Extraction of the sub-band gap density of states of Nb doped ZnO thin film transistors using C-V measurements

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The sub-band gap density of states (DOS) of Nb doped ZnO thin film transistors were extracted using a multi-frequency capacitance-voltage (C-V) method. The results can be represented by a two-term exponential DOS, representing the tail and deep states. The parameters for the tail and deep states are \( N_{\text{tail}} = 1.6 \times 10^{19} \text{ cm}^{-3} \), \( T_{\text{tail}} = 540 \text{ K} \), \( N_{\text{deep}} = 6.5 \times 10^{16} \text{ cm}^{-3} \) and \( T_{\text{deep}} = 4058 \text{ K} \) respectively. Furthermore, the DOS from C-V provides a good fit with current-voltage characteristics, using the multiple trap and release model.

Here, we extract the DOS in Nb doped ZnO (ZnO:Nb) TFTs using the multi-frequency C-V method outlined by Lee et al. [14] and Jang et al. [15]. This method is based on the derivation of an equivalent circuit for localized and free charge. The advantages of the technique are that optical illumination, temperature-dependent electrical characterization and numerical calculations are not required. The DOS parameters obtained from the C-V characteristics are compared with those extracted from I-V measurements, which were analyzed using the multi-trapping and release (MTR) model [18] allowing for a self-consistent check of the validity of the results.

1. Introduction

Zinc oxide (ZnO) based materials for active channel layers in thin-film transistors (TFTs) have attracted considerable attention for flat panel display applications due to their excellent optical and electrical properties compared to those of Si-based TFTs [1,2]. The carrier concentration in the active channel layer is required in determining the electrical characteristics of the TFTs. The carrier concentration in ZnO is highly dependent on the deposition technique and conditions [3]. Another alternative approach is to add dopants such as Ga and In [4,5], Si [6] or as demonstrated in our previous work, Nb [7] and Mg [8]. The sub-band gap density of states (DOS), \( g(E) \), is a key parameter for characterizing ZnO films and a number of techniques have been reported for their extraction. A numerical simulation technique was demonstrated by Kimura et al. [9] where the influence of the free carrier density was assumed negligible. Bae et al. [10] analyzed the variation in the sub-threshold slope in TFTs. The optical response of the DOS has been investigated in both capacitance-voltage (C-V) [11,12] and current-voltage (I-V) measurements [13]. A method based on multi-frequency C-V measurements has been outlined by Lee et al. [14] and Jang et al. [15] based on analysis of the frequency dispersion of C-V characteristics, to obtain a frequency-independent plot. Moreover, an extraction technique for the activation energy \( (E_a) \) based on the Meyer-Neldel rule was reported by Chen et al. [16] and Jeong et al. [17]. However, this method requires the temperature dependence of the I-V characteristics.

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transformed into the four-component \( Z_4 \) model shown in Fig. 2(a-ii). The four-component model separates the channel impedance and the contact resistances for source and drain \( (R_c) \). The impedance of the four-component model is represented as

\[
Z_4 = Z_3 + \frac{R_{ch}}{1 + (\omega C_{ch} R_{ch})^2} - j \frac{\omega C_{ch} R_{ch}}{1 + (\omega C_{ch} R_{ch})^2} + \frac{1}{\omega C_{gate}}
\]

(2)

where \( C_{ch} \) and \( R_{ch} \) are the channel capacitance and resistance respectively. It should be noted that the measured leakage current through the gate oxide is <30 pA over the full voltage range and the contact resistances for \( R_c \) are assumed to be frequency independent. The voltage dependent \( R_c \) is thus extracted and shown in Fig. 2(b). The inset in Fig. 2(b) demonstrates that \( R_c \) is determined by the minimum impedance for each applied voltage.

By assuming \( Z_2 = Z_4 \), the parameters \( C_{ch} \) and \( R_{ch} \) are obtained using

\[
C_{ch} = \frac{bC^2_{gate} - b^2 C_{gate}}{(a^2b^2 + 1)C^2_{gate}}
\]

(3)

where \( a = \left( \frac{D_s}{\alpha C_{ch}(1 + D_m^2)} - R_s \right) \), \( b = C_m(1 + D_m^2) \), and \( D_m = -\frac{1}{\alpha C_{ch} D_m} \).

The channel impedance, \( Z_{ch} \), is represented by

\[
Z_{ch} = \frac{R_{ch}}{1 + (\omega C_{ch} R_{ch})^2} - j \frac{\omega C_{ch} R_{ch}}{1 + (\omega C_{ch} R_{ch})^2}
\]

(5)

The four-component capacitance model is then transformed into the physics based model, where the channel charge is expressed \( Q_{loc} \) and \( Q_{free} \) charges. Fig. 2(a-iii) shows the equivalent circuit where \( \omega C_{ch} R_{ch} \) is the capacitance dependent on the voltage dependent \( Q_{loc} \) and \( Q_{free} \). The resulting capacitance and \( \omega C_{ch} R_{ch} \) is the capacitance due to the voltage dependent \( Q_{free} \). The total impedance for the physics based model (\( Z_{phys} \)) is then

\[
Z_{phys} = \frac{C^2_m R_{loc}}{\omega C^2_{ch} C_{free} R_{loc}^2 + (C_{loc} + C_{free})^2} - j \frac{\omega C^2_{loc} C_{free} R_{loc}^2 + (C_{loc} + C_{free})^2}{\omega C^2_{ch} C_{free} R_{loc}^2 + (C_{loc} + C_{free})^2}
\]

(6)

where it is assumed that \( R_{loc} \) and \( C_{loc} \) are frequency independent as their product determines the frequency dependence of \( Q_{loc} \). By using the relationship \( Z_4 = Z_{phys} \), Eq. (6) can be solved and equated for \( R_{loc} \) at the three measured frequencies. The resultant parameters \( C_{loc} \), \( C_{free} \), and \( R_{loc} \) obtained are frequency independent. By equating \( R_{loc} \) with 3 frequencies such that \( R_{loc}(f_1) = R_{loc}(f_2) = R_{loc}(f_3) \), the obtained \( C_{loc} \), \( C_{free} \), and \( R_{loc} \) are frequency independent. The frequency independent model for the gate capacitance is shown in Fig. 2(a-iv), with the C-V characteristics for this model depicted in Fig. 2(a-c); the model is seen to overlap the measured characteristics indicating excellent agreement. The frequencies used to obtain Fig. 2(c) are 100 Hz, 10 kHz and 100 kHz; a relatively wide range.

\[
R_{loc} = \sqrt{\frac{\omega^2 C^2_{ch} R^2_{loc} C_{loc} + C_{loc} + C_{free} - C_{ch} - C_{loc} + C_{free}}{\omega^2 C^2_{ch} R^2_{loc} C_{free} + 1 + \omega^2 C^2_{ch} R^2_{loc} C_{loc} - C_{free}}}
\]

(7)

The procedure associated with Eqs. (1)–(7) has involved the conversion of the frequency dependent C-V plots of Fig. 1, to frequency independent C-V characteristics by employing the equivalent circuit in Fig. 2(a-iv). The resultant C-V characteristics are shown in Fig. 2(c), where
it is evident that the model shows excellent agreement with the measured data. As $C_{loc}$ represents the voltage dependence of $Q_{loc}$, the DOS, $g(E)$ with units eV$^{-1}$ cm$^{-3}$, is obtained using

$$g(E) = \frac{C_{loc}(V_1) - C_{loc}(V_2)}{q^2 T_{ZnO:Nb}}$$

(8)

Finally, a relationship between the applied voltage on the gate and the surface potential ($\phi_s$) is required. The $\phi_s$ is obtained by integrating the frequency independent C-V characteristics between flat band voltage ($V_{FB}$) and $V$ shown by

$$\phi_s = \int_{V_{FB}}^{V} (1 - \frac{C}{C_{gate}}) dV$$

(9)

where $V_{FB}$ was determined from the fitting of I-V measurements using the MTR model. The value of $V_{FB}$ was slightly adjusted (<5%) to achieve a fit with the DOS derived from a TFT measurement taken on the same material, which is described next.

It is generally considered that the DOS associated with deep and tail states can be described by Gaussian distributions. Furthermore, it has been found that those can be approximated by exponential functions representing the tail of the Gaussian in an energy range most populated by carriers [18]. It is also worth noting that it has been recognised and demonstrated that the tail states alone dominate the response [18] and the DOS can be reasonably approximated by a single exponential term, thus allowing a closed form expression for the drain current of a ZnO:Nb TFT. The extracted $g(E)$ (symbols) is shown in Fig. 2(d) with the two-term exponential DOS model superimposed (lines) to account for the tail and deep states given as

$$g(E) = N_{tail} \exp\left(-\frac{E_c - E}{kT_{tail}}\right) + N_{deep} \exp\left(-\frac{E_c - E}{kT_{deep}}\right)$$

(10)

where $N_{tail}$ is the effective density of tail states, and $T_{tail}$ is the characteristic temperature of tail, $N_{deep}$ is the effective density of deep states, $T_{deep}$ is the characteristic energy of deep states and $E_c$ is the energy of the conduction band. By fitting Eq. (10), the parameters obtained are $N_{tail} = 1.6 \times 10^{19}$ cm$^{-3}$, $T_{tail} = 540$ K (49 meV), $N_{deep} = 6.5 \times 10^{16}$ cm$^{-3}$ and $T_{deep} = 4058$ K (350 meV).

A comparison of these results from the multi-frequency extraction technique is now made with the DOS obtained from fitting the MTR model to I-V data [7]. The measured I-V characteristics (symbols) and fits from the MTR (lines) and C-V measurements (dashes) are shown in Fig. 3. The I-V fits employ the MTR model with a single exponential DOS approximation, using a characteristic temperature, $T_o = 540$ K
(49 meV) and trap density, $N_t = 1 \times 10^{19} \text{ cm}^{-3}$. It is evident that there is good agreement with the number of trapping states ($N_t - N_{tail}$) and the characteristic temperatures ($T_o - T_{tail}$), demonstrating the dominance of the tail states in the conduction mechanism.

It should be noted that it is not apparent from the experimental C-V plots of Fig. 1 that the response has become independent of frequency and this implies there may be an associated error in the energy scale for the extracted DOS. The DOS extracted is therefore representative of those states probed in the measurement. The self-consistency between the DOS extracted from C-V and I-V techniques provides some confidence that the results can be used in the construction of a compact device model, as described in [18], which is the ultimate motivation for the work.

### 4. Conclusions

C-V measurements were conducted on ZnO:Nb TFTs over a frequency range from 100 to 100 kHz. The tail and deep state density of states were extracted using the multi-frequency method. The tail state DOS component was compared with that extracted from I-V measurements using the MTR model and good agreement found between the two extraction techniques with the qualification that it was necessary to adjust the C-V flat band voltage by ~5% to realise the fit.

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