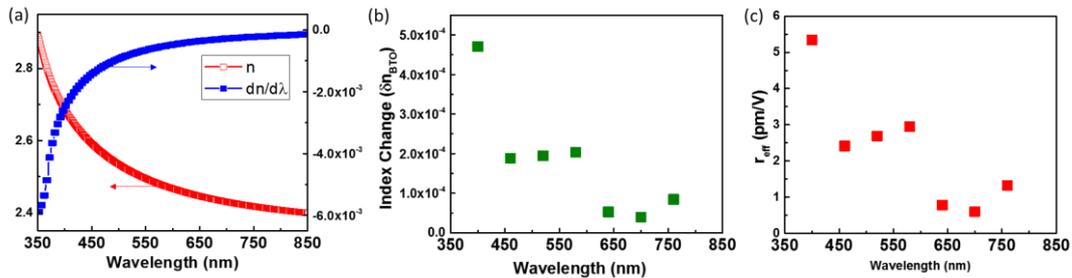


Figure 6. (a) The fitted index dispersion from SE as well as its derivative spectrum. (b) The calculated index change (δn_{BTO}) and effective pockels coefficient (r_{eff}) according to formula (3) and (4) respectively.

Conclusion

In most commercial SE, there is no additional signal amplifier making very challenging to look at EO phenomenon in the thin film materials by this technique. To overcome difficulties, in this work, we developed the TMM model to proceed not only designs of the top transparent electrode but also optimizations of EO measurement conditions. We successfully demonstrated high resolution δn $5\text{E-}5$ in the EO characterizations via non-destructive SE for MBE-grown BTO on Si.

References

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