Supplementary Information

m-Plane GaN Split-Well Direct-phonon Terahertz Quantum Cascade Laser

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Supplementary Methods

To further evaluate the robustness of the proposed split-well direct-phonon (SWDP) design, additional simulations were performed using the non-equilibrium Green's function (NEGF) formalism under the same conditions described in the main manuscript. All scattering mechanisms, including interface roughness (IFR), ionized impurity scattering, alloy disorder, and electron–electron interactions, were included self-consistently.
The interface roughness was modeled using an exponential correlation function with a correlation length of 80 Å. The roughness amplitude was varied systematically to evaluate its impact on the optical gain.

Supplementary Figures

To further understand the role of interface roughness scattering, we have investigated the sensitivity of the proposed SWDP design to increased interface roughness and compared it with previously proposed designs (RP and TW). The simulations were performed for increasing roughness amplitudes (Δ = 0–2.59 Å), while keeping the correlation length and all other scattering mechanisms fixed. As expected, increasing IFR leads to enhanced scattering, resulting in a clear reduction in the peak optical gain for all designs considered. Under ideal conditions (Δ = 0 Å), the SWDP structure exhibits the highest gain, significantly outperforming both the TW and RP designs. As the roughness amplitude increases, the optical gain decreases in all structures. Notably, for common interface roughness values ($\Delta \approx$ 1–1.3 Å), the SWDP design maintains the highest gain and remains well above the estimated waveguide losses, demonstrating its strong potential for practical implementation. However, for larger roughness amplitudes ($\Delta \approx$ 1.6 Å), the SWDP design shows a more pronounced degradation and falls below the estimated waveguide losses, while the RP structure retains gain above the losses. This indicates that although the SWDP design offers superior performance under common interface roughness values, it is more sensitive to severe interface roughness compared to more conventional designs.

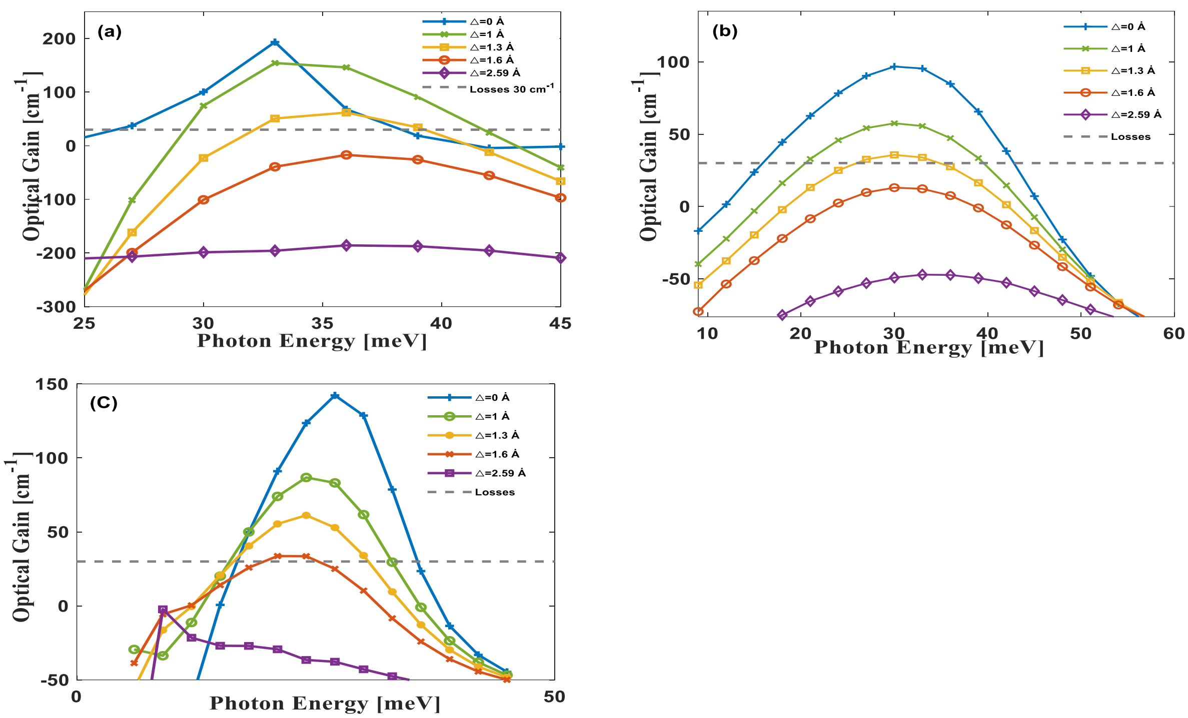

Figure S1. Optical gain as a function of photon energy for different interface roughness amplitudes (Δ) for (a) SWDP, (b) TW, and (c) RP designs, each evaluated at its respective alignment bias. The dashed horizontal line indicates the estimated waveguide losses of 30 cm^{-1}.

Table S1. Key simulation parameters used in the NEGF calculations for the proposed SWDP GaN/AlGaN THz QCL structure.

Parameter	Value	Description
Electron effective mass (GaN)	~ 0.2 m_0	Conduction band effective mass
LO phonon energy	~92 meV	Dispersionless LO phonon model
Conduction band offset (14% Al barrier)	~242 meV	Injection barrier
Conduction band offset (7% Al barrier)	~121 meV	Intra-well barrier
Interface roughness amplitude Δ	1 Å	IFR model
Correlation length Λ	80 Å	IFR model
IFR correlation model	Exponential	Interface correlation function
Electron–electron interaction	Hartree approximation	Self-consistent Poisson
Alloy disorder scattering	Included for $Al_{0.14}Ga_{0.86}N$ and $Al_{0.07}Ga_{0.93}N$ barriers	Standard alloy disorder model for AlGaN/GaN barriers
Ionized impurity scattering (IIS)	Included	Standard IIS within the NEGF formalism
Doping density (SWDP)	~1×10^{10} cm^{-2}	Optimized structure
Doping density (TW/RP)	~3×10^{11} cm^{-2}	Reference structures