

Well-width Compensation of the Polarization Field in Polar ZnO/MgZnO Triple-Barrier Resonant Tunneling Diodes Benchmarked Against GaN/AlN

Osama Bagi Aljewaw^{1,2}, Sulayman Mohamad Kabeer¹, Mohd Mustafa Awang Kechik¹, Mohd Hafiz Mohd Zaid¹, Izdihar Kamal¹, Muhammad Khalis Abdul Karim^{1,*}

¹*Department of Physics, Faculty of Science, Universiti Putra Malaysia, 43400 UPM Serdang Selangor, Malaysia*

²*Libyan Authority for Scientific Research, National Nanoscience and Nanotechnology Project, P.O. Box 30313, Tripoli - Libya*

**Corresponding author (email: mkhalis@upm.edu.my)*

*(Received: 1 September 2026 / Revised: 8 October 2026 / Accepted: 12 October 2026 /
Published online: 14 October 2026)*

© The Author(s) 2026. This article is licensed under a Creative Commons Attribution 4.0 International License (CC BY 4.0)

ABSTRACT

Built-in polarization fields tilt the barriers of polar resonant tunneling structures and detune the coupled wells of triple barriers. We modeled GaN/AlN and ZnO/Mg_{0.2}Zn_{0.8}O double and triple barriers using scattering-matrix transmission, polarization electrostatics with contact accumulation and depletion, injection from the emitter two-dimensional electron gas (2DEG) and area-conserving dephasing. For measured Ga-polar GaN/AlN diodes, the model reproduces the reverse level shift and collector barrier within 9% but overestimates the forward level shift by 36%. Without 2DEG injection the current is about 300 times too low; with it, a barrier one AlN monolayer thinner than nominal brings the model close to the measured peak current and a 10 fs dephasing time reproduces the measured peak-to-valley current ratio (PVCR). In polar ZnO/MgZnO triple barriers the well offset vanishes at zero bias for a 1.5 nm middle barrier or a second well widened from 3 to 3.82 nm, but that width aligns the wells only where almost no current flows. To place the first negative differential resistance (NDR) between 0.05 and 0.15 V, the polar second well must be 0.94–1.02 nm wider than the non-polar one at the sourced polarization contrast, a shift that grows by 0.066–0.077 nm per mC m⁻² of contrast and barely changes between dephasing times of 33 and 10 fs. Strong dephasing lowers the PVCR of the polar triple barrier to 1.3–1.9, against 5.8–8.0 for the non-polar reference, so interface quality likely limits polar triple barriers more than non-polar ones.

Keywords: resonant tunneling, polarization, GaN/AlN, ZnO/MgZnO, triple barrier

INTRODUCTION

Resonant tunneling diodes pass current through the quasi-bound states of a quantum well. Tsu and Esaki derived the current from the transmission through a finite superlattice and Chang, Esaki and Tsu observed resonant tunneling in GaAs/GaAlAs double barriers [1,2]. Nitride diodes took longer to establish, because early AlN/GaN double-barrier reports raised doubts over whether the negative differential resistance (NDR) came from resonant tunneling or from traps; repeatable NDR at room temperature was later reported in AlN/GaN and GaN/AlN diodes grown by molecular beam epitaxy [3]. Peak current densities have since risen above 1500 kA cm^{-2} and GaN/AlN triple-barrier diodes with electrically tunable oscillations have been demonstrated [4,5].

Wurtzite nitrides carry large spontaneous and piezoelectric polarization and the discontinuity at Al(In)GaN/GaN interfaces produces sheet charges and built-in fields that shift the transmission peaks, make nominally symmetric structures respond differently to forward and reverse bias and can be screened by heavily doped contacts [6,7]. Measured peak-to-valley current ratios (PVCRs) remain low, for example 1.20–1.60 and 1.23 in two recent high-current diodes [8,9]. Designs that counter the field in double barriers use asymmetric barriers, barrier-width modulation, polarization-matched AlInN/GaN or AlGaInN/AlInN layers, or cubic non-polar layers [10,11].

A triple barrier contains two wells whose ground states couple through the middle barrier and in a polar structure the field shifts them to different energies, so the coupled-well resonance splits and loses its unit peak transmission. Rong et al. simulated AlGaIn/GaN triple barriers with unequal wells (2 and 3.2 nm) and showed that narrowing the second well from 3.4 to 2.5 nm raises the peak voltage and can remove the second NDR region [12]. Encomendero et al. have now measured GaN/AlN triple-barrier diodes with 2 nm AlN barriers [5]. The width study of Rong et al. contains no non-polar reference, so it does not show how much of the width change compensates the polarization field; we have not found a study that separates this part, at zero bias or at the operating bias [12].

ZnO/MgZnO shares the wurtzite structure of GaN/AlN but has a much weaker polarization contrast, which makes it a useful second system for seeing how the effects scale with the field. The one experimental ZnO/MgZnO resonant tunneling device we know of was grown on c-plane sapphire and showed NDR at room temperature, recent ZnO simulations treat non-polar m-plane double and triple barriers and polar c-plane ZnO/MgZnO triple barriers have received little attention [13,14].

Here we model polar GaN/AlN and ZnO/Mg_{0.2}Zn_{0.8}O double and triple barriers with polarization electrostatics that include contact accumulation and depletion, scattering-matrix transmission on an adaptive energy grid, injection from the emitter two-dimensional electron gas (2DEG) and area-conserving dephasing. We first test the model against measured GaN/AlN double barriers, then use ZnO/MgZnO, whose weaker field leaves resonances with appreciable transmission at zero bias, to derive width rules for polar triple barriers at zero bias and at the operating bias and to find how dephasing changes their NDR [7].

MATERIALS AND METHODS

Structures

We model conduction-band electrons in GaN/AlN and ZnO/Mg_{0.2}Zn_{0.8}O double barriers (barrier/well/barrier = 2/3/2 nm) and triple barriers (2/3/2/3/2 nm), each placed between 2 nm undoped spacers and n-type contacts doped at $N_D = 10^{19} \text{ cm}^{-3}$, at $T = 300 \text{ K}$. Figure 1 shows the two GaN/AlN stacks. For GaN/AlN we also compute contacts doped at 10^{20} cm^{-3} . The 2 nm barriers match the AlN barriers of the GaN/AlN triple-barrier diodes of Encomendero et al. [5]. The Mg content $x = 0.2$ matches the ZnO/Zn_{0.8}Mg_{0.2}O resonant tunneling device of Krishnamoorthy et al. [13]. "Polar" denotes metal-face c-plane growth with the built-in polarization field; the "non-polar" reference keeps the same band offsets and masses but sets the polarization to zero. Positive bias lowers the collector, which lies on the metal-face side of the stack.

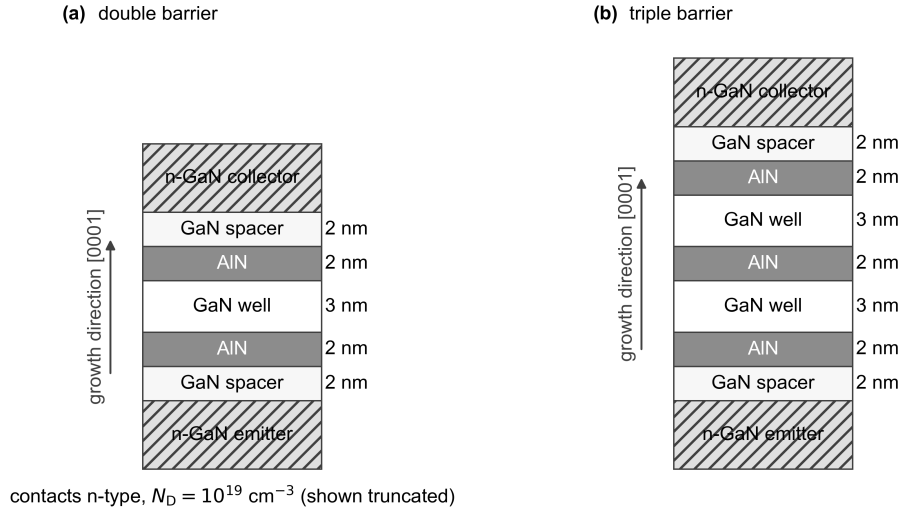


Figure 1. Cross-sections of the GaN/AlN structures. Layer stacks of the two GaN/AlN structures: (a) the double barrier (AlN/GaN/AlN = 2/3/2 nm) and (b) the triple barrier (2/3/2/3/2 nm). Each stack lies between 2 nm undoped GaN spacers and n-type GaN contacts doped at $N_D = 10^{19} \text{ cm}^{-3}$, drawn truncated. Growth is along [0001] (metal-face c-plane), with the emitter at the bottom and the collector at the top. Layer thicknesses are to scale. The ZnO/Mg_{0.2}Zn_{0.8}O structures use the same geometry with ZnO wells and Mg_{0.2}Zn_{0.8}O barriers

Material parameters

Table 1 lists the parameters. For GaN/AlN, only the polarization contrast ΔP between AlN and GaN enters the model, because the wells, spacers and contacts are all GaN. We set $\Delta P = 0.089 \text{ C m}^{-2}$ so that a pseudomorphic AlN barrier between flat GaN layers carries $F_\pi = \Delta P / (\epsilon_0 \epsilon_{\text{AlN}}) = 11 \text{ MV cm}^{-1}$, the barrier field extracted from measured reverse threshold voltages [7]. The polarization constants of Ambacher et al. give 11.9–14.4 MV cm⁻¹, depending on the permittivities and overshoot the measured thresholds [6]. Dreyer et al. likewise report that predicted AlGaIn/GaN sheet charges exceed most measured values [15]. For ZnO/Mg_{0.2}Zn_{0.8}O we take the spontaneous polarization $P_{\text{sp}} = -(0.057 + 0.066x) \text{ C m}^{-2}$ and neglect the piezoelectric term of the strained barrier, which

gives $\Delta P = 13.2 \text{ mC m}^{-2}$ at $x = 0.2$ [16]. Because this contrast is uncertain, we vary it from 0 to 1.5 times this value.

Table 1. Material parameters, with the source of each value in the last column. The parameters listed in the *Limitation* section still need checking against the primary source

Quantity	GaN/AlN	ZnO/Mg _{0.2} Zn _{0.8} O	Ref
Electron mass m^*/m_0 (well / barrier)	0.20 / 0.32	0.28 / 0.28	[17,23]
Static permittivity ϵ_r along c (well/barrier)	10.4 / 9.14	8.1 / 8.1	[24]
Conduction-band offset ΔE_c (eV)	1.75	0.3375	[17]
Polarization contrast ΔP (C m ⁻²)	0.089 (calibrated)	0.0132	[7,16]
Fermi level above band edge at $N_D = 10^{19} \text{ cm}^{-3}$ (meV)	77.1	49.3	
Screening length λ at $N_D = 10^{19} \text{ cm}^{-3}$ (nm)	1.89	1.48	

The ZnO/MgZnO offset follows $\Delta E_c = 0.675\Delta E_g$ with $\Delta E_g = 25 \text{ meV}$ per % Mg and the mass is the ZnO value used for both layers [17].

Polarization electrostatics

The barriers and wells hold no free charge, so the displacement is the same in every layer of the stack and equals its value in the well material next to the stack, where the field is F_s :

$$\epsilon_0 \epsilon_i F_i + P_i = \epsilon_0 \epsilon_w F_s + P_w \quad \Rightarrow \quad F_i = \frac{\epsilon_0 \epsilon_w F_s + P_w - P_i}{\epsilon_0 \epsilon_i}, \quad (1)$$

where F_i , P_i , ϵ_i and L_i are the field along the growth direction z , the polarization, the permittivity and the thickness of layer i , so that the electron potential energy rises by $eF_i L_i$ across the layer. The emitter side of the stack must then hold the areal charge $\sigma = \epsilon_0 \epsilon_w F_s$ and the collector side $-\sigma$, outside the stack. A side that must hold negative charge accumulates electrons against the outer barrier over a Thomas–Fermi screening length λ ; a side that must hold positive charge depletes its donors over a width $W = \epsilon_0 \epsilon_w |F_s| / (eN_D)$ beyond the undoped spacer. We solve for F_s with Brent's method so that the potential-energy drop across both sides and the stack equals the applied bias; equations (A1) to (A4) of the supplementary material give the contact Fermi level, the screening length and the two contact profiles. This is not a self-consistent Schrödinger–Poisson solution: quantization of the accumulation layer and charge stored in the wells do not feed back into the potential.

Transmission

We solve the one-dimensional effective-mass Schrödinger equation with the BenDaniel–Duke interface conditions (ψ and ψ'/m^* continuous), equation (A5) [18]. The potential is divided into constant slabs, following the multistep method of Ando and Itoh: 0.05 nm inside the stack for spectra and 0.1 nm for currents, with slabs twice as thick in the spacers and contact regions for currents [19]. The slabs are combined with a scattering-matrix (Redheffer star product) recursion instead of a product of transfer matrices, which loses precision through thick or high barriers; equations (A6) to

(A8) give the solution in a slab, the interface amplitudes and the recursion. The transmission probability is

$$T(E) = \frac{\text{Re}(k_R/m_R)}{\text{Re}(k_L/m_L)} |t|^2, \quad (2)$$

where t is the transmitted amplitude of the whole structure and k_L , k_R and m_L , m_R are the wavevectors and masses in the two leads.

Resolving narrow resonances

Resonances in the polar structures can be narrower than 10^{-11} eV, far below any practical uniform energy step. We therefore evaluate $T(E)$ on a uniform grid (step 0.5 meV for currents; 0.5 meV for GaN/AlN and 0.1 meV for ZnO/MgZnO spectra) and refine it in up to four passes. Each pass locates the local maxima, zooms onto each one with 21-point windows that shrink fourfold until the whole window lies on the flat top of the peak (relative variation below 10^{-9}), measures the full width at half maximum Γ and adds a cluster of points: a tangent-mapped core, $E = E_p \pm (\Gamma/2)\tan(u)$ with $0 < u \leq \arctan 20$, which reaches 10Γ from the peak position E_p and logarithmically spaced tails. Peaks closer than 5% of a known width to an existing resonance are merged.

Current density

The bulk-emitter current follows the Tsu–Esaki formula with transverse momentum conserved and the emitter mass in the supply function [1],

$$J_{3D} = \frac{em^*k_B T}{2\pi^2\hbar^3} \int_{E_{\min}}^{E_{\max}} T(E) \ln \frac{1 + e^{(E_F - E)/k_B T}}{1 + e^{(E_F - eV - E)/k_B T}} dE, \quad (3)$$

evaluated with the trapezoidal rule on the adaptive grid from the higher of the two lead band edges, $E_{\min} = \max(0, -eV)$, to $E_{\max} = \max(E_F, E_F - eV) + 15k_B T$. Here E is measured from the emitter band edge and E_F is the contact Fermi level of equation (1).

When a contact is in accumulation, its electrons also occupy quantized subbands E_n below the bulk band edge, which the bulk channel does not count. We find these subbands with a finite-difference BenDaniel–Duke eigensolver, take the areal density of each one from Fermi–Dirac statistics and let its electrons escape through the stack at a rate set by the amplitude of the bound state at the barrier and the transmission at that energy; equations (A9) to (A12) give the eigenproblem, the density, the escape rate and the resulting current. The total current is $J = J_{3D} + J_{2D}$.

Dephasing

Coherent transmission overestimates the height and underestimates the width of each resonance [20]. Following Stone and Lee, we keep the area $A_r = (\pi/2)T_r\Gamma_r$ of every resolved resonance r , with peak transmission T_r , width Γ_r and position E_r and widen it to $\Gamma'_r = \Gamma_r + \Gamma_\phi$ with $\Gamma_\phi = \hbar/\tau_\phi$, leaving the non-resonant background unchanged [20].

$$T_\phi(E) = T(E) + \sum_r A_r w\left(\frac{E - E_r}{\Gamma'_r}\right) \left[\frac{L(E - E_r; \Gamma'_r)}{\mathcal{N}} - L(E - E_r; \Gamma_r) \right], \quad (4)$$

where L is a Lorentzian and w a window that is flat to 3 and falls to zero at 5 broadened widths of area $N = 0.920$; equation (A13) gives both and T_ϕ is set to zero wherever it would be negative. We use $\tau_\phi = 33$ fs ($\Gamma_\phi = 19.9$ meV) and 10 fs ($\Gamma_\phi = 65.8$ meV), the

phonon-limited and interface-roughness-limited dephasing times quoted by Encomendero et al.; unless stated otherwise, results use 33 fs [7].

Scans and peak detection

We compute the J - V characteristics from -10 to 10 V in 25-mV steps for GaN/AlN and from -1 to 1 V in 4-mV steps for ZnO/MgZnO. A current peak is a local maximum; its valley is the lowest current before the current next exceeds the peak and the peak-to-valley current ratio (PVCR) is their ratio. For the operating-bias scan of the ZnO/MgZnO triple barrier we vary the second-well width w_2 from 1.5 to 5.5 nm in 0.1 nm steps at $w_1 = 3$ nm and compute the forward current from 0 to 0.6 V in 4-mV steps; for GaN/AlN with 10^{20} cm $^{-3}$ contacts we vary w_2 over 6–18 GaN monolayers (0.259 nm each) from 0 to 4 V in 20-mV steps. The "first NDR" is the lowest-bias peak with $J \geq 10^2$ A cm $^{-2}$ and $PVCR \geq 1.2$. We follow it as w_2 grows until it reaches zero bias, which happens at the zero-bias optimum w_2^* for the polar structure and at $w_2 = w_1$ for the non-polar one; a 10 fs point counts as the same resonance when it lies within 30 mV of the 33 fs position. Widths quoted at a chosen bias are interpolated: for each structure we interpolate the first-NDR bias linearly against w_2 and read off the width at that bias, which is why those widths carry more decimal places than the 0.1 nm scan grid.

The doublet splitting scan varies the middle-barrier thickness b_2 over 1–10 AlN monolayers (0.249 nm each) for GaN/AlN and from 0.5 to 5.0 nm in 0.25 nm steps for ZnO/MgZnO, stopping the polar ZnO/MgZnO scan at 3.5 nm. The zero-bias compensation map varies w_2 from 2.0 to 5.5 nm in 0.025 nm steps on an energy grid of 2001 points up to 0.2 eV; the sensitivity scan scales ΔP by 0 to 1.5 in steps of 0.25 and varies w_2 from 2.0 to 6.5 nm in 0.02 nm steps. To test the operating-bias rule against the uncertain contrast, we repeated the operating-bias scan of the polar ZnO/MgZnO triple barrier with ΔP scaled by 0.5, 0.75, 1, 1.25 and 1.5, at both dephasing times and ended each first-NDR family at the width where its bias is lowest.

Numerical checks

Ten checks pass; Table 2 groups them in eight rows, because the two symmetric-peak checks share a row and so do the two escape-rate checks. The code runs in Python 3.13.5 with NumPy 2.3.4 and SciPy 1.16.3 on 15 worker processes.

Table 2. Numerical checks

Check	Result
Single barrier with mass step versus analytic transmission	maximum relative error 3.6×10^{-15}
Current conservation $T + R = 1$, polar GaN/AlN triple barrier at 1 V	maximum deviation 1.1×10^{-12}
Symmetric non-polar double-barrier peaks (GaN/AlN, ZnO/MgZnO)	$T = 1$ at 0.12797 and 0.07180 eV
Slab-size convergence, polar GaN/AlN double barrier at 2 V	resonance shifts 0.01 meV between 0.05 and 0.025 nm
Current at zero bias	$J(0) = 0$
Fermi level at $T \rightarrow 0$ versus degenerate formula	0.08463 eV in both
$2\hbar\nu$ (escape through one barrier) versus exact resonance width	0.1% (GaN/AlN), 1.0% (ZnO/MgZnO)
Dephasing broadening: area and locality	area changes by 0.38%; transmission unchanged beyond 5 widths

Benchmark devices

For the benchmark we model the Ga-polar GaN/AlN double barriers of Encomendero et al.: a 3 nm GaN well between AlN barriers of $t_b = 1.5, 2.0$ and 2.4 nm, with 10 nm emitter and 6 nm collector spacers and contacts doped at $2 \times 10^{19} \text{ cm}^{-3}$ [7]. We compare four parameter sets: the Ambacher et al. polarization contrast (0.1085 C m⁻²) with permittivities 8.9/8.5 and 10.4/9.14 (GaN/AlN), a sheet charge of $6.5 \times 10^{13} \text{ cm}^{-2}$ with 10.4/9.14 and the calibrated set of table 1 [6]. The reverse threshold is $V_{\text{th}} = 2t_b F_\pi$ in this electrostatic model [7]. We obtain the forward and reverse level shifts γ_F and γ_R from linear fits to the bias dependence of the finite-difference well ground state E_0 , equation (A14). For comparison with the measured peak, we remove the series-resistance drop $J\rho_s = 0.77 \text{ V}$ quoted for the 1.5 nm device [7].

RESULTS AND DISCUSSION

Zero-bias band profiles and spectra

Polarization turns the flat barriers of the non-polar reference into steep ramps (Figure 2). In the polar GaN/AlN double barrier the field is 8.3 MV cm^{-1} in the AlN barriers and -2.4 MV cm^{-1} in the GaN well; the barrier carries less than the $F_\pi = 11 \text{ MV cm}^{-1}$ because that value applies to an AlN barrier between field-free GaN, whereas here the wells and spacers themselves carry -2.4 MV cm^{-1} (Eq. (1)). Electrons accumulate against the first barrier, where the band edge falls 0.45 eV below the emitter band edge and a 13.8 nm depletion region forms beyond the collector spacer, with a 2.1 eV potential hump. The triple barrier behaves the same way, with 7.9 and -2.7 MV cm^{-1} , a 0.51 eV accumulation well and a 15.5 nm, 2.6 eV collector hump. In ZnO/Mg_{0.2}Zn_{0.8}O the fields are about seven times weaker: 1.22 MV cm^{-1} in the barriers and -0.62 MV cm^{-1} in the well of the double barrier, with a 0.092 eV accumulation well and a 2.8 nm, 0.21 eV collector hump. The ZnO/MgZnO triple barrier gives 1.19 and -0.65 MV cm^{-1} and a 0.23 eV hump.

The non-polar structures show resonances with $T = 1$ (Figure 3): at 0.128, 0.512 and 1.138 eV in the GaN/AlN double barrier, at 71.8 meV in the ZnO/MgZnO double barrier and as a doublet at 69.6 and 74.1 meV in the ZnO/MgZnO triple barrier. In polar GaN/AlN the largest resonant transmission at zero bias is 5.6×10^{-6} for the double barrier (at 1.37 eV) and 1.2×10^{-2} for the triple barrier (at 1.50 eV), where the resonance is only $2.9 \times 10^{-12} \text{ eV}$ wide. The tilted barriers and the collector hump cause this loss. In polar ZnO/MgZnO the double-barrier resonance moves from 71.8 to 121.8 meV and its peak falls to $T = 0.51$. The triple-barrier doublet splits into a weak peak ($T = 2.5 \times 10^{-4}$ at 105 meV) and a stronger one ($T = 0.10$ at 147 meV), because the field shifts the two wells against each other.

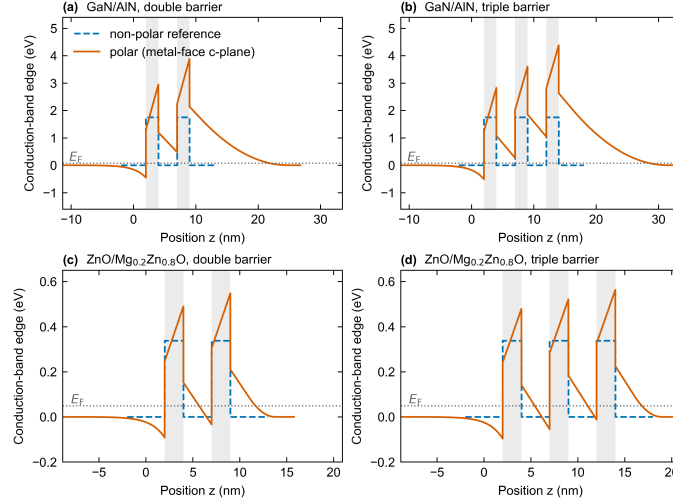


Figure 2. Conduction-band profiles at zero bias. Conduction-band edge of (a) GaN/AlN double barrier, (b) GaN/AlN triple barrier, (c) ZnO/Mg_{0.2}Zn_{0.8}O double barrier and (d) ZnO/Mg_{0.2}Zn_{0.8}O triple barrier at $V = 0$, for the polar structure (solid) and the non-polar reference (dashed). Grey bands mark the barrier layers. The dotted line is the emitter Fermi level E_F . In polar GaN/AlN the field is 8.3 MV cm^{-1} in the AlN barriers and -2.4 MV cm^{-1} in the GaN wells (double barrier). Electrons accumulate against the first barrier (band edge 0.45 eV below $E = 0$) and a $14\text{--}16 \text{ nm}$ depletion region forms beyond the collector spacer, raising the collector band edge by $2.1\text{--}2.6 \text{ eV}$. In ZnO/MgZnO the fields are about seven times weaker (1.2 MV cm^{-1} in the barriers) and the collector depletion region is 2.8 nm wide

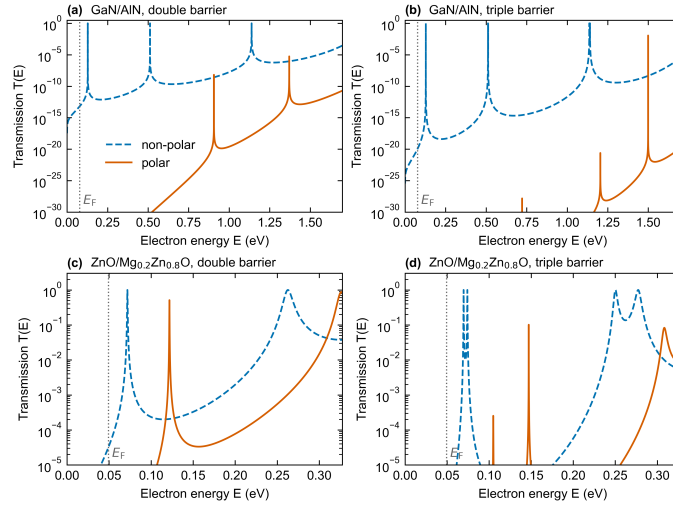


Figure 3. Transmission spectra at zero bias. Transmission probability $T(E)$ at $V = 0$ for the four structures of figure (log scale; values below the axis minimum are not shown). Non-polar structures show resonances with $T = 1$: single peaks in the double barrier (GaN/AlN at 0.128 , 0.512 and 1.138 eV ; ZnO/MgZnO at 71.8 meV) and doublets in the triple barrier (ZnO/MgZnO at 69.6 and 74.1 meV). In polar GaN/AlN the largest resonant transmission falls to 6×10^{-6} (double barrier, 1.37 eV) and 1×10^{-2} (triple barrier, 1.50 eV , a resonance only $3 \times 10^{-12} \text{ eV}$ wide) because of barrier tilt and the collector depletion barrier. In polar ZnO/MgZnO the double-barrier resonance moves from 71.8 to 121.8 meV and its peak drops to $T = 0.51$. The triple-barrier doublet splits into a weak peak ($T = 2.5 \times 10^{-4}$ at 105 meV) and a stronger one ($T = 0.10$ at 147 meV), because the field offsets the two wells. The energy grid is refined around every resonance, so peak heights are resolved; the narrowest resonances appear as vertical lines

Coupled-well doublet

In the non-polar triple barriers, the doublet splitting decays exponentially with the middle-barrier thickness b_2 (Figure 4): from 42.1 meV at one AlN monolayer to 0.0105 meV at ten, a factor of 2.5 per monolayer and in ZnO/MgZnO from 36.2 meV at 0.5 nm to 0.50 meV at 3.5 nm. In polar ZnO/MgZnO the splitting passes through a minimum of 8.1 meV at $b_2 = 1.5$ nm, close to the non-polar 9.0 meV. In our electrostatic model the offset Δ between the centres of the two wells is the sum of the potential drops across the middle barrier and across half of each well, equation (A15); at $b_2 = 1.5$ nm the two terms nearly cancel and $\Delta = -2.3$ meV. Away from the minimum the splitting follows the two-level estimate $\sqrt{(\Delta^2 + S_0^2)}$, equation (A16), with S_0 the non-polar splitting: at $b_2 = 2.0$ nm the estimate gives 42.3 meV against the calculated 42.2 meV. At the minimum the calculated splitting (8.1 meV) lies below the estimate (9.3 meV). The lower doublet peak of the polar structure falls to $T = 4.1 \times 10^{-8}$ at $b_2 = 3.0$ nm and beyond 3.0 nm the doublet can no longer be resolved.

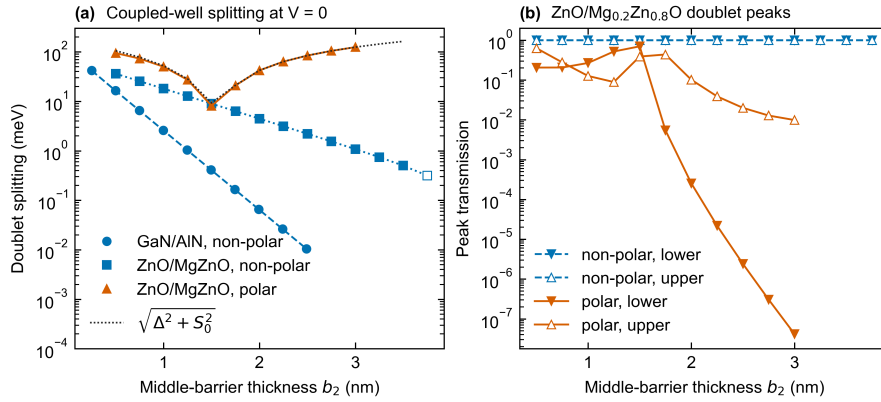


Figure 4. Coupled-well doublet versus middle-barrier thickness. (a) Splitting of the lowest triple-barrier doublet at $V = 0$ versus middle-barrier thickness b_2 (outer barriers 2 nm, wells 3 nm). GaN/AlN points are integer AlN monolayers (1–10 ML, 0.249 nm each). Open symbols: splitting smaller than the peak width (unresolved). Non-polar splitting decays exponentially, by a factor of about 2.5 per AlN monolayer (42 meV at 1 ML to 0.010 meV at 10 ML) and from 36 meV to 0.50 meV between 0.5 and 3.5 nm in ZnO/MgZnO. The polar ZnO/MgZnO splitting passes through a minimum at $b_2 = 1.5$ nm, where the electrostatic offset between the two wells crosses zero (-2.3 meV). There the splitting (8.1 meV) is close to the non-polar value (9.0 meV). The dotted line is the two-level estimate $\sqrt{\Delta^2 + S_0^2}$, with Δ the calculated well offset and S_0 the non-polar splitting. (b) Peak transmission of the two doublet peaks in ZnO/MgZnO. Both peaks stay at $T = 1$ in the non-polar case. In the polar case the lower peak falls to 4×10^{-8} at $b_2 = 3.0$ nm; beyond 3.0 nm it drops below $T = 10^{-10}$ and the doublet is no longer defined.

Well-width compensation at zero bias

With the reference 2 nm middle barrier, a wider second well can cancel the field-induced offset between the wells (Figure 5). In the polar ZnO/MgZnO triple barrier with $w_1 = 3$ nm, the two well states anticross at $w_2^* = 3.82$ nm rather than at $w_2 = w_1$. At $w_2 = 3$ nm the doublet peaks reach only $T = 2.5 \times 10^{-4}$ and 0.10. At w_2^* the weaker peak

reaches 0.34; close to w_2^* each peak in turn recovers to $T \approx 1$. w_2^* rises from 3.00 nm without polarization to 4.18 nm at 1.5 times the sourced contrast ($\Delta P = 19.8 \text{ mC m}^{-2}$), about 0.06 nm per mC m^{-2} of contrast; this zero-bias slope is smaller than the 0.066–0.077 nm per mC m^{-2} of the operating-bias width shift, which is a different quantity. At the sourced $\Delta P = 13.2 \text{ mC m}^{-2}$, $w_2^* = 3.82 \text{ nm}$. This width aligns the wells only near zero bias: its first current peak lies at 8 mV and carries $2.0 \times 10^2 \text{ A cm}^{-2}$.

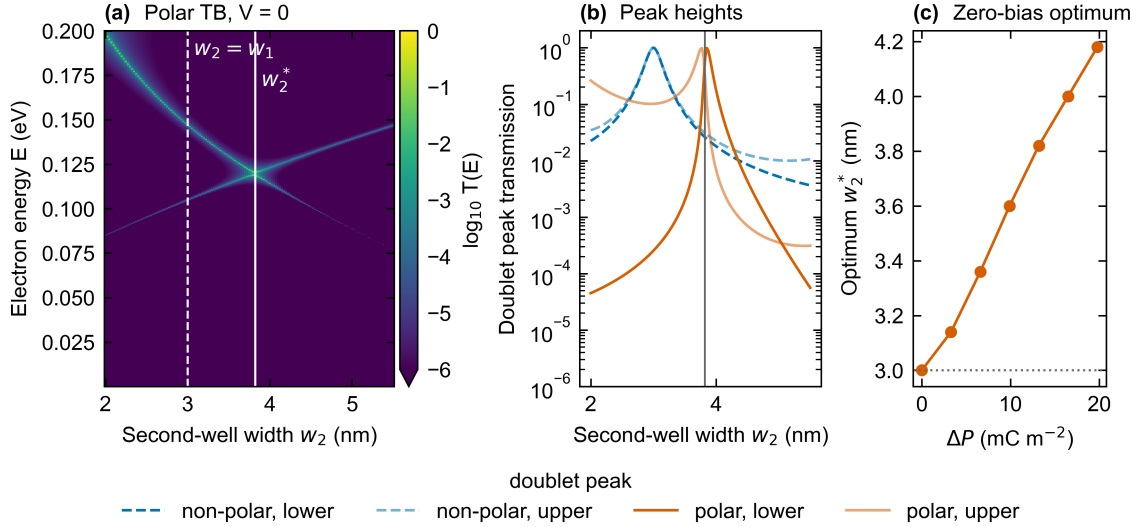


Figure 5. Restoring the triple-barrier resonance by well-width compensation (ZnO/Mg_{0.2}Zn_{0.8}O). (a) $\log_{10} T(E)$ at $V = 0$ for the polar triple barrier as the second-well width w_2 varies ($w_1 = 3 \text{ nm}$, all barriers 2 nm ; color scale clipped at 10^{-6}). The well-1 state (rising line) and the well-2 state (falling line) anticross at $w_2^* = 3.82 \text{ nm}$ (solid white line), not at $w_2 = w_1$ (dashed). (b) Peak transmission of the two doublet peaks versus w_2 . Non-polar (dashed): both peaks reach $T = 1$ at $w_2 = 3 \text{ nm}$. Polar (solid): at $w_2 = 3 \text{ nm}$ the peaks reach only 2.5×10^{-4} and 0.10 . Close to w_2^* each peak in turn recovers to $T \approx 1$; at the anticrossing itself the weaker of the two is 0.34, because the tilted barriers have unequal transparencies. (c) Optimum w_2^* versus the MgZnO/ZnO polarization contrast ΔP : w_2^* rises from 3.00 nm ($\Delta P = 0$) to 4.18 nm ($\Delta P = 19.8 \text{ mC m}^{-2}$), about $0.06 \text{ nm per mC m}^{-2}$. The sourced contrast for $x = 0.2$ is $\Delta P = 13.2 \text{ mC m}^{-2}$, giving $w_2^* = 3.82 \text{ nm}$

Current–voltage characteristics

Polar GaN/AlN structures conduct almost nothing below a threshold set by the collector hump (Figure 6). With 10^{19} cm^{-3} contacts the polar double barrier shows forward NDR peaks at 6.1 V (49 A cm^{-2} , PVCR 22) and 8.5 V ($2.0 \times 10^3 \text{ A cm}^{-2}$). With 10^{20} cm^{-3} contacts the first strong peak moves to 2.35 V ($4.1 \times 10^2 \text{ A cm}^{-2}$), followed by a peak at 4.75 V ($4.1 \times 10^4 \text{ A cm}^{-2}$, PVCR 8.0).

Polarization makes the ZnO/MgZnO double barrier strongly asymmetric. The polar structure peaks at $1.9 \times 10^5 \text{ A cm}^{-2}$ at $+0.34 \text{ V}$ (PVCR 7.3) and at $5.0 \times 10^3 \text{ A cm}^{-2}$ at -0.16 V (PVCR 1.5), a 39-fold difference. The non-polar reference peaks symmetrically at $\pm 0.12 \text{ V}$ with $7.6 \times 10^4 \text{ A cm}^{-2}$ and PVCR 6.5. The polar triple barrier peaks at 0.16 V with $2.4 \times 10^4 \text{ A cm}^{-2}$ and PVCR 6.8.

Stronger dephasing ($\tau_\phi = 10$ fs) leaves the peak positions nearly unchanged but lowers the PVCR: to 1.6 for the polar ZnO/MgZnO triple barrier, to 3.8 for the GaN/AlN double barrier at 2.35 V (10^{20} cm $^{-3}$) and to 1.2 for the forward peak of the polar ZnO/MgZnO double barrier.

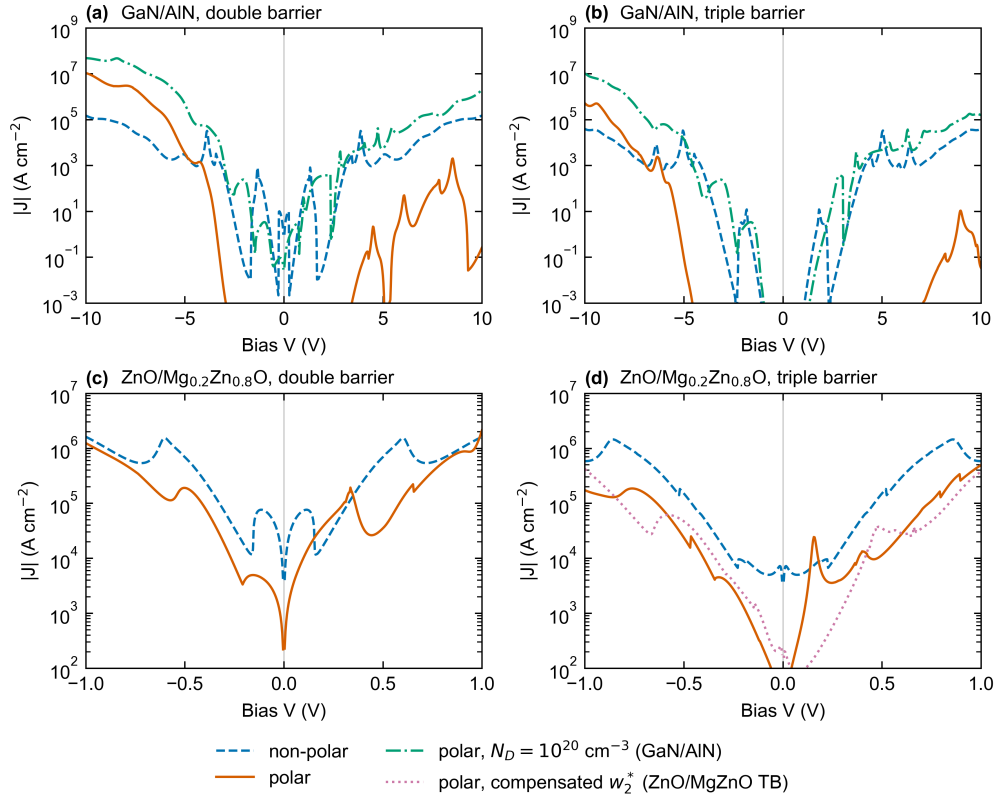


Figure 6. Current-voltage characteristics. Current density $|J|$ at 300 K versus bias (log scale; values below the axis minimum are not shown), summing the bulk-emitter and emitter-2DEG channels with resonances broadened by $\hbar/\tau_\phi$, $\tau_\phi = 33$ fs. Positive bias lowers the collector (top, metal-face side). (a, b) GaN/AlN double and triple barriers: non-polar (dashed), polar with $N_D = 10^{19}$ cm $^{-3}$ (solid) and polar with $N_D = 10^{20}$ cm $^{-3}$ (dash-dot). Polar structures conduct almost nothing below a threshold set by the collector depletion barrier. With $N_D = 10^{19}$ cm $^{-3}$ the polar double barrier shows NDR peaks at +6.1 V (49 A cm $^{-2}$) and +8.5 V (2.0×10^3 A cm $^{-2}$). With $N_D = 10^{20}$ cm $^{-3}$ the first strong peak moves to +2.35 V (4.1×10^2 A cm $^{-2}$), followed by +4.75 V (4.1×10^4 A cm $^{-2}$, PVCR 8). (c, d) ZnO/MgZnO double and triple barriers. Polarization makes the double-barrier characteristic strongly asymmetric: a forward peak of 1.9×10^5 A cm $^{-2}$ at 0.34 V (PVCR 7.3) against a reverse peak of 5.0×10^3 A cm $^{-2}$ at -0.16 V (PVCR 1.5). The non-polar reference peaks symmetrically at ± 0.12 V (7.6×10^4 A cm $^{-2}$, PVCR 6.5). The polar triple barrier peaks at 0.16 V (2.4×10^4 A cm $^{-2}$, PVCR 6.8); the dotted curve in (d) uses the zero-bias-compensated width $w_2^* = 3.82$ nm. With stronger dephasing ($\tau_\phi = 10$ fs) the peak positions barely change but the peak-to-valley ratios fall: to 1.6 for the polar ZnO triple barrier and 3.8 for the GaN/AlN double barrier at 2.35 V ($N_D = 10^{20}$ cm $^{-3}$). The forward peak of the polar ZnO double barrier at 0.34 V weakens to PVCR 1.2. Series resistance and self-heating are not included

Operating-bias design rule for the ZnO/Mg_{0.2}Zn_{0.8}O triple barrier

The zero-bias optimum w_2^* places the resonance where almost no current flows, so a device needs a rule for the width that places the NDR at a chosen bias (Figure 7). In both structures the first NDR moves to lower bias as w_2 grows: in the polar structure from 0.488 V at $w_2 = 1.5$ nm to 8 mV at 3.8 nm and in the non-polar structure from 0.192 V at 1.5 nm to 16 mV at 3.0 nm. Rong et al. report the same trend, a lower peak voltage for a wider second well, in their AlGa_N/Ga_N triple barriers [12]. With $\tau_\phi = 10$ fs, the first NDR lies within 12 mV (polar) and 8 mV (non-polar) of its 33 fs position wherever both calculations resolve the same resonance. To place the first NDR at 0.11 V, the polar second well must be 3.21 nm wide against 2.21 nm for the non-polar one. Across 0.05–0.15 V the difference stays between 0.94 and 1.02 nm.

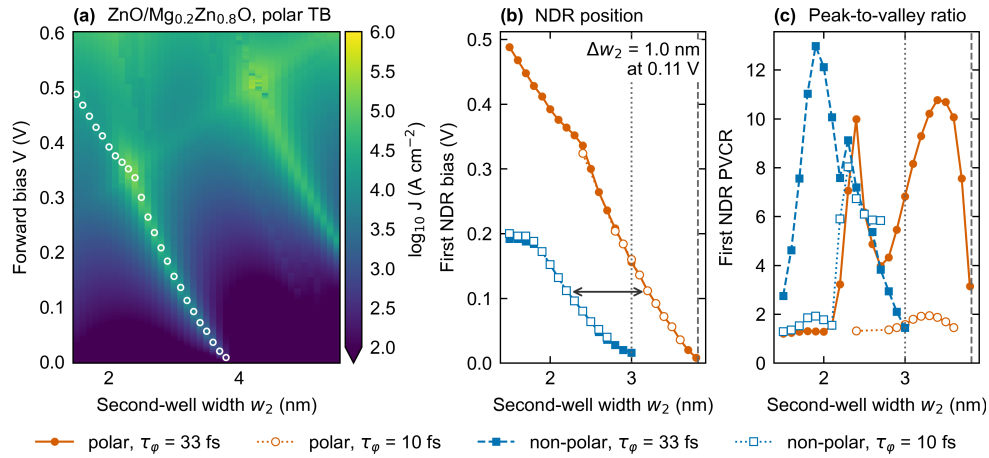


Figure 7. Operating-bias design rule for the ZnO/Mg_{0.2}Zn_{0.8}O triple barrier. (a) $\log_{10} J$ of the polar triple barrier versus second-well width w_2 and forward bias ($w_1 = 3$ nm, all barriers 2 nm, $\tau_\phi = 33$ fs; color scale clipped at 10^2 A cm⁻²). Circles mark the first negative-differential-resistance (NDR) peak: the lowest-bias NDR with $J \geq 10^2$ A cm⁻² and PVCR ≥ 1.2 . It moves to lower bias as w_2 grows and reaches zero bias at the zero-bias optimum $w_2^* = 3.82$ nm, where almost no current flows. (b) Bias of the first NDR versus w_2 for the polar (circles) and non-polar (squares) structures, with $\tau_\phi = 33$ fs (filled) and 10 fs (open). The 10 fs points are shown where that NDR is still resolved; there they agree with the 33 fs positions to within 12 mV. To place the NDR at a given bias, the polar second well must be about 1.0 nm wider than the non-polar one (arrow: 2.21 $\rightarrow$ 3.21 nm at 0.11 V; 0.94–1.02 nm between 0.05 and 0.15 V). (c) PVCR of the same NDR. With $\tau_\phi = 33$ fs both structures reach PVCR 10–13. With $\tau_\phi = 10$ fs the non-polar structure keeps PVCR 5.8–8.0 ($w_2 = 2.2$ –2.7 nm), while the polar structure falls to 1.3–1.9 ($w_2 = 2.4$ and 2.8–3.6 nm). Dotted line: $w_2 = w_1$. Dashed line: w_2^* . Series resistance is not included. Ga_N/Al_N is not shown: its currents change about eightfold per Al_N monolayer, so a width optimum would not be reliable

The two structures respond differently to dephasing. At $\tau_\phi = 33$ fs the first NDR reaches PVCR 10.8 in the polar structure ($w_2 = 3.4$ nm) and 13.0 in the non-polar one ($w_2 = 1.9$ nm). At $\tau_\phi = 10$ fs the non-polar structure keeps PVCR 5.8–8.0 for $w_2 = 2.2$ –2.7 nm, while the polar structure keeps only 1.3–1.9 ($w_2 = 2.4$ and 2.8–3.6 nm). For w_2

≤ 2.1 nm the polar structure has no NDR that meets the first-NDR criteria at 10 fs and at the remaining widths below 2.8 nm its first NDR belongs to a different resonance.

The width shift depends on the polarization contrast (Figure S1). At 0.11 V it is 0.44, 0.72, 1.00, 1.26 and 1.50 nm for $\Delta P = 6.6, 9.9, 13.2, 16.5$ and 19.8 mC m^{-2} , that is 0.066–0.077 nm per mC m^{-2} and 1.20–1.27 times the zero-bias shift $w_2^* - w_1$ at the same contrast. At $\tau_\phi = 10$ fs the first NDR lies within 16 mV of its 33 fs position wherever both calculations resolve the same resonance and the shift at 0.11 V is the same as at 33 fs for every contrast. At 10 fs the polar PVCR stays between 1.2 and 2.8 at every contrast, whereas at 33 fs its largest value rises from 6.6 at half the sourced contrast to 22.8 at 1.5 times.

Benchmark against measured GaN/AlN diodes

Every parameter set reproduces the linear growth of the reverse threshold with barrier thickness (Figure 8(a)); the Ambacher et al. constants overshoot the measured thresholds by 22–34%, depending on the permittivities and a sheet charge of $6.5 \times 10^{13} \text{ cm}^{-2}$ overshoots by 17–20% [7]. The calibrated set gives 3.30, 4.40 and 5.28 V against the measured 3.3, 4.3 and 5.2 V; this agreement follows from the calibration and does not test the model [7].

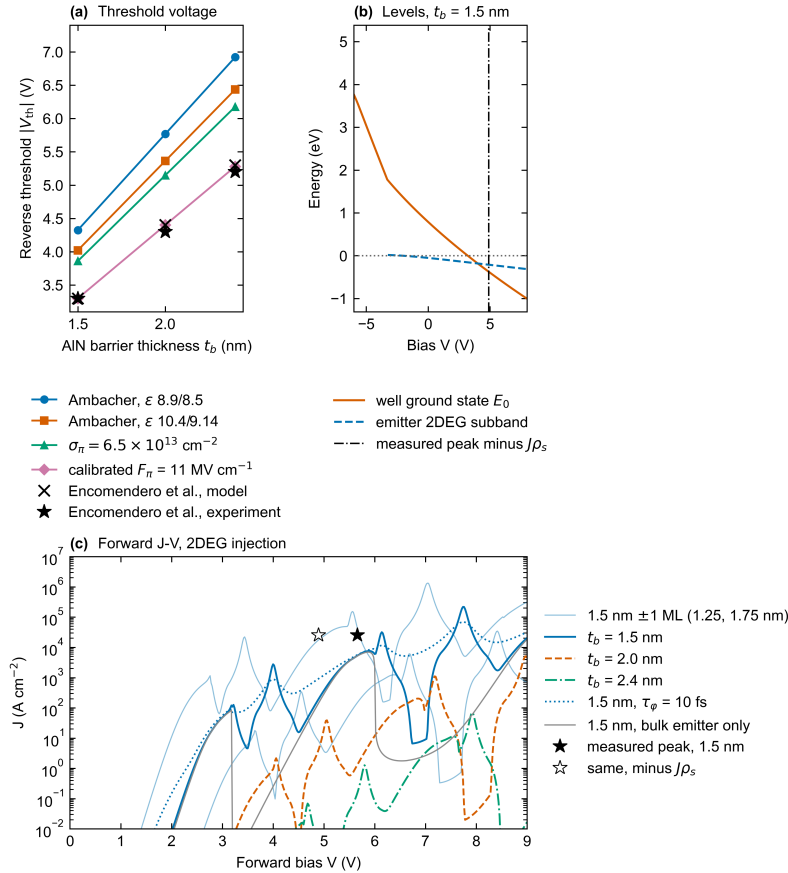


Figure 8. Benchmark against measured GaN/AlN resonant tunneling diodes. Comparison with the Ga-polar GaN/AlN double-barrier diodes of Encomendero et al: 3 nm GaN well, AlN barriers $t_b = 1.5, 2.0$ and 2.4 nm, 10 nm emitter and 6 nm collector spacers, contacts doped at about $2 \times 10^{19} \text{ cm}^{-3}$

Figure 8(a) shows the reverse threshold voltage $|V_{th}|$ versus t_b for four parameter sets (lines), with the model ($\times$) and measurements (star) of Encomendero et al. Every set reproduces the measured linear scaling $V_{th} = 2t_b F_\pi$. The Ambacher et al. polarization constants overshoot the measured thresholds by 22–34%, depending on the permittivities and a sheet charge of $6.5 \times 10^{13} \text{ cm}^{-2}$ overshoots by 17–20%. The calibrated set ($F_\pi = 11 \text{ MV cm}^{-1}$) matches within 2.3% by construction. Figure 8(b) shows the well ground state E_0 (solid) and lowest subband of the emitter accumulation layer (dashed) versus bias for $t_b = 1.5 \text{ nm}$, calibrated set. E_0 moves $244 \text{ meV} \cdot \text{V}^{-1}$ under forward bias (measured $\approx 180 \text{ meV} \cdot \text{V}^{-1}$) and $700 \text{ meV} \cdot \text{V}^{-1}$ under reverse bias (measured $\approx 770 \text{ meV} \cdot \text{V}^{-1}$); the kink at -3.3 V is the reverse threshold. The collector barrier at zero bias is 1.72 eV (measured $\approx 1.9 \text{ eV}$). E_0 crosses the 2DEG subband at 4.0 V ; the dash-dot line marks the measured peak (5.66 V) minus the series-resistance drop $J\rho_s = 0.77 \text{ V}$. Figure 8(c) shows the forward current density including injection from the emitter 2DEG, with resonances broadened by $\hbar/\tau_\phi$ (calibrated set). Solid, dashed and dash-dot lines: $t_b = 1.5, 2.0$ and 2.4 nm with $\tau_\phi = 33 \text{ fs}$ ($\Gamma_\phi = 20 \text{ meV}$). Thin lines: $1.5 \text{ nm} \pm$ one AlN monolayer (1.25 and 1.75 nm). Dotted: 1.5 nm with $\tau_\phi = 10 \text{ fs}$ ($\Gamma_\phi = 66 \text{ meV}$). Grey: the bulk-emitter model without the 2DEG channel. Filled star: measured peak for $t_b = 1.5 \text{ nm}$; open star: the same with the series-resistance drop removed. For $t_b = 1.5 \text{ nm}$ the ground-state resonance (well ground state aligned with the lowest 2DEG subband) gives $2.8 \times 10^3 \text{ A cm}^{-2}$ at 4.0 V with $\tau_\phi = 33 \text{ fs}$ and $8.7 \times 10^2 \text{ A cm}^{-2}$ with PVCR 2.9 with $\tau_\phi = 10 \text{ fs}$. The measured values are $2.55 \times 10^4 \text{ A cm}^{-2}$ and PVCR 1.55 and one monolayer thinner barriers give $2.2 \times 10^4 \text{ A cm}^{-2}$. The measured peak also lies close to the model's next resonance (6.1 V , $3 \times 10^4 \text{ A cm}^{-2}$), so the assignment of the measured peak is not settled. Without the 2DEG channel the model gives only 82 A cm^{-2} .

The level shifts and the collector barrier are independent tests (Figure 8(b)): for $t_b = 1.5 \text{ nm}$ the well ground state moves $244 \text{ meV} \cdot \text{V}^{-1}$ under forward bias against a measured $\approx 180 \text{ meV} \cdot \text{V}^{-1}$ (+36%) and $700 \text{ meV} \cdot \text{V}^{-1}$ under reverse bias against $\approx 770 \text{ meV} \cdot \text{V}^{-1}$ (−9%) and the collector barrier at zero bias is 1.72 eV against $\approx 1.9 \text{ eV}$ (−9%) [7]. The well ground state aligns with the lowest emitter-2DEG subband at 4.0 V , 18% below the measured peak of 4.89 V after the series-resistance drop is removed ($5.66 - 0.77 \text{ V}$); the error in γ_F accounts for this offset [7].

Injection from the emitter 2DEG sets the peak current (Figure 8(c)): without it the model gives at most 82 A cm^{-2} for $t_b = 1.5 \text{ nm}$, about 300 times below the measured $2.55 \times 10^4 \text{ A cm}^{-2}$ [7]. With it the ground-state resonance carries $2.8 \times 10^3 \text{ A cm}^{-2}$ ($\tau_\phi = 33 \text{ fs}$, PVCR 177) or $8.7 \times 10^2 \text{ A cm}^{-2}$ (10 fs , PVCR 2.9), against a measured PVCR of 1.55 [7]. Barriers one AlN monolayer thinner (1.25 nm) raise the peak to $2.2 \times 10^4 \text{ A cm}^{-2}$, so the measured current lies within one monolayer of the model, but the model's peak current changes by a factor of 8.0–8.2 per monolayer against 3.6 per monolayer measured between the 1.5 nm and 2.4 nm devices [7]. For $t_b = 2.4 \text{ nm}$ the model shows no ground-state NDR above 10 A cm^{-2} whereas the measured peak is $2.5 \times 10^2 \text{ A cm}^{-2}$ and the next resonance of the 1.5 nm model (6.14 V , $3.2 \times 10^4 \text{ A cm}^{-2}$) lies close to the measured peak, so the assignment of the measured peak to the ground state is not settled [7]. The quantized 2DEG holds 1.2–1.9 times the accumulation charge required by the electrostatics and 1.7 times at the ground-state resonance, because the accumulation layer is not solved self-consistently.

A width rule for polar triple barriers that holds under dephasing

In a polar triple barrier, the built-in field sets an electrostatic offset Δ between the two wells and its sign and size depend on the middle-barrier thickness. The offset can be removed in two ways: with a middle barrier near 1.5 nm, where the field drops across barrier and well cancel, or with a wider second well, whose ground state lies lower. Zero-bias compensation is of little use in a diode, because the wells then align only where almost no current flows. The operating-bias scans give a direct rule. To place the first NDR at a chosen bias between 0.05 and 0.15 V, make the polar second well about 1.0 nm wider than the non-polar well that places it at the same bias, for the sourced contrast. The shift grows almost in proportion to ΔP , which supports our reading that it compensates the polarization offset between the wells; the built-in field fixes this offset and it changes little over the 0.1 V operating range. The rule holds at both dephasing times because the broadening leaves each resonance centered where it was and the NDR position follows the alignment of the resonance with the emitter supply. The rule is only as accurate as the contrast: the width shift changes by 0.066–0.077 nm per mC m^{-2} , so an error of 3 mC m^{-2} in ΔP moves it by about 0.2 nm and a 25% error moves it from 1.0 nm to 0.72 or 1.26 nm. Pinning down ΔP , including the piezoelectric term of the MgZnO barrier that we neglect, is therefore a precondition for applying the rule to a device.

Dephasing sets the peak-to-valley ratio

Dephasing lowers the PVCR of the polar ZnO/MgZnO triple barrier far more than that of the non-polar one. Area-conserving broadening lowers a resonance of coherent width Γ and height T_p to a height of about $T_p \Gamma / (\Gamma + \Gamma_\phi)$. Once Γ_ϕ exceeds Γ , the strength of a resonance therefore scales with its coherent area $T_p \Gamma$ rather than with T_p . Both dephasing widths used here exceed the width of every zero-bias resonance of the ZnO/MgZnO triple barriers, which is at most 0.25 meV. The tilted barriers of the polar structure shrink this area: at $w_2 = 3$ nm and zero bias the stronger polar doublet peak has a $T_p \Gamma$ 44 times smaller than either non-polar peak, or even at w_2^* the weaker peak reaches only $T = 0.34$. We think this smaller area explains why the polar NDR falls to PVCR 1.3–1.9 at $\tau_\phi = 10$ fs while the non-polar NDR keeps 5.8–8.0. If so, interface quality matters more for polar triple barriers than for non-polar ones, because interface roughness sets the shorter of the two dephasing times [7].

In our benchmark only $\tau_\phi = 10$ fs reproduces the measured PVCR of 1.55; 33 fs gives 177 [7]. PVCRs computed in the coherent limit or with weak dephasing are therefore upper bounds. Rong et al. report PVCRs of up to 12.3 from ballistic calculations of AlGaIn/GaN triple barriers, similar to our 33 fs values of 10.8–13.0; our 10 fs results suggest that values of this size need weak dephasing [12].

What the GaN/AlN benchmark tests

The calibration fixes the thresholds, so the level shifts, the collector barrier and the current are the independent tests: the reverse level shift and the collector barrier agree within 9%, but the forward level shift is 36% too large. A forward lever arm that is too large brings the well ground state into alignment too early, which fits the model peak lying 18% below the measured one. The missing forward-bias drop most likely lies in the emitter accumulation layer, because our Thomas–Fermi profile ignores its

quantization and the quantized 2DEG holds 1.2–1.9 times the charge the electrostatics requires.

The emitter 2DEG carries almost all of the resonant current: at the ground-state peak of the 1.5 nm device the bulk-emitter channel contributes 0.37 of $2.8 \times 10^3 \text{ A cm}^{-2}$, so a bulk-emitter Tsu–Esaki model underestimates the current of polar GaN/AlN diodes with an accumulated emitter, here by a factor of about 300. With the 2DEG channel, a barrier one AlN monolayer thinner brings the peak current close to experiment, but the current depends too steeply on barrier thickness (a factor of 8.0–8.2 per monolayer against 3.6 measured); Encomendero et al. also report an exponential dependence of current on barrier thickness [7]. We have not tested the candidate causes of the steeper model dependence: band nonparabolicity in AlN, monolayer thickness fluctuations and the uncertain AlN mass and band offset. Because of this sensitivity we give no width rule for GaN/AlN and a measurement that resolves both the ground-state and the excited-state resonance would settle which resonance the measured peak is.

Comparison with other polar structures

Encomendero et al. showed that heavily doped contacts screen the polarization field and recover negative differential conductance under both polarities [21]. In our model, raising N_D from 10^{19} to 10^{20} cm^{-3} moves the first strong forward peak of the polar GaN/AlN double barrier from 6.1 V to 2.35 V. Wang et al. measured asymmetric NDR in AlGaIn/GaN double barriers (PVCR 1.4 forward against 1.08 reverse) and attributed it to polarization [22]. Our polar ZnO/MgZnO double barrier shows the same kind of asymmetry with a field about seven times weaker than in GaN/AlN, giving a 39-fold difference in peak current. The only ZnO/MgZnO resonant tunneling device we know of, grown on c-plane sapphire, used 7 nm barriers [13]. Recent ZnO simulations treat non-polar m-plane layers [14,17]. Testing our c-plane predictions therefore needs new devices with barriers of about 2 nm [13].

Limitations

The accumulation layer is not solved self-consistently, so the 2DEG current is uncertain by roughly the factor of 1.2–1.9 between the quantized and the electrostatic charge. Dephasing enters only as an energy-independent broadening and phonon- and defect-assisted valley currents are missing, so even the 10 fs PVCRs may be too high. Bands are parabolic and interfaces ideal and the J – V curves include neither series resistance nor self-heating. Four parameters still need checking against primary sources: the AlN/GaN band offset (1.75 eV, against a literature range reaching 2.1 eV), the c-axis permittivities of GaN and AlN, the ZnO/MgZnO permittivity and the piezoelectric term of the MgZnO barrier. We made two choices after inspecting the results: the first-NDR criterion replaced an earlier largest-peak criterion and the screened emitter spacer, the 2DEG channel and the dephasing broadening entered the model after the first comparison with the GaN/AlN measurements. The benchmark is therefore partly a calibration of the model rather than an independent test. A self-consistent Schrödinger–Poisson treatment of the accumulation layer, as used by Rong et al. and transport with energy-dependent scattering would address the first two limitations [12].

CONCLUSIONS

For the measured GaN/AlN diodes, the model reproduces the reverse level shift and collector barrier within 9% and, with 2DEG injection, comes close to the measured peak current when the barrier is one AlN monolayer thinner; it overestimates the forward level shift by 36% and the thickness dependence of the current. In polar ZnO/MgZnO triple barriers the field-induced offset between the wells vanishes at zero bias with a middle barrier near 1.5 nm or a second well of 3.82 nm. For a diode operating between 0.05 and 0.15 V, the polar second well must be wider than its non-polar counterpart by 0.066–0.077 nm per mC m^{-2} of polarization contrast, about 1.0 nm at the sourced 13.2 mC m^{-2} , at both dephasing times studied. The polar triple barrier loses most of its NDR under strong dephasing (PVCR 1.3–1.9 against 5.8–8.0 for the non-polar structure at $\tau_\phi = 10$ fs), so interface quality is likely to decide whether polar triple barriers show useful NDR.

ACKNOWLEDGMENTS

This work was supported by Universiti Putra Malaysia under Geran Putra Berimpak (GPB/9810400).

AUTHOR CONTRIBUTIONS

Osama Bagi Aljewaw: conceptualization, methodology, software, formal analysis, investigation, data curation, visualization, writing (original draft). Muhammad Khalis Abdul Karim: conceptualization, methodology, validation, supervision, project administration, funding acquisition, writing (review and editing). Sulayman Mohamad Kabeer, Mohd Mustafa Awang Kechik, Mohd Hafiz Mohd Zaid and Izdiyar Kamal: validation, writing (review and editing).

CONFLICT OF INTEREST

The authors declare no competing interests.

DATA AVAILABILITY

The simulation code and the data that support the findings of this study are available from the corresponding author on reasonable request.

REFERENCES

- [1] Tsu R, Esaki L. Tunneling in a finite superlattice. *Applied Physics Letters*. 1973;22(11):562–564. doi:10.1063/1.1654509
- [2] Chang LL, Esaki L, Tsu R. Resonant tunneling in semiconductor double barriers. *Applied Physics Letters*. 1974;24:593–595.

- [3] Encomendero J, Faria FA, Islam SM, Protasenko V, Rouvimov S, Fay P, et al. New Tunneling Features in Polar III-Nitride Resonant Tunneling Diodes. *Physical Review X*. 2017;7:041017. doi:10.1103/PhysRevX.7.041017
- [4] Liu F, Xue J, Yao J, Wu G, Li Z, Liu R, et al. Record peak current density of over 1500 kA/cm² in highly scaled AlN/GaN double-barrier resonant tunneling diodes on free-standing GaN substrates. *Applied Physics Letters*. 2024;124(7):073501. doi:10.1063/5.0180145
- [5] Encomendero J, Pieczulewski N, Chung E, Protasenko V, Muller DA, Jena D, et al. Electrically Tunable Room-Temperature Microwave Oscillations in GaN/AlN Triple-Barrier Resonant Tunneling Diodes. *Advanced Electronic Materials*. 2026;12(9):e00419. doi:10.1002/aelm.202500419
- [6] Ambacher O, Majewski J, Miskys C, Link A, Hermann M, Eickhoff M, et al. Pyroelectric properties of Al(In)GaN/GaN hetero- and quantum well structures. *Journal of Physics: Condensed Matter*. 2002;14(13):3399–3434. doi:10.1088/0953-8984/14/13/302
- [7] Encomendero J, Protasenko V, Sensale-Rodriguez B, Fay P, Rana F, Jena D, et al. Broken Symmetry Effects due to Polarization on Resonant Tunneling Transport in Double-Barrier Nitride Heterostructures. *Physical Review Applied*. 2019;11(3):034032. doi:10.1103/PhysRevApplied.11.034032
- [8] Growden TA, Zhang W, Brown ER, Storm DF, Hansen K, Fakhimi P, et al. 431 kA/cm² peak tunneling current density in GaN/AlN resonant tunneling diodes. *Applied Physics Letters*. 2018;112(3):033508. doi:10.1063/1.5010794
- [9] Zhang H, Xue J, Sun Z, Li L, Yao J, Liu F, et al. 1039 kA/cm² peak tunneling current density in GaN-based resonant tunneling diode with a peak-to-valley current ratio of 1.23 at room temperature on sapphire substrate. *Applied Physics Letters*. 2021;119(15):153506. doi:10.1063/5.0064790
- [10] Rong T, Yang LA, Yang L, Hao Y. Theoretical investigation into negative differential resistance characteristics of resonant tunneling diodes based on lattice-matched and polarization-matched AlInN/GaN heterostructures. *Journal of Applied Physics*. 2018;123(4):045702. doi:10.1063/1.5009397
- [11] Imaizumi H, Mase A, Egawa T, Miyoshi M. Design and Simulation of III-Nitride-Based Polarization-Matched Resonant-Tunneling Diodes with Quaternary AlGaInN Quantum Wells and Ternary AlInN Double Barriers. *Physica Status Solidi (RRL) - Rapid Research Letters*. 2025;19(12):e202500199. doi:10.1002/pssr.202500199
- [12] Rong T, Yang LA, Zhao Z, Zhang K, Hao Y. Theoretical Modeling of Triple-Barrier Resonant-Tunneling Diodes Based on AlGaIn/GaN Heterostructures. *Physica Status Solidi (a)*. 2019;216(23):1900471. doi:10.1002/pssa.201900471
- [13] Krishnamoorthy S, Iliadis AA, Inumpudi A, Choopun S, Vispute RD, Venkatesan T. Observation of resonant tunneling action in ZnO/Zn_{0.8}Mg_{0.2}O devices. *Solid-State Electronics*. 2002;46(10):1633–1637. doi:10.1016/S0038-1101(02)00117-X
- [14] Sirkeli VP, Vatavu SA, Yilmazoglu O, Preu S, Hartnagel HL. Negative differential resistance in ZnO-based resonant tunneling diodes. In: *2019 44th International Conference on Infrared, Millimeter and Terahertz Waves (IRMMW-THz)*; 2019. doi:10.1109/IRMMW-THz.2019.8874570

- [15] Dreyer CE, Janotti A, Van de Walle CG, Vanderbilt D. Correct Implementation of Polarization Constants in Wurtzite Materials and Impact on III-Nitrides. *Physical Review X*. 2016;6(2):021038. doi:10.1103/PhysRevX.6.021038
- [16] Yano M, Hashimoto K, Fujimoto K, Koike K, Sasa S, Inoue M, et al. Polarization-induced two-dimensional electron gas at $\text{Zn}_{1-x}\text{Mg}_x\text{O}/\text{ZnO}$ heterointerface. *Journal of Crystal Growth*. 2007;301--302:353–357. doi:10.1016/j.jcrysgro.2006.11.114
- [17] Atić A, Wang X, Vuković N, Stanojević N, Demić A, Indjin D, Radovanović, J. Resonant tunnelling and intersubband optical properties of ZnO/ZnMgO semiconductor heterostructures: impact of doping and layer structure variation. *Materials*. 2024;17(4):927. doi:10.3390/ma17040927.
- [18] BenDaniel DJ, Duke CB. Space-Charge Effects on Electron Tunneling. *Physical Review*. 1966;152:683. doi:10.1103/PhysRev.152.683
- [19] Ando Y, Itoh T. Calculation of transmission tunneling current across arbitrary potential barriers. *Journal of Applied Physics*. 1987;61(4):1497–1502. doi:10.1063/1.338082
- [20] Stone AD, Lee PA. Effect of Inelastic Processes on Resonant Tunneling in One Dimension. *Physical Review Letters*. 1985;54(11):1196–1199. doi:10.1103/PhysRevLett.54.1196
- [21] Encomendero J, Protasenko V, Rana F, Jena D, Xing HG. Fighting Broken Symmetry with Doping: Toward Polar Resonant Tunneling Diodes with Symmetric Characteristics. *Physical Review Applied*. 2020;13:034048. doi:10.1103/PhysRevApplied.13.034048
- [22] Wang D, Chen ZY, Wang T, Yang LY, Sheng BW, Liu HP, et al. Repeatable asymmetric resonant tunneling in $\text{AlGaIn}/\text{GaIn}$ double barrier structures grown on sapphire. *Applied Physics Letters*. 2019;114(7):073503. doi:10.1063/1.5080470
- [23] Vurgaftman I, Meyer JR. Band parameters for nitrogen-containing semiconductors. *Journal of Applied Physics*. 2003;94(6):3675–3696. doi:10.1063/1.1600519
- [24] Barker AS, Illegems M. Infrared Lattice Vibrations and Free-Electron Dispersion in GaIn . *Physical Review B*. 1973;7(2):743–750. doi:10.1103/PhysRevB.7.743

APPENDIX A

MODEL EQUATIONS

This appendix gives the equations behind the model where the main text states the four that define it.

The contacts hold fully ionized donors, so for a parabolic band with Fermi–Dirac statistics their Fermi level E_F above the band edge and their linear screening length λ follow from

$$N_D = N_c \mathcal{F}_{1/2} \left(\frac{E_F}{k_B T} \right), \quad N_c = 2 \left(\frac{m^* k_B T}{2\pi \hbar^2} \right)^{3/2},$$

$$\lambda = \left[\frac{\varepsilon_0 \varepsilon_w k_B T}{e^2 N_c \mathcal{F}_{-1/2}(E_F/k_B T)} \right]^{1/2}, \quad (\text{A1})$$

where $\mathcal{F}_j$ is the normalized Fermi–Dirac integral of order j and m^* and ε_w are the mass and permittivity of the well and contact material; table 1 lists the resulting values.

On a side that must hold negative charge, the band edge in the accumulation layer follows

$$U(z) = \Delta U_e \frac{e^{(z-z_1)/\lambda} - e^{-6}}{1 - e^{-6}}, \quad z_1 - 6\lambda \leq z \leq z_1, \quad (\text{A2})$$

where z_1 is the emitter edge of the first barrier and energies are measured from the emitter band edge; an accumulating collector has the same exponential form, steepest next to the last barrier.

The potential-energy change across each side is therefore

$$\Delta U_{e,c} = \begin{cases} eF_s (L_s + W/2) & (\text{depletion}), \\ eF_s \lambda & (\text{accumulation}), \end{cases} \quad (\text{A3})$$

and the field F_s next to the stack follows from the condition that the total potential-energy drop equals the applied bias,

$$\Delta U_e(F_s) + e \sum_i F_i(F_s) L_i + \Delta U_c(F_s) = -eV. \quad (\text{A4})$$

We solve the one-dimensional effective-mass Schrödinger equation

$$-\frac{\hbar^2}{2} \frac{d}{dz} \left[\frac{1}{m^*(z)} \frac{d\psi}{dz} \right] + U(z) \psi = E \psi \quad (\text{A5})$$

with ψ and ψ'/m^* continuous at every interface.

In slab j , of thickness d_j , band edge U_j and mass m_j , the wavefunction is

$$\psi_j(z) = a_j e^{ik_j(z-z_j)} + b_j e^{-ik_j(z-z_j)}, \quad \hbar k_j = \sqrt{2m_j(E - U_j)}, \quad (\text{A6})$$

with $\text{Im } k_j > 0$ where $E < U_j$.

At the interface between slabs $j-1$ and j , the interface conditions give the reflection and transmission amplitudes for incidence from the left (r , t) and from the right (r' , t'):

$$\begin{aligned}
r &= \frac{\rho_j - 1}{\rho_j + 1}, & t &= \frac{2\rho_j}{\rho_j + 1}, & r' &= \frac{1 - \rho_j}{1 + \rho_j}, & t' &= \frac{2}{1 + \rho_j}, \\
\rho_j &= \frac{k_{j-1}/m_{j-1}}{k_j/m_j},
\end{aligned} \tag{A7}$$

while a slab reflects nothing and multiplies the transmitted amplitudes by $e^{ik_j d_j}$.

Adding the next element (r_2, t_2, r_2', t_2') to the part already combined (r_1, t_1, r_1', t_1') gives the Redheffer star product

$$\begin{aligned}
r &= r_1 + \frac{t_1' r_2 t_1}{1 - r_1' r_2}, & t &= \frac{t_2 t_1}{1 - r_1' r_2}, \\
r' &= r_2' + \frac{t_2 r_1' t_2'}{1 - r_1' r_2}, & t' &= \frac{t_1' t_2'}{1 - r_1' r_2},
\end{aligned} \tag{A8}$$

so the recursion contains no growing exponentials: the only propagation factors are $e^{ik_j d_j}$, whose modulus is at most 1.

The subbands of an accumulated contact come from a finite-difference BenDaniel–Duke eigensolver on a grid of step $h = 0.01$ nm that spans a 40 nm pad of contact, the accumulation region and the adjacent barrier, with $\psi = 0$ at both ends:

$$-\frac{\hbar^2}{2h^2} \left[\frac{\psi_{j+1} - \psi_j}{m_{j+1/2}} - \frac{\psi_j - \psi_{j-1}}{m_{j-1/2}} \right] + U_j \psi_j = E_n \psi_j, \tag{A9}$$

where $m_{j\pm 1/2}$ is the mass midway between grid points j and $j\pm 1$.

Each subband holds the areal density

$$n_n = \frac{m^* k_B T}{\pi \hbar^2} \ln [1 + e^{(\mu - E_n)/k_B T}], \tag{A10}$$

where μ is the Fermi level of the accumulating contact.

Next to the barrier, at z_b , the normalized bound state is a standing wave $A_n e^{ik_n z} + B_n e^{-ik_n z}$ with $|A_n| = |B_n|$, so that

$$|A_n|^2 = \frac{1}{4} \left[\psi_n'(z_b)^2 + \frac{\psi_n^2(z_b)}{k_n^2} \right], \quad \hbar k_n = \sqrt{2m^*(E_n - U_b)}, \tag{A11}$$

where U_b is the band edge next to the barrier. Electrons in the subband escape through the stack at the rate $\nu_n = (\hbar k_n / m^*) |A_n|^2 T(E_n)$, where T is the transmission of the stack seen from a lead at the local band edge.

The net 2DEG current uses the same difference of Fermi functions as equation (3) of the main text,

$$J_{2D} = e \sum_n \nu_n \frac{m^* k_B T}{\pi \hbar^2} \left\{ \ln [1 + e^{(\mu_s - E_n)/k_B T}] - \ln [1 + e^{(\mu_d - E_n)/k_B T}] \right\}, \tag{A12}$$

with source and drain Fermi levels $\mu_s = E_F$ and $\mu_d = E_F - eV$ for the emitter; a collector that accumulates electrons under reverse bias contributes with μ_s and μ_d exchanged and the opposite sign.

The Lorentzian and the window of equation (4) of the main text are

$$L(x; \Gamma) = \frac{\Gamma/2\pi}{x^2 + \Gamma^2/4}, \quad w(u) = \begin{cases} 1, & |u| \leq 3, \\ \frac{1}{2} \left\{ 1 + \cos \left[\frac{\pi}{2} (|u| - 3) \right] \right\}, & 3 < |u| < 5, \\ 0, & |u| \geq 5, \end{cases} \quad (\text{A13})$$

where $N = \int L(x;1) w(x) dx = 0.920$ is the area of the windowed unit Lorentzian and T_ϕ is set to zero wherever it would be negative.

The level shifts of the benchmark are linear fits to the bias dependence of the well ground state E_0 ,

$$\gamma_F = -\frac{dE_0}{dV} \quad (0.5 \leq V \leq 3 \text{ V}), \quad \gamma_R = \left| \frac{d(E_0 + eV)}{dV} \right| \quad (-3 \leq V \leq -0.5 \text{ V}), \quad (\text{A14})$$

so that γ_R measures the level against the band edge of the injecting collector, $-eV$.

In our electrostatic model the offset between the centers of the two wells is

$$\Delta = e \left[F_w \frac{w_1 + w_2}{2} + F_b b_2 \right], \quad (\text{A15})$$

Away from the minimum the splitting follows the two-level estimate

$$S \approx \sqrt{\Delta^2 + S_0^2}, \quad (\text{A16})$$

SUPPLEMENTARY FIGURE

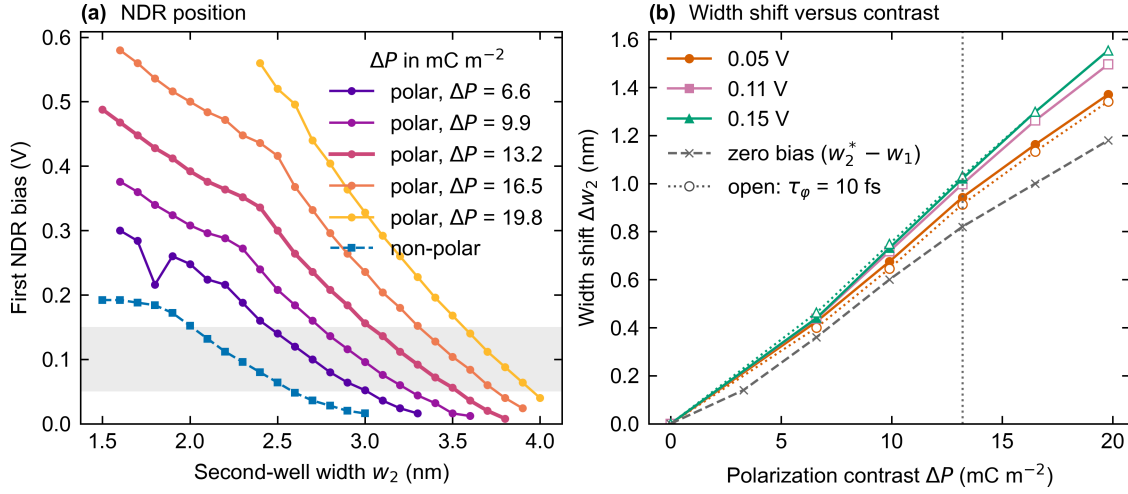


Figure S1. Sensitivity of the operating-bias width rule to the polarization contrast (ZnO/Mg_{0.2}Zn_{0.8}O). (a) Bias of the first NDR versus second-well width w_2 for the polar triple barrier at five MgZnO/ZnO polarization contrasts ΔP , 0.5 to 1.5 times the sourced 13.2 mC m^{-2} (thick line) and for the non-polar reference (dashed), with $\tau_\phi = 33$ fs ($w_1 = 3$ nm, all barriers 2 nm; first NDR defined as in figure). Each polar curve ends where its first NDR reaches its lowest bias, at or below the zero-bias optimum $w_2^* - w_1$. The grey band marks 0.05–0.15 V. (b) Width shift Δw_2 between the polar and non-polar second wells that place the first NDR at 0.05, 0.11 and 0.15 V, versus ΔP , for $\tau_\phi = 33$ fs (filled) and 10 fs (open; only where the 10 fs NDR lies within 30 mV of its 33 fs position; at 0.11 V the two coincide). At $\Delta P = 0$ the polar structure is identical to the non-polar one. At 0.11 V, Δw_2 rises from 0.44 nm (6.6 mC m^{-2}) through 1.00 nm (13.2 mC m^{-2} , dotted line) to 1.50 nm (19.8 mC m^{-2}) and lies above the zero-bias shift $w_2^* - w_1$ (dashed) at every contrast. Series resistance is not included