Electronic Supplementary Information

The Structural, Optical and Electrical Characterization of High-Performance, Low-Temperature and Solution-Processed Alkali Metal-Doped ZnO TFTs

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We modified equation of optical absorption coefficient as follows,\textsuperscript{[1]}

\[
T_{ZnO/glass} = e^{-(\alpha_{ZnO}d_{ZnO})} \cdot e^{-(\alpha_{g}d_{g})}, \quad T_g = e^{-\alpha_g d_g} \]

\[
T_{relativeZnO} = \frac{T_{ZnO/glass}}{T_{glass}} = e^{-\alpha_{ZnO}d_{ZnO}} \]

\[
-\frac{1}{d} \ln T_{relativeZnO} \equiv \alpha \]

We estimated the optical bandgap from the intersection of the linear extrapolated line with the horizontal axis,\textsuperscript{[2]}

\[
(\alpha hv)^n = A(hv - E_{opt}) \tag{1} \]

The value of n in equation (1) was obtained the best straight line fit to the experimental data for n=2 when \( \alpha \) was plotted against \( hv \). The measured optical bandgap (\( E_{opt} \)) was defined as follows,

\[
E_{opt} = E_g - \Delta E \tag{2} \]
The Burstein-Moss shift, $\Delta E$, could be expressed as,

$$\Delta E = \frac{\hbar^2 E_b}{8\pi^3}, \quad E_b = \frac{N_e^3}{m_e^*}$$  \hspace{1cm} (3)

Thus, equation (2) could be written as follow.

$$E_{\text{opt}} = E_g + \frac{\hbar^3 N_e^3}{8m_e^*\pi^3}$$  \hspace{1cm} (4)

$N$ is carrier concentration. Assuming the effective mass $m_e^*$ to be independent of doping concentration, we could determine the optical bandgap of pristine ZnO film and the average value of $m_e^*$ from the UV transmittance plot.\cite{3} To calculate the optical bandgap, the linear data region of pristine ZnO film was selected. Generally, the band gap of intrinsic ZnO is $\sim 3.3\text{eV}$, however, the calculated optical bandgap of pristine ZnO film which we selected was $3.24\text{eV}$. Under the same linear data region ($3.5\text{eV} \sim 3.64\text{eV}$) of $(ah\nu)^2$ vs. photon energy plot, the $E_{\text{opt}}$ of Li-doped ZnO films (1mol%~15mol%) was calculated respectively.
Figure S1. Output curves and transfer curves of ZnO TFTs. (a) and (b) pristine ZnO. (c) and (d) Li-ZnO (Li 1mol%). (e) and (f) Li-ZnO (Li 10mol%). (g) and (h) Li-ZnO (Li 15mol%). The gate voltage was varied between 0 V and 60 V in steps of 12 V. The channel length and width were 50 and 1000 μm, respectively.
**Figure S2.** The box chart of optical band gap vs. Li doping concentration.
**Figure S3.** The average field effect mobility of Li-doped ZnO TFTs as one run at 300°C. (a) pristine ZnO. (b) Li-doped ZnO (1mol%). (c) Li-doped ZnO (10mol%). (d) Li-doped ZnO (15mol%).
**Figure S4.** The TGA data of various alkali metal-doped ZnO films.
Figure S5. XPS spectra of alkali metals doped ZnO films. (a) Li peaks at 55.7 eV in Li-doped ZnO films (10 mol%). (b) Na peaks at 55.7 eV in Na-doped ZnO films (1 mol%).
Figure S6. XPS spectra of Li 1s for Li-doped ZnO film (10 mol%).
Figure S7. TOF-SIMS results of (a) pristine and (b) Li-doped ZnO (Li 10 mol\%) film. Etching rate and analysis area was 0.4 Å/s and 100 x 100 μm, respectively.
Figure S8. EDS results of (a) pristine and (b) Li-doped ZnO (Li 1 mol%) films. (c) Li-doped ZnO (Li 10 mol%) films. (d) Li-doped ZnO (Li 15 mol%) films. Note that nitrogen doping was not observed in the ZnO films. All films were annealed at 300 °C for 1 hour.

Reference