Supporting Information

Title: Effect of thickness on the optical and electrical properties of ITO/Au/ITO sandwich structures.

Authors: Ka Kin Lam¹, Sheung Mei Ng¹, Hon Fai Wong¹, Linfeng Fei¹, Yukuai Liu¹, Ka Ho Chan¹, Hui Ye², Chi Wah Leung¹, Chee Leung Mak^{1, *}

¹Department of Applied Physics, The Hong Kong Polytechnic University, Hong Kong SAR,

China

²State Key Laboratory of Modern Optical Instrumentation, Department of Optical Engineering, Zhejiang University, Hangzhou,310027, P. R. China **Omega Scan of ITO (400) peak of the top ITO layer for different trilayer structures**



Figure S1(a) The rocking curve of top ITO (400) peak of samples with different top layer thickness (b) the FWHM of the ITO (400) rocking curve as a function of top layer film thicknesses.

Figure S1(a) shows the XRD omega scan of the ITO (400) peak observed in different trilayer samples with various top layer thickness. Figure S1(b) displays the full-width half-maximum (FWHM) of the rocking curve as a function of top ITO thickness. In general, the FWHM of the rocking curves of all samples were over 14°, and this indicated that all the top ITO film samples were having low crystallinity. It is noticed that the crystallinity of the top layer was improved with increasing top layer thickness, as indicated by the decrease of FWHM of ITO (400) peak with increasing thickness. This also indicated that the average grain size of the top ITO layer became larger as the layer thickness increased. Therefore, we believed that the improvement in electrical properties such as increment in carrier mobility was arisen from the large grain size and thus less grain boundaries, resulting in reduction of grain boundary scattering.

XRR measurement of Set B samples

Figure S2 shows the XRR measurement and the corresponding fitting results. From the graph, we estimated the individual layer thickness of the trilayer thickness. From the measurements, we confirmed that the trilayer structure with asymmetric geometry was successfully fabricated as the position of the gold insertion layer being shifted upward or downward within the ITO sandwich structure i.e. this asymmetric geometry was achieved by controlling the top and bottom ITO film thickness using different deposition time. This set of sample was based on the S3 sample (ITO_t (20 nm)/Au (3 nm)/ITO_b (20 nm) symmetric geometry) through shifting the Au layer upward and downward 10 nm and 15nm with respect to the center of the ITO sandwich.



Figure S2 XRR pattern of ITO (40-t nm)/Au (2.9 nm)/ITO (t nm) asymmetric trilayer structures.

Permittivity profile of the gold layer

Figure S3 shows the permittivity profile of the gold thin film which was obtained from the buildin profile of the ellipsometer. The permittivity is assumed to be constant among all samples for calculation. Indeed, from the TEM microscopy, all the gold layers in our trilayer structures were continuous and uniform.



Figure S3 The permitivity profile of gold thin film.

Transmittance spectra of the trilayer structure

To verify the validity of the ellipsometry data, a simulation calculation based on the transfer matrix method was used to calculate the transmittance spectra of the multilayer structures. The transfer matrix method (TMM) described by Stenzel¹ was employed to calculate the transmittance and reflectance of the multilayer thin films based on the complex refractive index and film thickness. Since the light source of UV-Vis spectrometry was incident normally on the sample. The transmitting s/p polarization of the light would be the same. In our calculation, only the s-polarized mode was considered. The algorithm is listed in the following equations, and the complex matrix multiplication was done by Microsoft Excel.

The initial parameters were refractive index n and extinction coefficient k which were obtained by our ellipsometry measurements. The schematic diagram showing the effective medium approximation (EMA) described in the paper is shown in Figure S4. The complex refractive index is given by equation (3).

$$n = \sqrt{\frac{|\tilde{\varepsilon}_{\perp}| + \tilde{\varepsilon}_{\perp,r}}{2}} \tag{1}$$

$$\kappa = \sqrt{\frac{|\tilde{\varepsilon}_{\perp}| - \tilde{\varepsilon}_{\perp,r}}{2}}$$
(2)

$$\tilde{n} = n + i\kappa \tag{3}$$

The transfer matrix by one-layer thin film is given:

$$M = \begin{pmatrix} \cos(k_o \tilde{n} d \cos \psi) & \frac{-i}{\tilde{n} \cos \psi} \sin(k_o \tilde{n} d \cos \psi) \\ -i\tilde{n} \cos \psi \sin(k_o \tilde{n} d \cos \psi) & \cos(k_o \tilde{n} d \cos \psi) \end{pmatrix}$$
(4)

$$M_{multilayer} = \prod_{j=1}^{N} M_j(n_j, d_j)$$
(5)

where k_o is the wave vector of incident light and ψ is the angle between the normal of film and propagation vector. It was taken $\psi = 0$ for normal incident wave. \tilde{n} and d are the complex refractive index and the thickness of film. The overall transfer matrix for n layers thin film is the product of transfer matrix of each layers. The transmission coefficient t can be calculated by the matrix element of transfer matrix

$$t = \frac{2}{(m_{11} + m_{12}n_s) + m_{21} + m_{22}n_s}$$
(6)

where m11, m12, m21 and m22 are the matrix elements of the overall transfer matrix M. The overall transmittance of the light across n layers thin films is given by:

$$T = \frac{n_{substrate}}{n_{air}} |t|^2 \tag{7}$$



Figure S4 Schematic diagram of TMM modeling trilayer structure by effective media approximation (EMA).



Figure S5 The effective refractive index and extinction coefficient of trilayer structure using effective media approximation.



Figure S6 Camparision of the simulated transmittance using EMA and measured transmittance of trilayer structure with different ITO top and bottom thickness.

In this part, the transmittance of the multilayer structure was calculated directly by the data retrieved form the ellipsometry measurement without using the EMA.



Figure S7 schamatic diagram of TMM modeling trilayer structure by direct calculation



Figure S8 (a) simulated transmittance calculated by the refractive index of individual layer and (b) measured spectral transmittance data of the trilayer samples.

Similar to the spectra calculated by the effective medium approximation, the simulation can model the transmittance with the from NIR to visible range including the transmittance response in the transition.

References

1. Stenzel, O., *The Physics of Thin Film Optical Spectra*. Springer: 2005.

Corresponding Author

*C.L.M.: e-mail, apaclmak@polyu.edu.hk; phone, (852)2766 5667; fax, (852)23337629.