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SPECTRAL-ENVIRONMENTAL PERFORMANCE MODELING AND MULTI-SCENARIO DESIGN OF A SELF-POWERED ZNO/SI ULTRAVIOLET PHOTODETECTOR

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ABSTRACT

Dust, humidity, and temperature act at the same time in service, yet their combined effect on self-powered ZnO/Si ultraviolet detectors is rarely evaluated. A reduced-order model was therefore assembled for an n-ZnO/p-Si device. It links wavelength-dependent ZnO absorption and thickness-dependent carrier collection with an Ångström soiling term, humidity-dependent surface transport, thermally activated dark current, shot and Johnson noise, and adsorption-controlled transients. Calibration used one quantity only: the clean zero-bias responsivity at 365 nm. With the adopted idealized noise expression, D^* was 4.10×10^{13} Jones, compared with 3.5×10^{13} Jones in the reference device (17.2% higher). This comparison was used as a plausibility check and was not a fitting target. Performance retention was summarized by a weighted geometric Reliability Index (RI). The design was then tested by changing the RI weights and passivation penalty, refining the numerical grid, and checking Monte Carlo convergence. The practical grid selected 225 nm and the refined grid 226 nm, giving a conditional thickness region of 220–235 nm. By contrast, the preferred passivation index changed with the assumed coating penalty. For the harsh case (0.35 mg cm^{-2} dust, 85% RH, and 325 K), optimization raised RI from 0.255 to 0.483. In 12,000 conditional uncertainty realizations, the median was 0.738 and the 5th–95th percentile range was 0.671–0.806. The model can be used to screen designs before fabrication, but it does not qualify device reliability. Measurements are still needed to identify the coating and material parameters.

Keywords: ZnO/Si Heterojunction, Self-Powered Ultraviolet Photodetector, Environmental Degradation, Surface Passivation, Multi-Scenario Optimization, Monte Carlo Uncertainty

1 INTRODUCTION

Ultraviolet photodetectors are used in flame monitoring, environmental sensing, optical communication, biomedical instrumentation, and industrial process control. ZnO is attractive for these applications because of its direct wide band gap near the ultraviolet-A/visible boundary, relatively low-cost processing, and potential for high photoconductive gain associated with oxygen-sensitive surface states. The same surface chemistry, however, makes the photoresponse

sensitive to humidity, oxygen adsorption, and ageing, creating a substantial gap between laboratory figures of merit and field performance [1–3].

A ZnO/Si heterojunction can work at zero bias because its built-in field separates photogenerated carriers. Recent self-powered devices give responsivities close to 0.1 A W^{-1} and specific detectivities of about 10^{13} Jones. Much larger responsivities have been reported for biased vertical bilayers, where gain contributes to the measured signal [4, 5]. Most of these values come from controlled optical tests, so they say little about operation under dust, humidity, and temperature changes. Natural soiling attenuates ultraviolet and blue light more strongly than longer wavelengths; a modified Ångström relation provides a useful description of that trend [6]. Water adsorption also competes with oxygen at the ZnO surface. Depending on the device architecture, increasing RH can lower the illuminated current and change recovery times by several orders of magnitude [2, 7]. Higher temperature adds another loss mechanism through junction leakage and the associated electrical noise.

Published surface treatments are not directly interchangeable, so protection is represented here by a general passivation index. PMMA has been processed on ZnO nanorod photodetectors [18], and SiO_2/ZnO multilayers have been used to modify ultraviolet selectivity and carrier transport [19]. In another device configuration, atomic-layer-deposited Al_2O_3 reduced defects at a ZnO interface [20]. Postica et al. reported lower humidity sensitivity and better long-term stability for ZnO films covered by 10–20 nm SiO_2 [21]. These observations justify testing a protection term, but they do not justify assigning the same numerical value to coatings made from different materials or used in different junctions. UV-assisted self-cleaning has also been observed for ZnO/epoxy surfaces [27]; that photocatalytic process is separate from the transparent barrier considered in the present model.

This study combines the principal optical, electrical, and environmental terms in one reduced-order model. The calculation follows ultraviolet absorption and carrier collection, then applies surface soiling, humidity-dependent transport, thermal leakage and noise, and the measured-time-scale response. Its outputs are wavelength-resolved retention maps and a design objective evaluated over several operating conditions. Only the clean responsivity scale is calibrated. Separate analytical checks and convergence tests are used to verify the implementation. The analysis also examines the robustness of the thickness result to changes in numerical resolution and RI weights, as well as the sensitivity of the passivation result to the assumed coating penalty. Manufacturing and environmental variations are propagated explicitly, and the final section describes measurements that could be used to test the model on fabricated devices. The RI is intended for comparison among cases; it should not be interpreted as a survival probability or a formal reliability certificate.

The calculations are designed to answer three questions. First, does the competition between absorption and carrier collection produce a broad thickness optimum, and does this optimum persist when the grid resolution or RI weights are varied? Second, does surface protection remain advantageous after accounting for its optical and response-time penalties? Finally, are the predicted variations near the selected thickness driven primarily by environmental conditions rather than by small errors in thickness? These questions must be considered separately because a numerically stable result may still depend on material parameters that have not yet been measured.

2 PHYSICAL MODEL AND PERFORMANCE METRICS

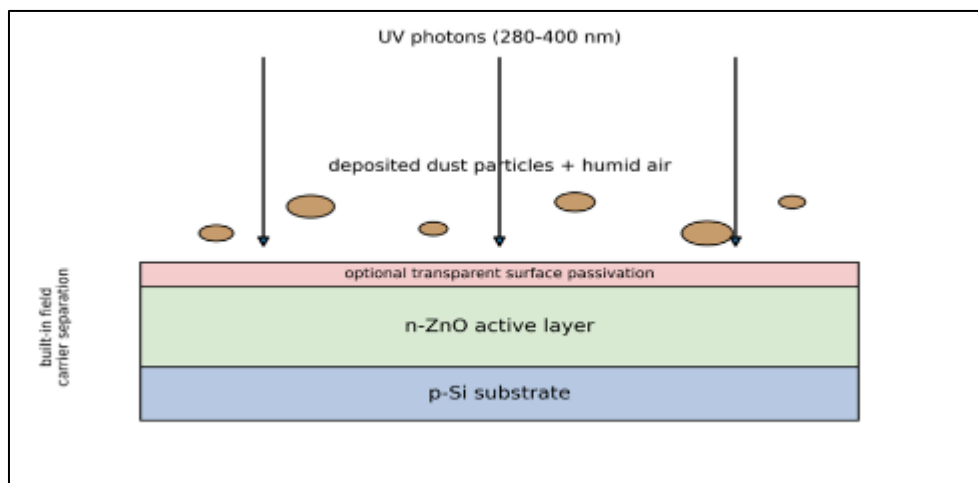


Figure 1: ZnO/Si structure used in the model and the environmental pathways acting at its surface

2.1 Spectral Absorption and Carrier Collection

For photon energies above the ZnO band gap, the absorption coefficient is represented using a smoothed direct-transition relation. At each wavelength, the external quantum efficiency (EQE) is then calculated as the product of four contributions: the absorbed fraction, a thickness-dependent carrier-collection factor, the junction-transfer efficiency, and a smooth band-edge function:

$$\alpha(\lambda) = \alpha_0 \frac{\left[\frac{\max\left(\frac{hc}{\lambda} - E_g, 0\right)}{E_0} \right]^{1/2}}{1 + b_\alpha \left(\frac{hc}{\lambda} - E_g\right)} \quad (1)$$

$$EQE_0(\lambda, d) = \eta_j [1 - \exp(-\alpha(\lambda)d)] \eta_c(d) S_{edge}(\lambda) \quad (2)$$

$$\eta_c(d) = \exp \left[- \left(\frac{d - d_c}{\sigma_d} \right)^2 \right] \quad (3)$$

$$S_{edge}(\lambda) = \left[1 + \exp \left(\frac{\lambda - \lambda_c}{s_\lambda} \right) \right]^{-1} \quad (4)$$

$$R_0(\lambda, d) = \left(\frac{q\lambda}{hc} \right) EQE_0(\lambda, d) \quad (5)$$

Very thin ZnO layers do not absorb enough incident light, whereas very thick layers incur a greater recombination penalty through the collection term. Equation (3) defines a Gaussian function that provides a compact representation of this trade-off. Before evaluating αd in Eq. (2), d is converted from nanometres to centimetres. The resulting thickness range is useful for design screening, but it is not a substitute for a drift-diffusion or technology computer-aided design (TCAD) simulation. The location of the predicted optimum depends on the adopted values of α_0 , d_c , and σ_d and should therefore be validated experimentally.

2.2 Spectral Dust Attenuation

$$T_{dust}(\lambda) = \exp \left[- \kappa_d L_{eff} \left(\frac{\lambda_0}{\lambda} \right)^\gamma \right] \quad (6)$$

$$L_{eff} = L(1 - \xi p) \quad (7)$$

In Eqs. (6) and (7), L denotes the dust mass deposited per unit area, and $\lambda_0 = 365\text{nm}$ is the reference wavelength. The exponent γ describes the spectral dependence. The dimensionless variable p ranges from 0 to 1, while ξ specifies the maximum fractional reduction in retained dust permitted by the model. Using a dimensionless p enables candidate surface treatments to be compared before experimental measurements are available to relate each value of p to a specific physical coating.

2.3 Humidity, Temperature, and Leakage Current

$$F_{RH} = 1 - a_{RH}(1 - b_p p) u_{RH}^m, \quad u_{RH} = \text{clip} \left(\frac{RH - 40}{50}, 0, 1 \right) \quad (8)$$

$$F_T = 1 - \beta_T(T - 300) \quad (9)$$

$$I_{dark} = I_{s0} \left(\frac{T}{300} \right)^n \exp \left[\frac{E_a}{k_B} \left(\frac{1}{300} - \frac{1}{T} \right) \right] \exp [\beta_{RH}(1 - c_p p) u_{RH}] \quad (10)$$

$$R = R_0 T_{dust} F_{RH} F_T (1 - \delta_p p) \quad (11)$$

The environmental terms are incorporated into the responsivity calculation through Eq. (11). A higher value of p results in lower dust retention and a weaker humidity dependence, but also in reduced optical transmission. The exponential term in Eq. (10) is evaluated using E_a in electronvolts and $k_B = 8.617333262 \times 10^{-5} \text{ eV K}^{-1}$. The same unit convention is used for the activation exponent. By contrast, the Johnson-noise term in Eq. (16) uses the SI value $k_B =$

1. $380649 \times 10^{-23} \text{ J K}^{-1}$. The humidity response of the bare device is intentionally modelled conservatively because a single universal response to adsorbed water cannot be assumed for all ZnO morphologies and contact designs.

2.4 Experimental Identification of the Passivation Index

The model variable p should not be interpreted as the thickness of a universal coating. Candidate experimental series could include an ultrathin Al_2O_3 interfacial layer deposited by atomic layer deposition (ALD), a 10–20 nm SiO_2 overlayer, and a PMMA treatment adapted to the selected fabrication route [18–21]. Because these materials behave differently, each treatment should be evaluated against its own otherwise identical uncoated control. The inverse expressions in Eqs. (12)–(14), derived from Eqs. (7), (8), and (10), allow the experimental passivation index p_{exp} to be inferred from paired measurements. In Eq. (13), ΔR_{RH} denotes the fractional loss in responsivity relative to each sample's own baseline at $\text{RH} = 40\%$, with dust loading and temperature held constant. For Eq. (14), measurements at the stated RH endpoints of 40% and 90% should likewise be performed at the same temperature. This inversion assumes that the change in leakage current between these endpoints arises only from the modelled humidity term and that the other leakage channels remain unchanged. Until such measurements are performed, a value such as $p = 0.87$ should be regarded solely as a position within the model's design space. It represents neither a physical coating thickness nor a transferable material constant.

$$p_{\text{dust}} = \text{clip}\left(\frac{1 - L_{\text{eff,coat}}/L_{\text{eff,bare}}}{\xi}, 0, 1\right) \quad (12)$$

$$p_R = \text{clip}\left(\frac{1 - \Delta R_{\text{RH,coat}}/\Delta R_{\text{RH,bare}}}{b_p}, 0, 1\right) \quad (13)$$

$$p_I = \text{clip}\left(\frac{1 - \ln(I_{90}/I_{40})_{\text{coat}}/\ln(I_{90}/I_{40})_{\text{bare}}}{c_p}, 0, 1\right) \quad (14)$$

$$p_{\text{exp}} = \text{clip}\left(\frac{p_{\text{dust}} + p_R + p_I}{3}, 0, 1\right) \quad (15)$$

2.5 Noise, Detectivity, and Temporal Response

$$i_{\text{noise}} = \left(2qI_{\text{dark}} + \frac{4k_B T}{R_{\text{sh}}}\right)^{1/2} \quad (16)$$

$$D^* = \frac{R_\lambda A^{1/2}}{i_{\text{noise}}} \quad (17)$$

$$PDCR = \frac{I_{ph}}{I_{\text{dark}}} = \frac{R_\lambda P_{in}}{I_{\text{dark}}} \quad (18)$$

$$I_{\text{rise}}(t) = I_0 + \Delta I \left[1 - \exp\left(-\frac{t}{\tau_r}\right)\right] \quad (19)$$

$$I_{\text{decay}}(t) = I_0 + \Delta I \exp\left(-\frac{t}{\tau_d}\right) \quad (20)$$

$$\tau_r = \tau_{r,\text{ref}} \exp(-k_r u_{\text{RH}})(1 + \zeta_r p) \quad (21)$$

$$\tau_d = \tau_{d,\text{ref}} \exp(-k_d u_{\text{RH}})(1 + \zeta_d p) \quad (22)$$

The multiplier $(1 + \zeta p)$ adds a modest response-time cost as protection becomes stronger. This choice reflects the possibility that a barrier which preserves signal amplitude and limits leakage may also slow exchange at the surface. Without this term, the temporal part of RI would reward passivation without accounting for that cost.

2.6 Proposed Reliability Index

$$RI = \left(\frac{R}{R_{\text{ref}}}\right)^{w_R} \left(\frac{D^*}{D_{\text{ref}}^*}\right)^{w_D} \left(\frac{PDCR}{PDCR_{\text{ref}}}\right)^{w_P} S_\tau^{w_\tau} \quad (23)$$

$$S_{\tau} = \text{clip} \left[\left(\frac{\tau_{r,ref} \tau_{d,ref}}{\tau_r \tau_d} \right)^{1/2}, 0.75, 1.15 \right] \quad (24)$$

RI compares each environmental case with the clean reference state through a dimensionless weighted geometric mean. The geometric form reduces compensation between components but does not eliminate it, and RI is not mathematically bounded to the interval 0–1. The baseline weights are [0.32, 0.32, 0.26, 0.10] for responsivity, detectivity, PDCR, and the temporal term, respectively. Responsivity and detectivity receive the same nominal exponent, PDCR retains a separate margin related to dark current, and speed receives the lowest weight. These are design preferences. D* and PDCR both depend algebraically on responsivity and dark current, so the four components are not independent measurements and their effective influence is not set by the displayed weights alone. The value RI = 0.80 is used as an exploratory screening level. It is not a standard and does not represent a probability of failure. Results are therefore also reported for different weights and for RI thresholds of 0.70 and 0.90.

3 COMPUTATIONAL METHODOLOGY AND VERIFICATION

3.1 Parameter Domain and Coefficient Disclosure

Table 1: Variables and ranges used in the simulations

Parameter	Range/value	Role
ZnO thickness, d	80–500 nm	Design variable
Dust loading, L	0–0.50 mg cm ⁻²	Environmental variable
Relative humidity	20–90%	Environmental variable
Temperature	280–340 K	Environmental variable
Passivation index, p	0–1	Generalized design descriptor
Wavelength	280–500 nm	Spectral simulation
Active area	0.04 cm ²	Fixed
UV irradiance	3 mW cm ⁻²	PDCR calculation

Table 2: Coefficients adopted in the reduced-order model

Symbol/group	Value	Status and role
E _g	3.30 eV	ZnO band gap; literature-informed
α ₀	1.20 × 10 ⁵ cm ⁻¹	Assumed absorption scale
E ₀	1.00 eV	Normalization energy
bα	0.35 eV ⁻¹	Band-edge smoothing
η _j	0.81214	Calibrated only to R ₃₆₅ = 0.110 A W ⁻¹
dc / σd	180 / 180 nm	Collection-surrogate center/breadth
λ _c / sλ	370 / 2.5 nm	Logistic cutoff parameters
κd	1.466 cm ² mg ⁻¹	Surface-soiling attenuation scale
γ	1.25	Ångström spectral exponent
λ ₀	365 nm	Reference wavelength in the Ångström-type attenuation law
ξ	0.55	Maximum dust-retention reduction
aRH / bp / m	0.259 / 0.82 / 1.25	Humidity-response coupling
β _T	1.20 × 10 ⁻³ K ⁻¹	Responsivity temperature coefficient
I _{s0}	8.00 × 10 ⁻¹³ A	Clean dark-current reference

n / Ea	2.0 / 0.195 eV	Thermal leakage parameters
βRH / cp	0.956 / 0.88	Humidity leakage/passivation terms
δp	0.035	Optical penalty per unit p
Rsh	$5.20 \times 10^{11} \Omega$	Johnson-noise shunt resistance
A / Pin	$0.040 \text{ cm}^2 / 1.20 \times 10^{-4} \text{ W}$	Active area / incident power
τ _{r,ref} / τ _{d,ref}	0.127 / 0.298 s	Clean effective time constants
kr / kd / ζτ	1.00 / 1.62 / 0.22	Humidity kinetics / barrier trade-off
RI weights	0.32 / 0.32 / 0.26 / 0.10	R / D* / PDCR / temporal
λ _p	0.109	Quadratic passivation-demand penalty
Scenario weights	0.15 / 0.30 / 0.30 / 0.25	Clean / moderate / warm-humid / harsh
Monte Carlo N / seed	12,000 / 42	Sample size used for the reported uncertainty

3.2 Calibration and External Benchmark

Only η_j was calibrated. It was selected to reproduce the clean, zero-bias responsivity of $R = 0.110 \text{ A W}^{-1}$ reported for the ZnO quantum-dot/Si device at 365 nm under an irradiance of 3 mW cm^{-2} [5]. Detectivity was not included in this calibration. The model subsequently predicts $D^* = 4.10 \times 10^{13}$ Jones using shot-noise and Johnson-noise contributions to the current-noise amplitude spectral density. Compared with the reference value of 3.5×10^{13} Jones, the relative difference is 17.2%. Here, i_{noise} denotes the one-sided amplitude spectral density in $\text{A Hz}^{-1/2}$, while the device area A is entered in cm^2 in Eq. (17). This comparison supports the plausibility of the calculated detectivity scale; it neither replaces a measured noise spectrum nor validates the environmental terms.

The remaining model construction was independent of this calibration. Literature evidence was used to determine the expected directions of the soiling and humidity responses, whereas the other reduced-order coefficients were assumed. Except for η_j , the coefficients were not fitted to outputs dependent on dust loading, humidity, temperature, or passivation. Consequently, the reliability maps, predicted optimum, and uncertainty results should be regarded as model predictions. The reported checks demonstrate numerical consistency and compatibility with the clean-state scale, but they do not constitute device-level validation under environmental exposure.

3.3 Multi-Scenario Design Optimization

Four operating scenarios were assigned fixed weights: clean/cool ($L = 0$, RH = 30%, $T = 290 \text{ K}$; 0.15), moderate (0.10 mg cm^{-2} , 50%, 300 K; 0.30), warm-humid (0.20 mg cm^{-2} , 70%, 315 K; 0.30), and harsh (0.35 mg cm^{-2} , 85%, 325 K; 0.25). The scenario-weighted objective was:

$$J(d, p) = \sum_s \omega_s RI_s(d, p) - \lambda_p p^2, \quad \sum_s \omega_s = 1 \quad (25)$$

The first search used steps of 5 nm in d and 0.01 in p . A second search reduced the steps to 1 nm and 0.0025 to check whether the selected point moved with grid resolution. We also repeated the calculation with other RI weights and swept the penalty assigned to passivation. Those tests show which conclusions follow from the numerical surface and which depend on a design preference. The objective in Eq. (25) is used for engineering screening across the four scenarios. It is not a worst-case, chance-constrained, or distributionally robust criterion.

3.4 Independent Numerical Verification and Uncertainty Analysis

A second implementation was written independently from the MATLAB-form equations. It reproduced five analytical identities, including the conversion between EQE and responsivity, the PDCR definition, and the shot-plus-Johnson expression for detectivity. Four grids were used for the convergence test. Monte Carlo sample sizes of 3000, 6000, 12,000, and 24,000 were then run with the same truncated-normal definitions and controlled random seed. For the reported uncertainty case, the inputs were $d = 225 \pm 18 \text{ nm}$, $p = 0.87 \pm 0.075$, $L = 0.14 \pm 0.04 \text{ mg cm}^{-2}$, RH = $55 \pm 6\%$, $T = 310 \pm 3 \text{ K}$, and $\gamma = 1.25 \pm 0.15$. Samples were independent and were truncated at the limits of the model domain. Spearman coefficients were used to describe monotonic sensitivity. This calculation includes the stated input variation while holding the model coefficients fixed. Uncertainty in those coefficients and in the structure of the model remains outside the calculation.

4 RESULTS AND DISCUSSION

4.1 Spectral and Environmental Behavior

The simulated photoresponse is centered near the ZnO absorption edge. Insufficient absorption occurs in very thin films, whereas excessive thickness reduces the collection surrogate. The resulting response has a broad optimum at approximately 220–235 nm. Dust attenuation is spectrally non-neutral and is strongest in the near-ultraviolet interval used by the detector, in agreement with optical measurements of natural soiling [6].

For the conservative bare-device branch, increasing RH from 40 to 90% reduces responsivity by 25.9% and increases dark current by a factor of 2.60. Thermally activated leakage increases and detectivity decreases between 300 and 330 K. The humidity-assisted acceleration of recovery is therefore not interpreted as an overall improvement in detector performance.

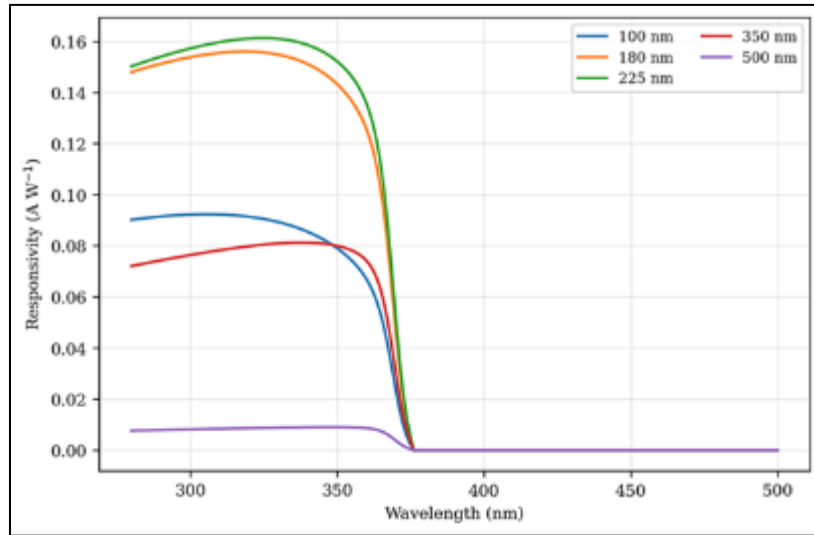


Figure 2: Clean spectral responsivity for selected ZnO thicknesses

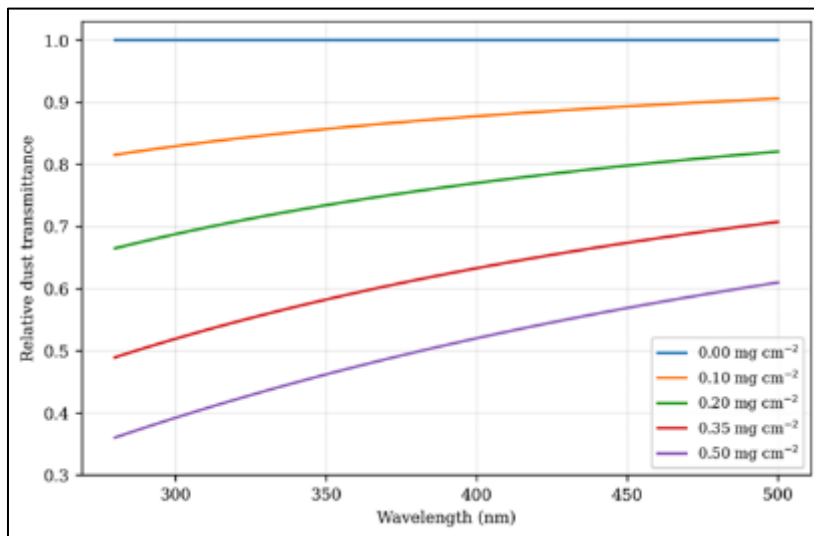


Figure 3: Predicted relative transmittance of deposited dust

4.2 Spectral–Environmental Reliability Maps

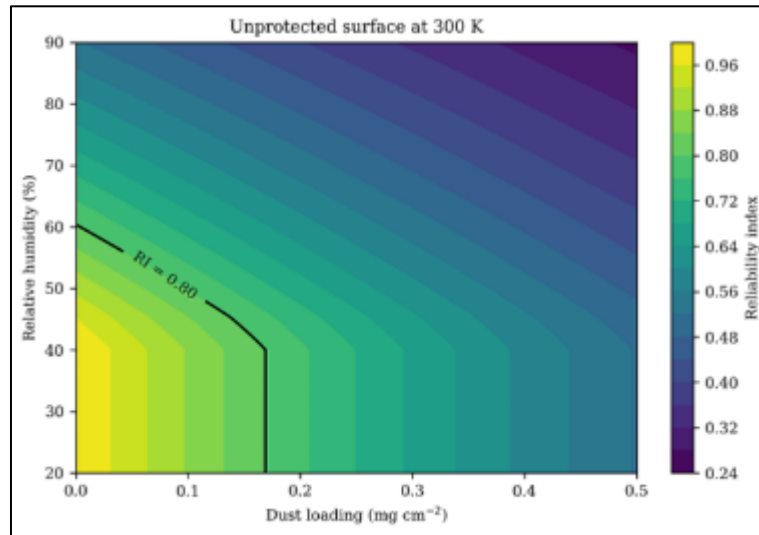


Figure 4: Reliability map of the unprotected device at 300 K; the contour denotes RI = 0.80

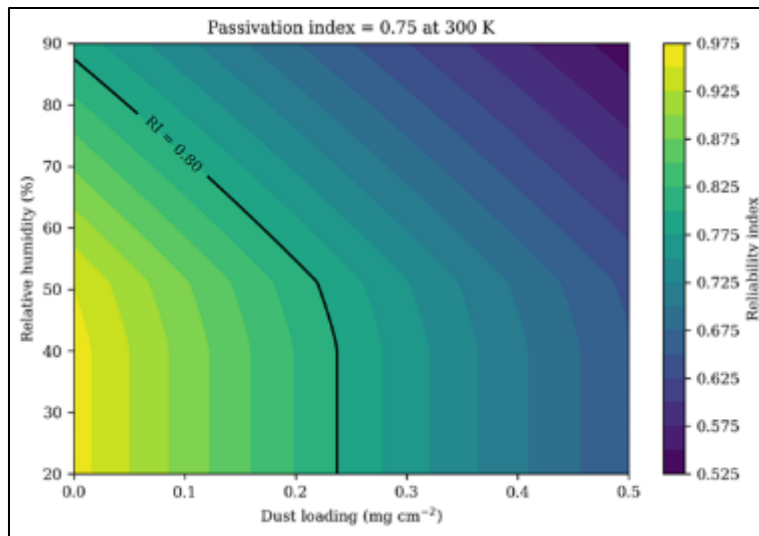


Figure 5: Reliability map at $p = 0.75$ and 300 K

At 300 K and 40% RH, the unprotected design reaches $RI = 0.80$ at $L = 0.169 \text{ mg cm}^{-2}$. With $p = 0.75$, the corresponding critical loading increases to 0.237 mg cm^{-2} . At 80% RH, the unprotected detector is already below $RI = 0.80$ without dust, whereas the protected design maintains the criterion up to approximately 0.048 mg cm^{-2} . The numerical boundary shifts when thresholds of 0.70 and 0.90 are used, but the comparative advantage of protection remains. These contours should be interpreted as model-based maintenance or screening boundaries, not as experimentally certified safe operating limits.

4.3 Transient Response and the Passivation-Speed Trade-Off

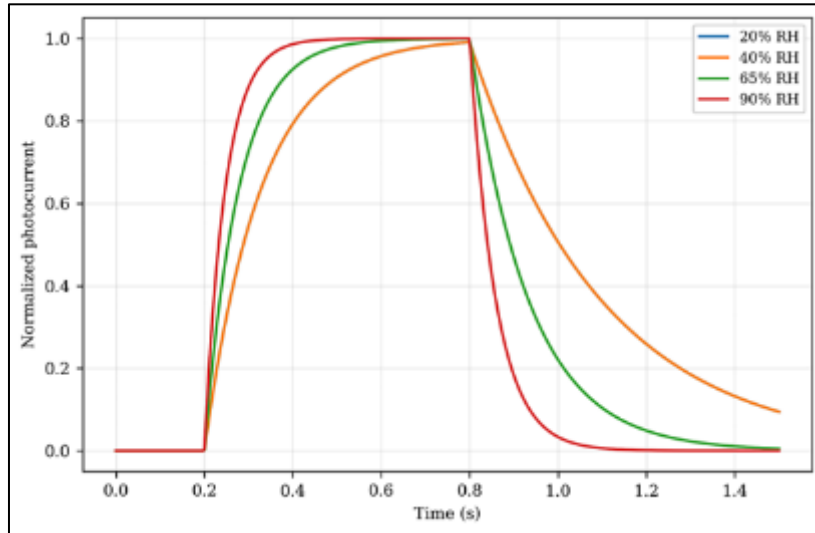


Figure 6: Normalized on/off response at different humidity levels for the unprotected detector

For the unprotected detector, the fitted recovery time becomes shorter as RH rises. This trend has the same direction as the oxygen/water competition observed in ZnO nanowires [2]. It should not be mistaken for better overall performance: signal amplitude, detectivity, and the dark-current margin deteriorate at the same time. The factors in Eqs. (21) and (22) add a small slowing term to protected devices so that passivation does not gain an unrealistic advantage from the temporal component of RI.

4.3.1 Multi-Scenario Design Optimization and Sensitivity

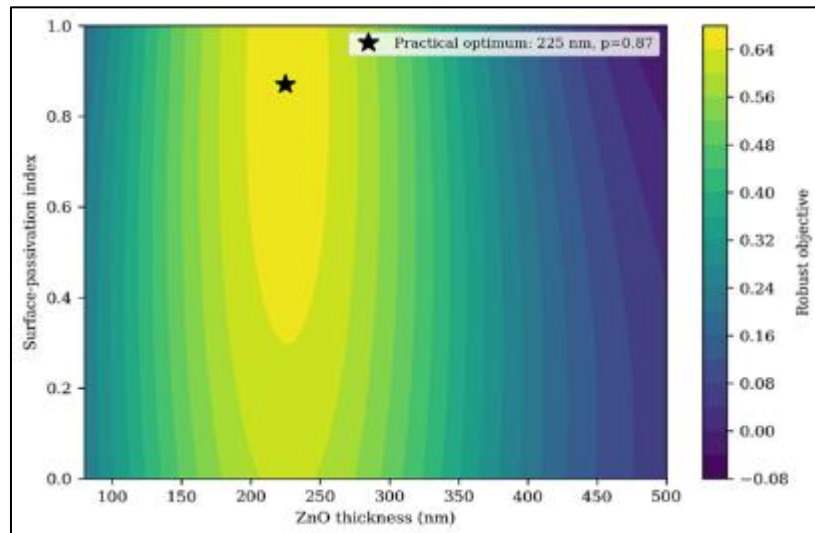


Figure 7: Scenario-weighted objective calculated across the ZnO thickness and passivation design space

On the practical grid, the maximum occurs at $d = 225$ nm and $p = 0.87$. Reducing the increments to 1 nm and 0.0025 moves it slightly, to $d = 226$ nm and $p = 0.875$. The objective differs by only 0.057% between the coarsest and finest grids. Grid convergence is therefore adequate for the adopted coefficients, and the result is better reported as a thickness interval than as a one-nanometer target. This numerical test does not cover uncertainty in α_0 , d_c , or σ_d , so it cannot establish that the interval is physically robust. The extra decimals in p are also numerical. A value transferable to fabrication can only be assigned after the coating penalty and p_{exp} have been obtained from measurements.

All deterministic weight schemes retain $d = 225$ nm, whereas p varies from 0.69 to 0.98. Under 1000 randomized $\pm 20\%$ perturbations of the baseline weights, every realization retains $d = 225$ nm; the 5th, median, and 95th percentiles of p are 0.84, 0.87, and 0.91. By contrast, varying λp from 0.07 to 0.15 moves p from 1.00 to 0.56 while leaving d unchanged. Thickness is therefore the more stable design conclusion, whereas passivation strength remains an experimentally testable and penalty-dependent recommendation.

Table 3: Sensitivity of the multi-scenario optimum to alternative RI weights

Scheme	wR	wD	wP	w τ	d_opt (nm)	p_opt	J_max
Baseline	0.32	0.32	0.26	0.10	225	0.87	0.6636
Equal	0.25	0.25	0.25	0.25	225	0.72	0.7001
Responsivity priority	0.42	0.28	0.20	0.10	225	0.81	0.6791
Detectivity priority	0.24	0.42	0.24	0.10	225	0.90	0.6588
PDCR priority	0.24	0.24	0.42	0.10	225	0.98	0.6430
Temporal priority	0.27	0.27	0.21	0.25	225	0.69	0.7073

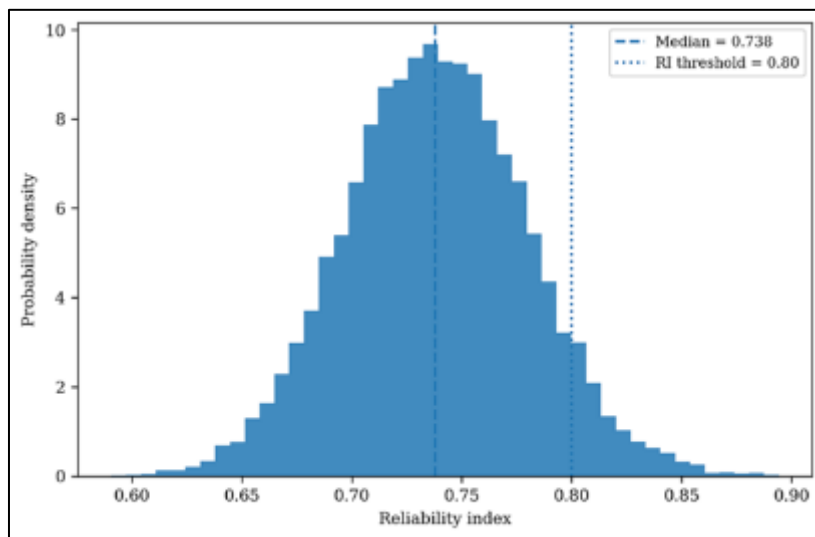
Together with the broad spectral response in Fig. 2, these tests support reporting 220–235 nm as the model-predicted thickness region for the stated parameter set. Within that region, small thickness changes influence the objective less than the unresolved mapping between p and a real coating. The thickness window is therefore the more numerically stable design output, whereas both its physical location and the recommended passivation strength require experimental identification.

Table 4: Selected simulated operating cases at 365 nm

Case	R (A W ⁻¹)	EQE (%)	D* (Jones)	I _{dark} (A)	PDCR	τ_r/τ_d (s)	RI
Clean	0.110	37.4	4.10×10^{13}	8.00×10^{-13}	1.65×10^7	0.127/0.298	1.000
Moderate	0.0918	31.2	3.14×10^{13}	9.69×10^{-13}	1.14×10^7	0.104/0.216	0.797
Harsh	0.049	16.8	8.66×10^{12}	3.97×10^{-12}	1.50×10^6	0.052/0.069	0.255
Harsh + optimized	0.074	25.2	1.78×10^{13}	2.05×10^{-12}	4.34×10^6	0.062/0.083	0.483

Under the harsh condition, the optimized design increases R from 0.0494 to 0.0741 A W⁻¹, reduces dark current from 3.97×10^{-12} to 2.05×10^{-12} A, and increases RI from 0.255 to 0.483. The protected response is deliberately slower than the unprotected harsh response because the model includes a barrier-induced surface-exchange penalty. The RI gain is therefore a comparative model result rather than evidence that the 0.80 screening criterion is achieved under the harsh state.

4.4 Monte Carlo Uncertainty and Global Sensitivity

**Figure 8: Monte Carlo distribution of RI for the optimized design under conditional input uncertainty**

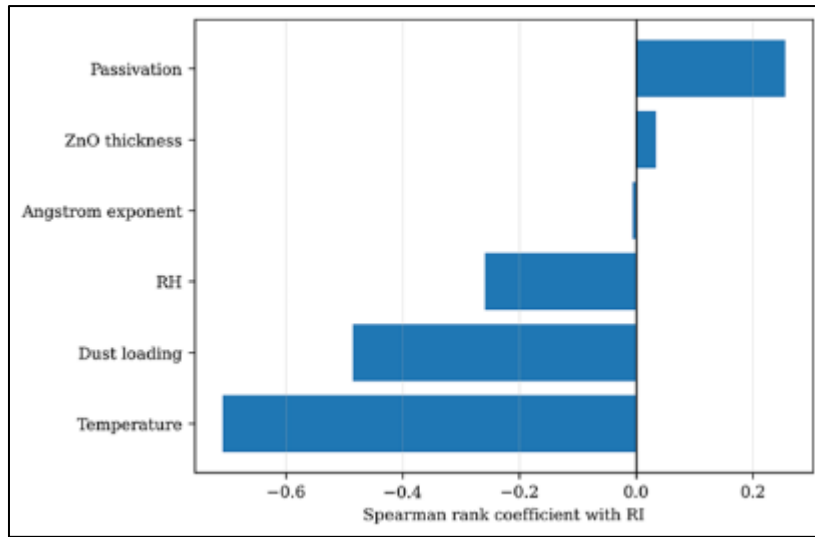


Figure 9: Spearman rank sensitivity coefficients for RI

At $N = 12,000$, RI has a median of 0.738 and a 5th–95th percentile interval of 0.671–0.806. Only 6.83% of the samples reach $RI \geq 0.80$. Temperature has the largest monotonic association with RI ($\rho = -0.708$), followed by dust loading ($\rho = -0.486$) and RH ($\rho = -0.259$). Because $\lambda = \lambda_0$ at 365 nm, γ has no direct effect on the single-wavelength result; its small sampled rank coefficient reflects finite-sample variation. The exponent would matter in a broadband calculation. Passivation is positively associated with RI, while thickness has little influence inside the broad optimum. The 6.83% figure is simply the fraction that crosses the chosen threshold for the stated truncated-normal inputs. It is not a reliability probability, since no chance constraint was imposed during optimization.

4.5 Numerical Verification and External Literature Context

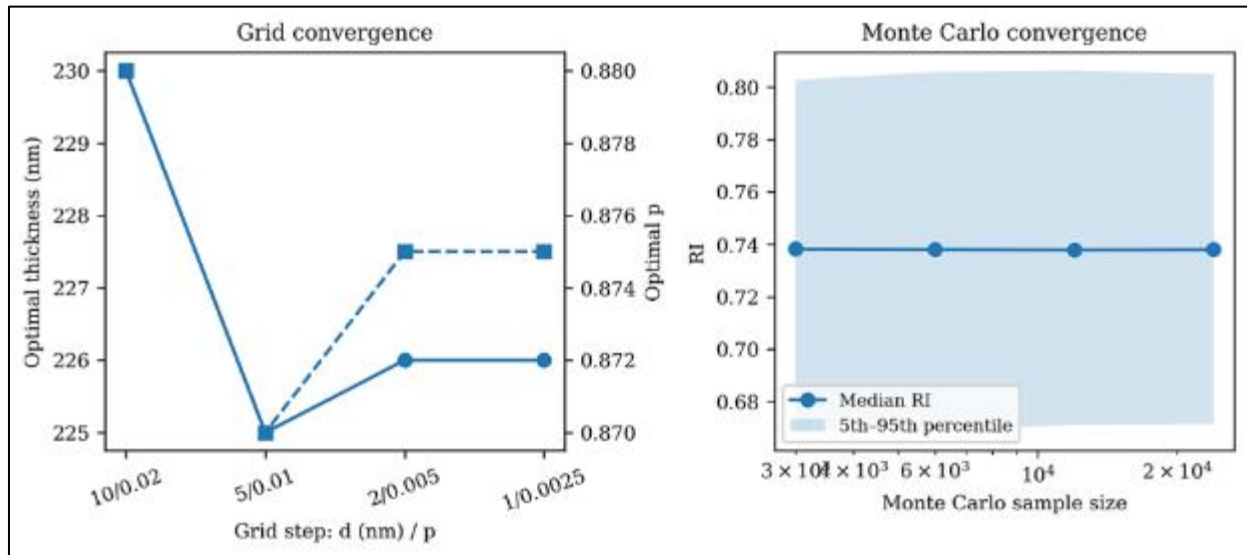


Figure 10: Grid-refinement and Monte Carlo sample-size convergence

Table 5: Numerical checks and comparison with the external clean-state scale

Verification item	Reference/target	Model result	Assessment
Analytic EQE identity	37.4150% from R	37.4150%	$<10^{-12}$ relative difference
Analytic PDCR identity	1.6522×10^7	1.6522×10^7	Machine-precision agreement
Analytic D* identity	4.1034×10^{13} Jones	4.1034×10^{13} Jones	Machine-precision agreement
External R benchmark [5]	0.110 A W^{-1}	0.11015 A W^{-1}	0.13% (calibration quantity)
External D* plausibility benchmark	3.5×10^{13} Jones	4.10×10^{13} Jones	17.2% difference; not forced
Grid-refinement check	230/0.88 226/0.875	→ J spread 0.057%	Converged
Monte Carlo sample-size check	N = 3000–24,000	Median spread 0.00033	Converged

Changing N from 3000 to 24,000 shifts the Monte Carlo median by 0.00033. Over the same range, the estimated share of samples above RI = 0.80 changes by 1.09 percentage points. That variation is expected for a small tail probability of about 6–7%. Quantitative comparison with Ref. [5] is limited to the matched conditions of zero bias and 365 nm illumination. Values reported for other ZnO, graphene/Si, oxide-heterojunction, and self-powered devices are used only to indicate scale [8–17, 25]. Their bias, irradiance, active area, geometry, and noise bandwidth differ too much for a common ranking plot to be meaningful.

Table 6: Literature values used for comparison and the purpose of each comparison

Study/device	Condition	Reported observation	Role in this study
Chen et al. [5], ZnO QD/Si	0 V, 365 nm	$R = 0.110 \text{ A W}^{-1}$; $D^* = 3.5 \times 10^{13}$ Jones	Direct scale benchmark
Song et al. [4], 90 nm ZnO/Si	2 V, 360 nm	$E_g = 3.258 \text{ eV}$; $R = 9 \text{ A W}^{-1}$; fast/slow kinetics	Band-edge and biased-gain context
Li et al. [2], ZnO nanowires	Variable RH	High RH lowers illuminated current; decay changes 2–3 orders	Humidity direction and kinetics
Hassan et al. [26], ZnO NR/p-Si	0 V, 395 nm	Rise/recovery = 25/22 ms; sensitivity 8000%	Fast-junction lower-bound context
Chen et al. [20], Al ₂ O ₃ -modified NiO/ZnO	0 V, 380 nm	$R = 1.4 \text{ mA W}^{-1}$; response < 0.04 s	Interface-defect passivation precedent
Postica et al. [21], SiO ₂ /ZnO	Humidity/aging tests	Reduced humidity effect and improved stability	10–20 nm SiO ₂ humidity-barrier precedent

5 PRACTICAL IMPLICATIONS AND VALIDATION

5.1 Engineering Interpretation

The calculations can inform three decisions before fabrication: which ZnO thicknesses deserve priority, whether a protective surface treatment is worth testing, and when cleaning or recalibration may be needed. After calibration on a real device, the RI boundary could also be used as a warning level if temperature, RH, and a suitable soiling proxy are monitored. Such a warning would be specific to that detector. It should not be reported as a certified lifetime or as a probability of failure.

5.2 Limitations and Scope of Validity

The calculation intentionally uses a reduced-order formulation. Dust attenuation is represented by an empirical Ångström law rather than a particle-resolved scattering model, while carrier collection is described by a Gaussian

function rather than a drift–diffusion model. The current formulation also neglects dust composition, irregular particle shapes, electrostatic adhesion, condensation, contact resistance, spatial nonuniformity, and defect formation during long-term operation.

Several additional limitations affect the interpretation of the results. The model is calibrated only against the clean responsivity. The environmental coefficients are either assumed or inferred from qualitative trends in the literature and have not been fitted to measurements from this device. The detectivity calculation includes shot and Johnson noise but does not include measured $1/f$, generation–recombination, or instrumental noise over a specified bandwidth. Moreover, responsivity, D^* , and PDCR share common algebraic terms; consequently, their RI weights should not be interpreted as independent evidence. In the uncertainty analysis, the inputs are sampled independently from truncated normal distributions. The analysis therefore omits correlations among environmental variables, uncertainty in the model coefficients, and model-form uncertainty. Consequently, the reported 220–235 nm interval remains conditional on the selected absorption and collection coefficients. Similarly, the optimised value of p cannot be converted into a physical coating thickness without measurements for a specific coating material and device structure.

5.3 Experimental Validation Plan

A validation study should fabricate ZnO layers with thicknesses of approximately 180, 225, and 300 nm, together with bare controls and architecture-appropriate protective treatments. Candidate series could include an ultrathin ALD Al_2O_3 interface layer selected to avoid carrier blocking, a 10–20 nm SiO_2 overlayer, and a fabrication-appropriate PMMA treatment [18–21]. At least three independently fabricated devices should be tested per condition. Required measurements include spectral responsivity, reflectance/transmittance, dark current, noise spectral density at a declared bandwidth, rise and recovery times, contact angle, dust retention, and repeated switching over RH = 20–90% and T = 300–330 K. Coating-specific p_{exp} values should be calculated from Eqs. (12)–(15). Coefficients should be fitted on a predefined training subset and assessed blindly on withheld dust–humidity–temperature combinations. Current photodetector metrology guidance [22–24] should then be used to quantify drift and long-term stability under thermal–humidity cycling and accelerated ageing.

6 CONCLUSIONS

This work investigated the combined effects of dust, humidity, and temperature on a self-powered ZnO/Si ultraviolet photodetector. The model was calibrated only against the clean responsivity reported for a recent zero-bias device. The predicted detectivity was 17.2% higher than the reported value and was therefore used as a scale check rather than as a second calibration target. The analytical-identity, grid-refinement, and Monte Carlo sample-size tests produced numerically consistent results. The practical and refined grid searches selected ZnO thicknesses of 225 and 226 nm, respectively. For the assumed absorption and collection coefficients, these results support a conditional design interval of 220–235 nm. The selected thickness showed little sensitivity to changes in grid resolution and RI weights, whereas the optimal passivation index remained strongly dependent on the assumed coating-demand penalty. Under the harsh conditions, optimisation increased the RI from 0.255 to 0.483 and approximately doubled the detectivity relative to the unprotected case; however, the RI remained below the exploratory screening level of 0.80. The model is therefore most useful for selecting experiments and screening candidate designs before fabrication. Measurements on fabricated devices are required to establish the thickness interval, determine the environmental coefficients, characterise the complete noise spectrum, assess model-form error, and relate p to a physical coating.

STATEMENTS ON COMPLIANCE WITH ETHICAL STANDARDS

Data and code availability

The numerical data, coefficient definitions, random seed, and MATLAB code may be requested from the corresponding author.

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