Quantitative Simulation of Strained and Unstrained InP-Based Resonant Tunneling Diodes

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State-of-the-art InP-based resonant tunneling diodes (RTDs) are being developed for circuit applications such as low power memory cells[1] and high speed adders.[2] Depending on the application RTDs must be designed to provide either a low[1] or a high[2] current density. Quantitative modeling of such devices is expected to reduce the device development cycle time significantly.[3] We have expanded our interactive design and analysis software NEMO (Nanoelectronic Modeling)[4,5] to quantitatively model pseudomorphic InP-based RTDs which can include lattice matched $In_{0.53}Ga_{0.47}As$, $In_{0.52}Al_{0.48}As$, and pseudomorphic AlAs and InAs. We present the world's first quantitative simulations of strained and unstrained InP-based RTDs that include quantum charge self-consistency (Hartree) in a full band (sp^3s^*) model.

The quantitative modeling of these devices requires accurate modeling of the bandstructure for each material. The strained AlAs barriers and InAs wells have altered bandgaps, band-offsets, effective masses and relative line-ups of Γ and X valley from their respective bulk values. Important bandstructure features to be modeled are the non-parabolicity of the $In_{0.53}Ga_{0.47}As$ and InAs and the complex band wrapping in the $In_{0.52}Al_{0.48}As$ and AlAs barriers. All these features combined required us to develop sp^3s^* bandstructure parameters optimized for the conduction and valence bands including spin-orbit interactions.[6] Not only is accurate bandstructure necessary, but a self-consistent calculation of the electrostatic potential with the quantum charge in both the quantized emitter and well states is required for predictive accuracy.

We find quantitative agreement between simulation and experiment for a test matrix of unstrained InGaAs/InAlAs and strained InGaAs/AlAs high current density RTDs in which barrier, well, and spacer widths are varied systematically. The material parameters are fixed and only structural changes from one device to the next are changed for all the simulations.

Our charge self-consistency model is evaluated with structures which have intentional barrier asymmetry. We quantitatively model the charge accumulation/depletion inside an RTD in the forward/reverse bias direction and achieve good agreement between theory and experiment.

Our comparisons between experimental and calculated I-Vs show that the room temperature valley current of InGaAs/InAlAs and InGaAs/AlAs RTDs is determined by thermionic emission through the first excited state rather than incoherent scattering. Preliminary calculations of state-of-the-art RTDs with the InAs notched well indicate that the regime has been reached in which the room temperature valley current is determined by incoherent scattering processes rather than thermionic emission. NEMO can now be used to design devices quantitatively to address issues like the improvement of the peak-to-valley-ratio.

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[6] T. Boykin *et al.*, submitted to Phys. Rev. B (1997).

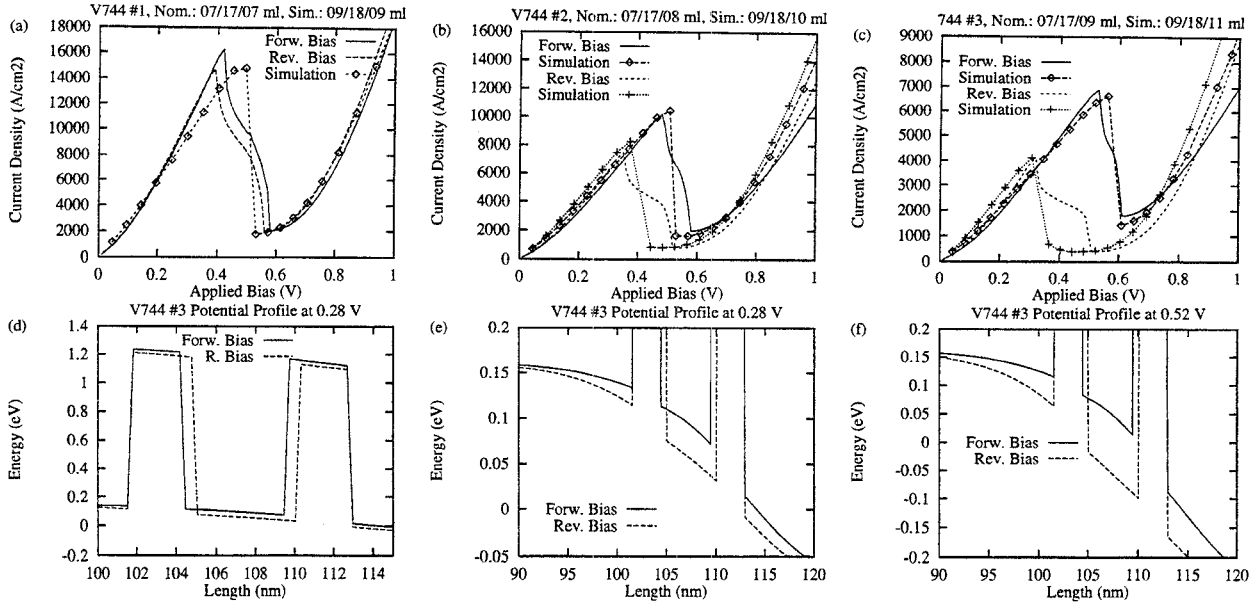

Figure 1: Test matrix of a strained InGaAs/AlAs RTD system. *One* of the AlAs barriers is increased in thickness by one mono-layer at the time. The nominally symmetric device V744 #1 has nominal well and barrier thicknesses of 30Å/10 mono-layer (ml) and 47Å/16ml, respectively. The devices are symmetrically clad with 20Å/7ml undoped, 500Å low doping ($1 \times 10^{18} cm^{-3}$) and 500Å high doping ($5 \times 10^{18} cm^{-3}$) spacer/contact layers. a-c) Comparison of experimental and simulated I–V's. Forward bias (thicker collector barrier) shows a higher peak current at a higher voltage. d-f) Potential profiles calculated for device #3 in forward and reverse bias for biases 0.28 V and 0.52 V. For comparison we reverse the spatial order of the layers for the reverse bias device. d) 0.28 V bias. The forward bias direction implies a thicker collector barrier. e) Zoom of (d). Reverse bias has a linear potential drop in the well indicating negligible electron charge in the well. Forward bias shows curvature in the well indicating electron accumulation resulting in a potential difference of about 40meV. f) 0.52V bias. Potential difference in the well is about 90meV due to charge accumulation in forward bias. A higher bias must be applied to the RTD to turn off the RTD.

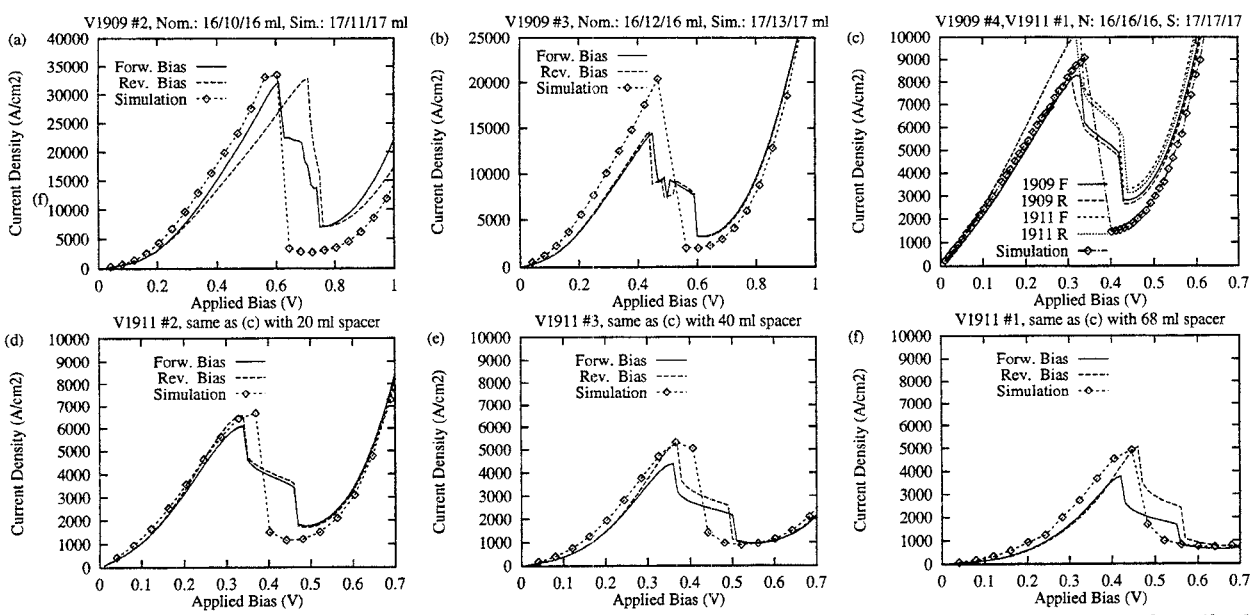

Figure 2: Test matrix of an unstrained InGaAs/InAlAs RTD system. The cladding is the same as described in Figure 1. a-c) Variation of the well thickness ((a) 11 ml, (b) 12 ml, (c) 16 ml). c-f) Variation of the undoped spacer layer ((c) 7ml, (d) 20 ml, (e) 40 ml, (f) 68 ml).