Supporting Information: Optoelectronic devices on index-near-zero substrates

Lisa J. Krayer1,2, Jongbum Kim2, Joseph L. Garrett2, and Jeremy N. Munday1,2

1Electrical and Computer Engineering Department, 2Institute for Research in Electronics and Applied Physics.
University of Maryland, College Park, MD 20742, USA

The transfer matrix method
Maxwell’s equations for light traveling through stratified media can be solved using a method called the transfer matrix method. In this method, the characteristic matrix for each layer, \( M_j \), is multiplied together to form the characteristic matrix of the full system, \( M \). For a TE wave, the characteristic matrix for the \( j^{th} \) layer is:

\[
M_j = \begin{bmatrix}
\cos \left( \frac{2\pi}{\lambda_0} h_j p_j \right) & -\frac{i}{p_j} \sin \left( \frac{2\pi}{\lambda_0} h_j p_j \right) \\
-ip_j \sin \left( \frac{2\pi}{\lambda_0} h_j p_j \right) & \cos \left( \frac{2\pi}{\lambda_0} h_j p_j \right)
\end{bmatrix}, \tag{S1}
\]

where \( p_j = \hat{n}_j \cos \theta_j \), \( \hat{n}_j \) is the complex refractive index of the \( j^{th} \) layer, \( \theta_j \) is the angle that the electromagnetic wave makes with the normal axis as determined by Snell’s law, \( \lambda_0 \) is the optical wavelength in free space, and \( h_j \) is the film thickness of the \( j^{th} \) layer. The total characteristic matrix, \( M \), that describes all \( N \) distinct layers can then be calculated (Eq S2, below), and the amplitudes of the reflected, \( E_r \), and transmitted, \( E_t \), waves can be obtained from Eq S3:

\[
M = \prod_{j=1}^{N} M_j = \begin{bmatrix}
m_{11} & m_{12} \\
m_{21} & m_{22}
\end{bmatrix}
\]

\[
\begin{bmatrix}
E_0 + E_r \\
p_1(E_0 - E_r)
\end{bmatrix} = M \begin{bmatrix}
E_t \\
p_N E_t
\end{bmatrix}, \tag{S2}
\]

where 1 and \( N \) represent the first and last media in the stratified stack, and \( E_0 \), \( E_r \), and \( E_t \) are the amplitudes of the incident, reflected, and transmitted waves, respectively. This system can then be solved to find the reflection, \( r \), and transmission, \( t \), coefficients.

\[
r = \frac{E_r}{E_0} = \frac{(m_{11}+m_{12}p_N)p_1 - (m_{21}+m_{22}p_N)}{(m_{11}+m_{12}p_N)p_1 + (m_{21}+m_{22}p_N)} \tag{S4}
\]

\[
t = \frac{E_t}{E_0} = \frac{2p_1}{(m_{11}+m_{12}p_N)p_1 + (m_{21}+m_{22}p_N)} \tag{S5}
\]

Finally, the reflectivity, \( R \), and transmittivity, \( T \), are determined by:

\[
R = |r|^2 \quad \text{and} \quad T = \frac{p_N}{p_1} |t|^2 \tag{S6}
\]

For a TM wave, a simple modification is made to the above equations by replacing \( p_j \) with \( q_j = \frac{\cos \theta_j}{\hat{n}_j} \).
Figure S1. Effect of non-ideal INZ on the absorption resonance when $n_{top} = n_Si$. The metal film ($n_f + i\kappa_f$) on an INZ substrate ($n_{INZ} + i\kappa_{INZ}$) is illuminated through silicon, and the absorption is determined within the thin film. The diagonal line in each contour plot corresponds to $n_f = \kappa_f$. Absorption is calculated for 17 nm-thick films at normal incidence with $\lambda = 1300$ nm. The maximum absorption moves to higher $n_f$ as $\kappa_{INZ}$ increases, and the value of maximum absorption decreases with increasing $n_{INZ}$. The dots represent the optical indices of real materials showing that the absorption peak moves away from common materials for high optical loss in the INZ material.
Figure S2. Optical design considerations for INZ materials to enhance absorption in Pt and Cr. The grey contour lines show increments of 10% absorption with the line closest to the origin showing 90% absorption. Refractive indices of INZ materials at $\lambda = 1300$ nm from literature are shown by the white dots. Of these materials, the absorption at $\lambda = 1300$ nm is maximized by ITO from reference [19], GZO from reference [33], AZO from reference [9] and GZO from reference [18]. When deposited on these substrates, the calculated absorption in thin film Cr and Pt is >70% and >60% when illuminated through air and ≥90% and >84% when illuminated through silicon, respectively. The absorption within the metal is calculated for optimized film thickness at each data point. For illumination through air, the optimized thicknesses ranged from 4 to 12 nm for Cr and 3 to 7 nm for Pt. The 90% absorption contour line for Cr and Pt intersects the $n_{\text{INZ}}$ axis at 0.11 and 0.07 and intersects the $\kappa_{\text{INZ}}$ axis at 0.65 and 0.24, respectively. For illumination through silicon, the optimized thicknesses ranged from 17 to 25 nm for Cr and from 11 to 14 nm for Pt. The 90% absorption contour line for Cr and Pt intersects the $n_{\text{INZ}}$ axis at 0.38 and 0.19, respectively. For Cr, the 90% absorption contour line does not intersect with the $\kappa_{\text{INZ}}$ axis in this range, however, for Pt, the line intersects the $\kappa_{\text{INZ}}$ axis at 0.66.
Figure S3. Absorption in Pt, Ti, Cr, and Fe on INZ substrates with optical properties found in literature.

(a) Optical properties for ITO from reference [1] (blue), ITO from reference [3] (green), and the AZO fabricated for this paper (red). Absorption in Pt, Ti, Cr and Fe was calculated, and the range of absorption obtained using these four metals is shown for (b) illumination from air \( n_{\text{top}} = n_{\text{air}} \) and (c) illumination from silicon \( n_{\text{top}} = n_{\text{Si}} \). The shaded regions span the calculated absorption maximized for film thickness in all four metals when placed on the three examples of INZ materials from literature. These metals obtain \( \sim 75\% \) absorption on INZ substrates when illuminated through air and \( \sim 90\% \) when illuminated through silicon. The absorption reaches maximum at a wavelength 50-70 nm longer than \( \lambda_{\text{ENZ}} \), i.e. the wavelength where \( n_{\text{INZ}} = \kappa_{\text{INZ}} \), and then decreases because \( \kappa_{\text{INZ}} \) increases and moves the absorption resonance away from the optical properties of the thin metal films. As expected, the ITO with larger \( n_{\text{INZ}} \) has lower absorption.
**Figure S4.** AZO has index-near-zero behavior. Images of AZO deposited on (a) glass and (c) silicon show the thickness gradient on each substrate. The real (solid lines) and imaginary (dashed lines) refractive indices of all thicknesses of AZO on (b) glass and (d) silicon as determined from ellipsometry analysis. $\lambda_{ENZ}$ is blue shifted for decreasing thickness on glass and red shifted on silicon.
**Figure S5.** Current-voltage relationship for the Si/Pt photodiode. The data was recorded using a Keithley 2400 source meter with a LabView script that swept voltage and read current and resistance. The barrier height extracted from the forward bias region using thermionic emission theory is 0.7 eV with an ideality factor of 3.56. This result suggests that there is a PtSi or Pt$_2$Si region at the interface reducing the quality of the junction.

**Figure S6.** Kelvin probe force microscopy scan of Pt and AZO edge. (a) Topography and, (b) work function difference between Pt and AZO. Using a Pt probe, the work function was measured using the heterodyne KPFM method. (c) The histogram of the H-KPFM data showing a 131 ± 75 mV work function difference between Pt and AZO.