Simulation of heat flux through multilayer structures

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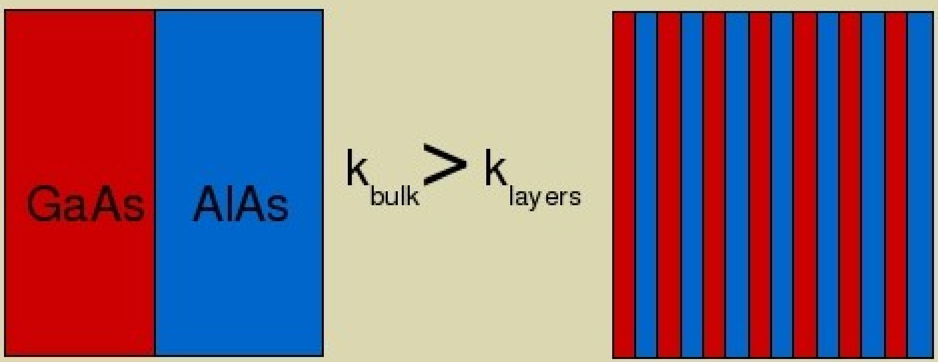
Presentation outline

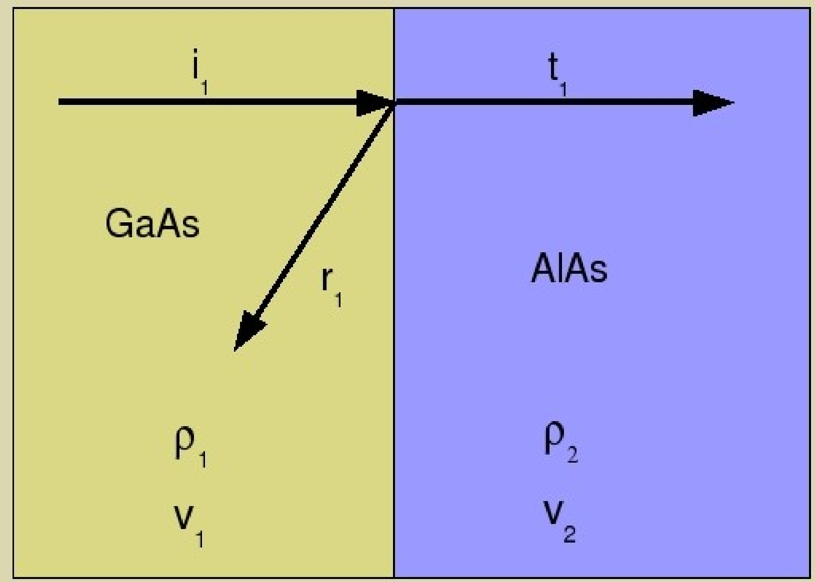
- Heat flow through structures with multiple epitaxial layers
  - Thermal conductivity of structures with multiple interfaces
  - Thermal boundary resistance (TBR)
- Heat flow in 1.3μm dilute nitride edge-emitting lasers
  - Full electro-opto-thermal simulations
  - Introduction of TBR into the model
- Discussion of effect in other (dilute nitride) devices
- Conclusions

Thermal conductivity of superlattices

- GaAs/AlAs superlattices have a much lower thermal conductivity than one would predict from the bulk values alone.[1] (3x-10x lower)

  - Bulk GaAs/AlAs thermal conductivity = $58.4m^{-1}K^{-1}$
  - Superlattice thermal conductivity = $5.0m^{-1}K^{-1}$





i = incident wave
r = reflected wave
t = transmitted wave

- This effect is mainly due to phonon scattering/reflections at material interfaces

- TBR first observed by Kapitza (1941)[2]

[1] W.S. Capinski *et. al.*, Phys. Rev. B Vol. 59, No. 12, p.8105 (1999).
[2] Collected papers of P.L. Kapitza, Vol. 2, Pergamon, Oxford, p. 581 (1965).

How does structure size affect the conductivity?

Consider a superlattice with a period L, where Λ is the average phonon mean free path (20-140nm)

One can distinguish two regimes:

1) $L \approx \Lambda$ A bulk thermal conductivity can be used between the interfaces by placing a thermal resistance at each boundary (TBR)

2) $L \ll \Lambda$ The situation becomes more complicated with phonons reflecting off multiple layers and gaps forming in the dispersion relations

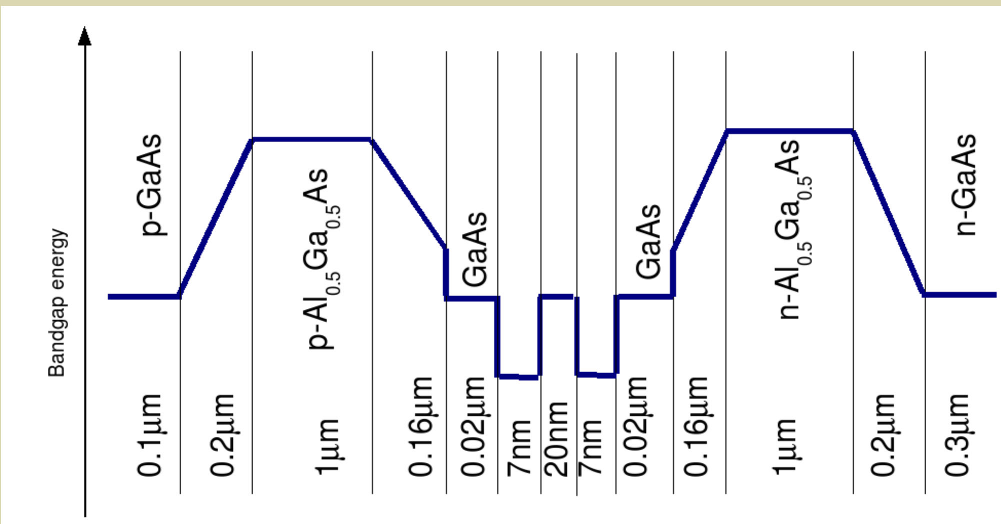
- **Edge-emitting lasers fall within the $L \approx \Lambda$ regime**

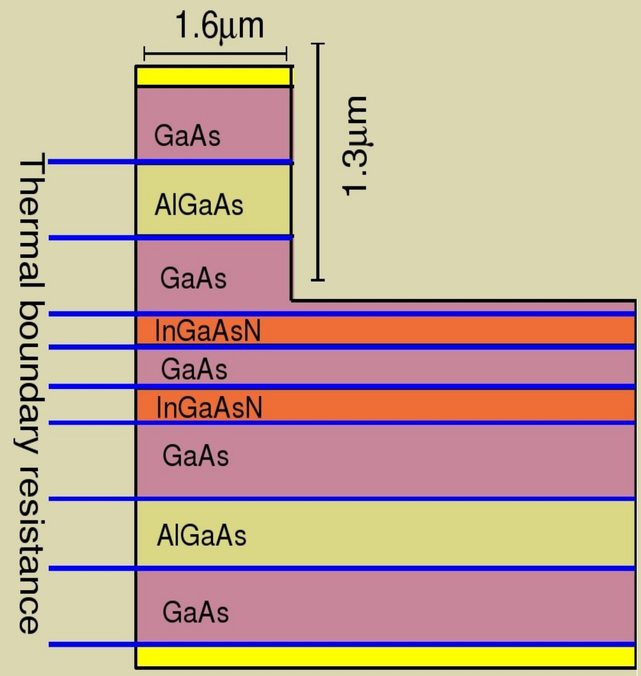
How does TBR affect dilute nitride EELs?

QW material: $Ga_{0.613}In_{0.387}NAs$ with 1.2% nitrogen

Number of QWs: 2

Front facet output power: P_{out} = 10 – 15 mW





- Half space simulations
- TBR introduced at each epitaxial interface

What values of TBR should be used?

- Values of TBR are depend on:
  - The acoustic mismatch of the materials
    - Masses - Elastic constants -> Speed of sound in materials
    - Similar to Snell's law
  - The quality of epitaxial interfaces
    - E.g. nitrogen plasma damage (dilute nitride devices)
  - Layer thickness
- Exhaustive experimental characterization of the effect is not complete
  - Still no real consensus on microscopic models for TBR
- Diffuse mismatch model is used in this work
  - Has shown some agreement with experiment
  - A range of values will be used to examine the impact of TBR

Typical values of TBR from experiment

Interface	*TBR value (m^2K/W)*	*Method*	*Device*
GaAs/AlGaAs/InGaAsN	*≈ $1.2x10^{-9}$*	*DMM*	*EEL*
GaN/Si[1]	$7x10^{-8}$	experiment	HEMT
GaN/SiC[1]	$1.2x10^{-7}$	experiment	HEMT
AlN/Si[1]	$7-8x10^{-8}$	experiment	Thin film

- TBR is a known problem in nitride HEMTs
- TBR is less well studied in EELs

1) J. Kuzmík *et.al.*, J. Appl. Phys. Vol. 101, 054508 (2007).

Device simulator

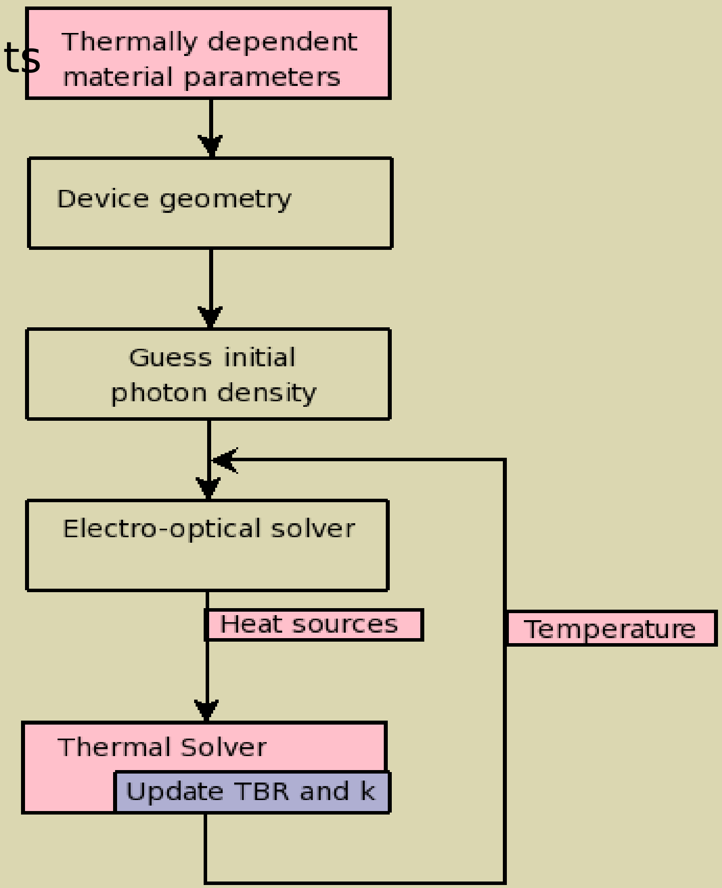
Electro-thermal Model

- Bipolar 2D Drift Diffusion (DD) model (0^{th} and 1^{st} moments of the Boltzmann Transport Equation (BTE))
- Poisson’s equation
- QW capture/escape equations for each QW
- 2D lattice heat equation
  - Heat sources derived from 2^{nd} moment of BTE

Optical Model

- Photon rate equation
- Valance band structure calculated using 4x4 band ***k.p***
- Band anti-crossing model for the conduction band
- Fermi's Golden rule used to calculate stimulated/spontaneous emission rates

All equations solved using Newton's method



Discretization scheme for inclusion of TBR

- The lattice heat equation is commonly solved in thermal models:

$$\rho_L C_L \frac{\partial T}{\partial t} = \nabla \cdot \left(k \nabla T \right) + H$$

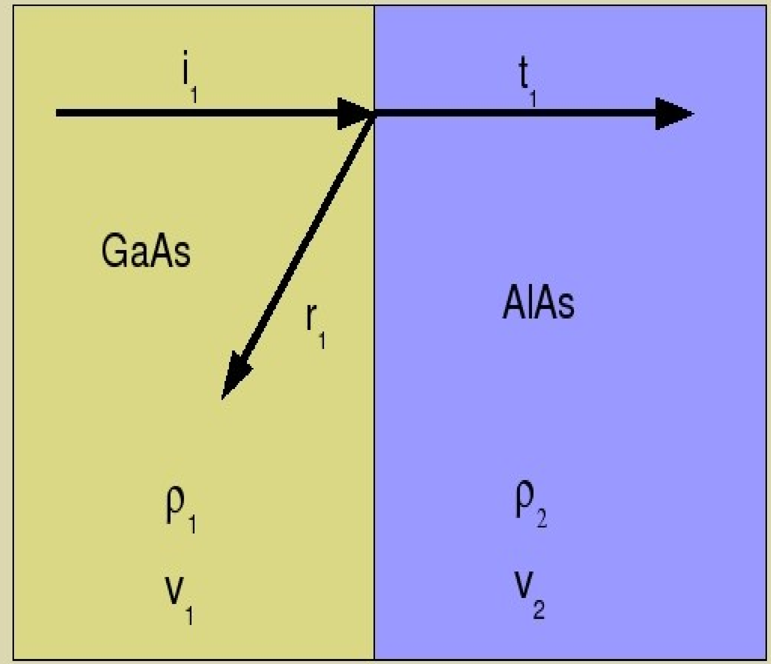
- However, because of abrupt thermal resistances at epitaxial interfaces one must solve:

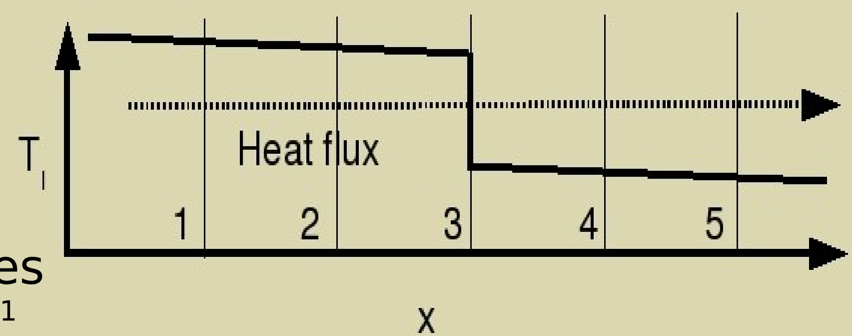
(1) $$\left(\frac{\partial T}{\partial x} \right)^3_{r+1/2} k_1 = k_2 \left(\frac{\partial T}{\partial x} \right)^4_{r+1/2}$$

- Introduce a step in temperature proportional to the boundary resistance:

(2) $$T^{(3)}_{r+1/2} - T^{(4)}_{r+1/2} = R k_2 \left(\frac{\partial T}{\partial x} \right)^3_{r+1/2}$$

- Adapted from a scheme to model discontinuities Quasi-TE modes of semiconductor waveguides[1]

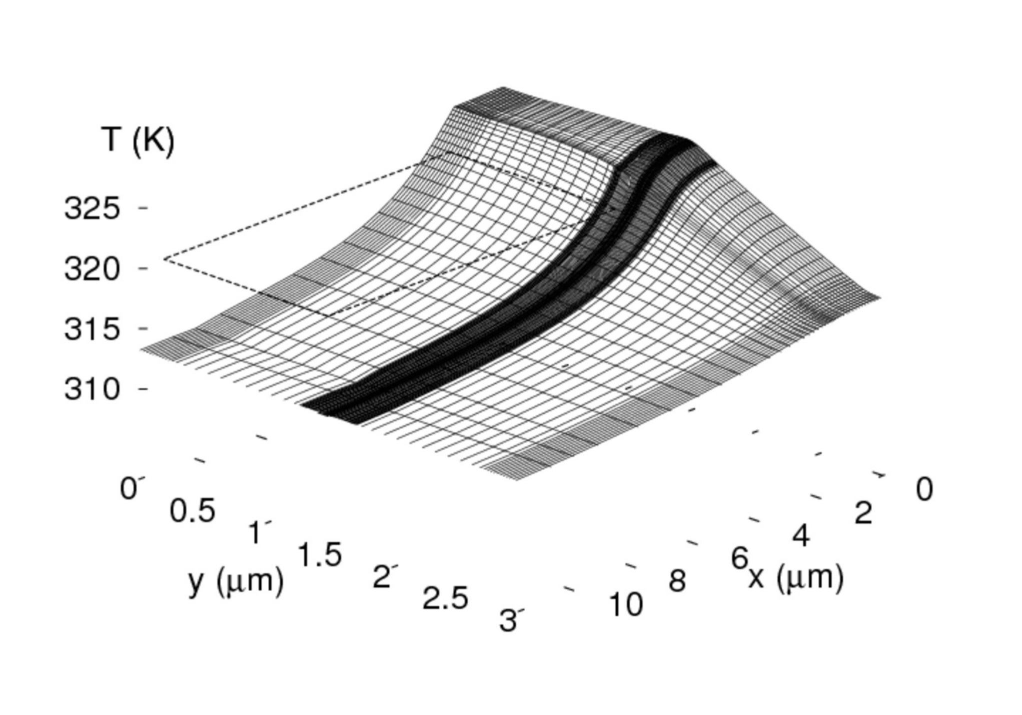




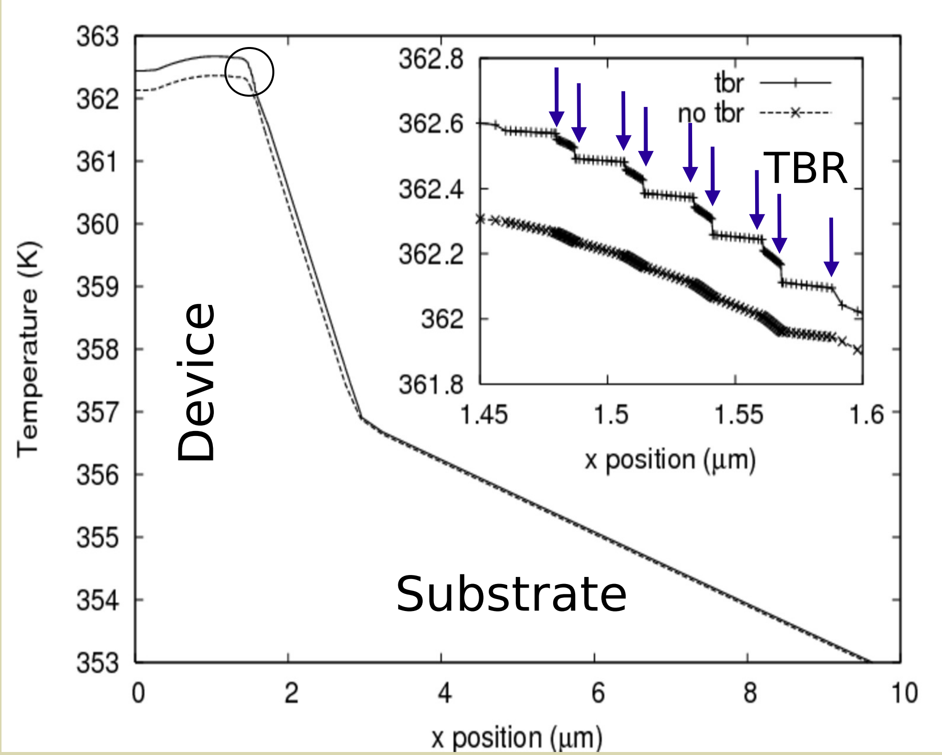
1) M.S. Stern, IEE Proc. Vol. 135, pp. 56-63 (1998).

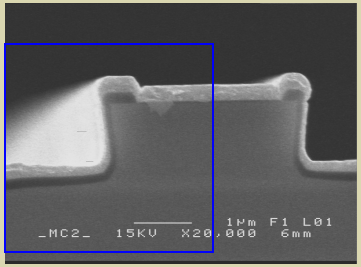
Thermal profile with and with out TBR

Half-space 2D thermal profile



Thermal profile with & without TBR

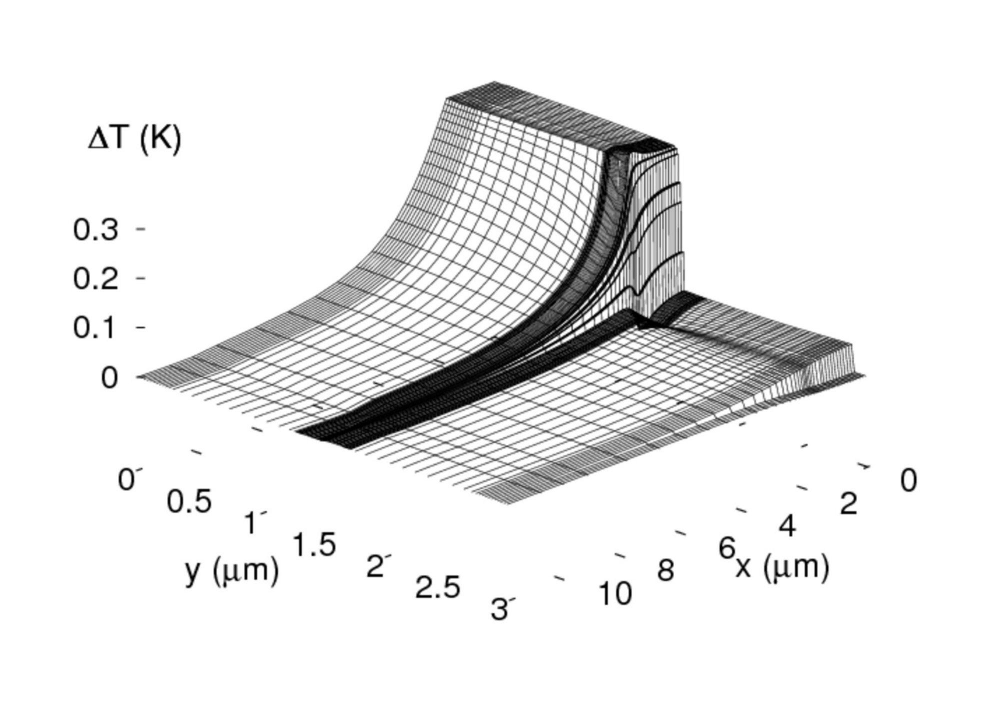




- Up to half a degree difference in peak temperature of device
- Small temperature differences are important for accurate models

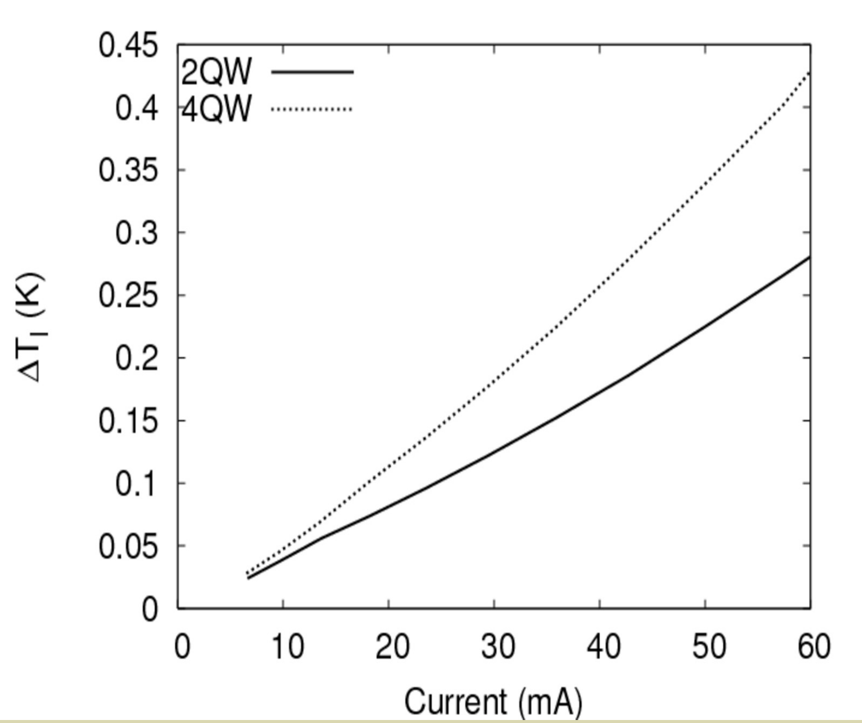
Thermal profile with and with out TBR

Difference between simulations with and without TBR



- Joule heating and free carrier absorption in ridge
  - High heat flux out of ridge
  - TBR has a large effect at bottom of ridge

Change in QW temperature due to TBR vs. injection current

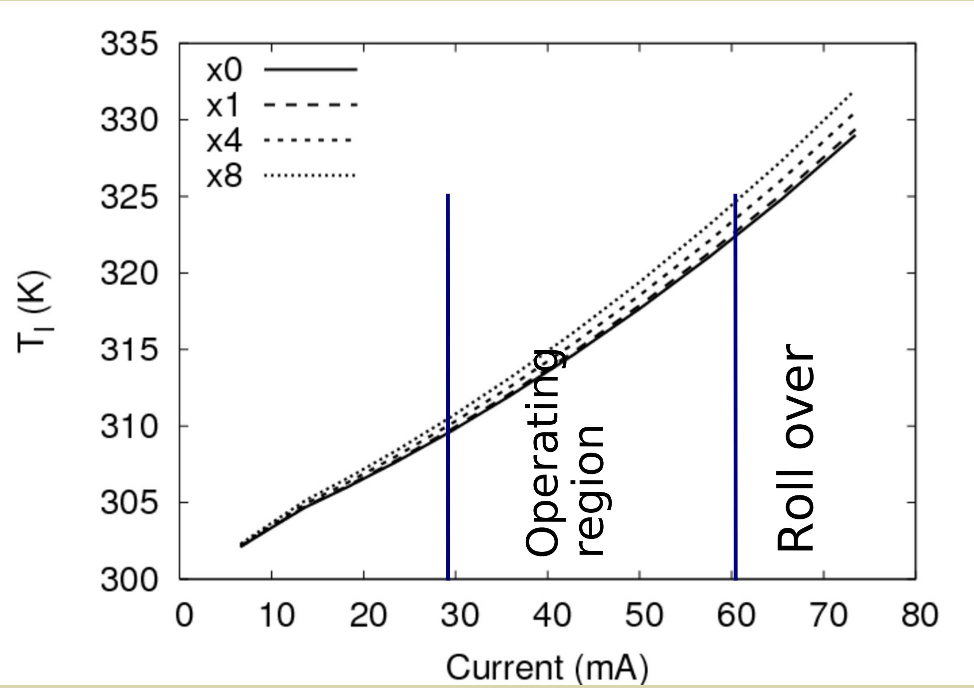


- The interfaces introduce a small increase in QW temperature

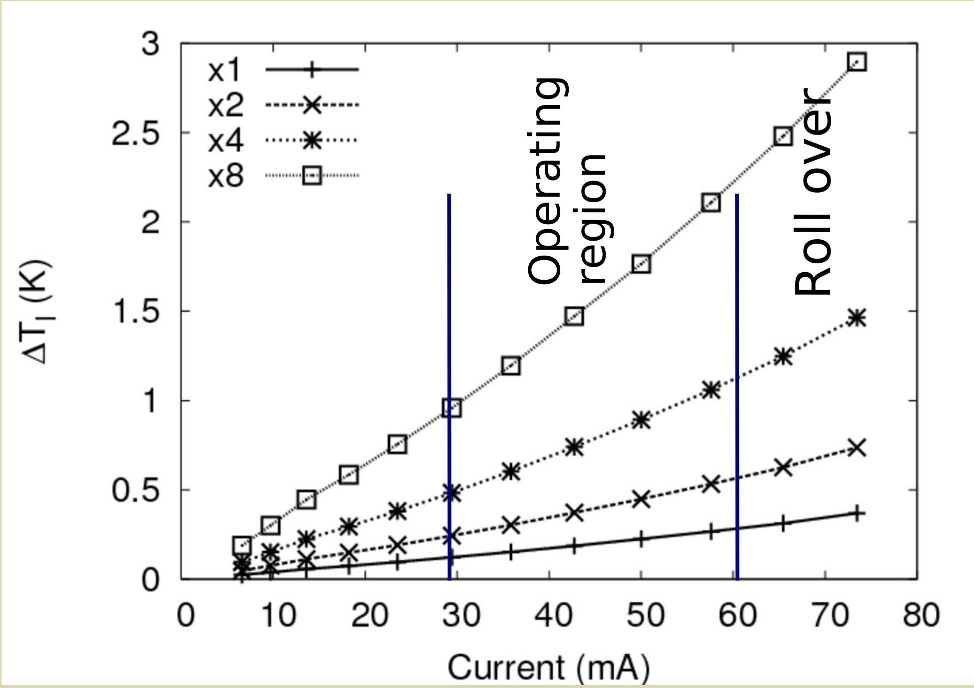
Impact of TBR on QW temperature

The University of Nottingham

Temperature of QW for various TBR values



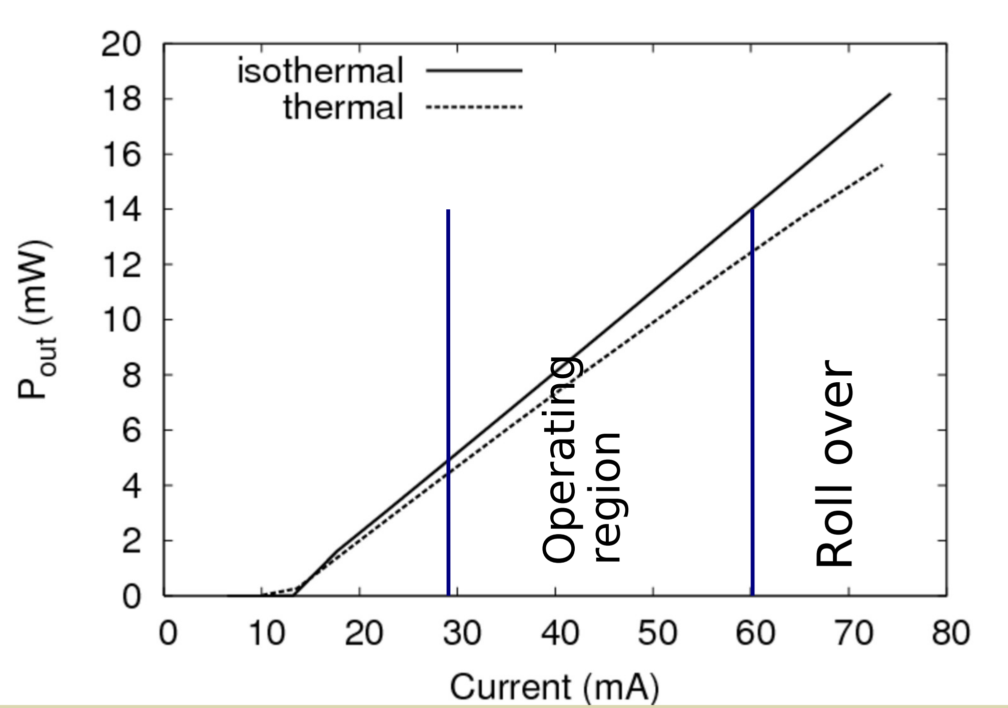
Difference in QW temperature due to TBR



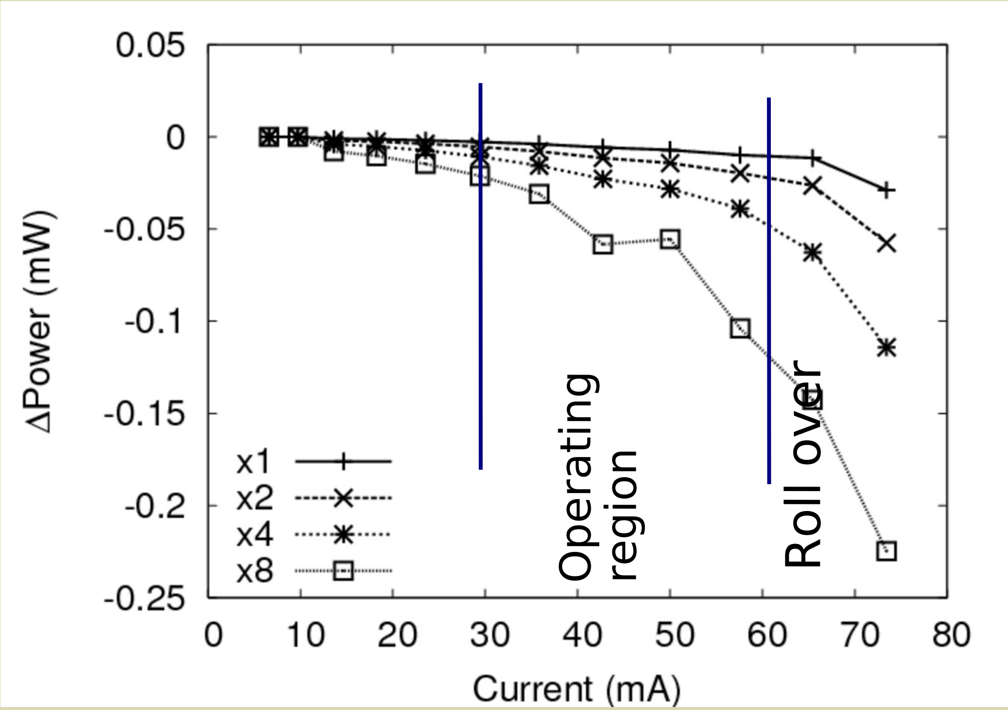
- A small increase in QW temperature can be seen
  - Although small, the effect may need to be included in some cases

Impact of TBR on output power

L-I curves for isothermal, ordinary thermal and thermal with TBR



Difference in L-I curves compared to ordinary thermal case



- x1,x2,x4 and x8 times the value predicted by TBR
- A small decrease in power due to the temperature increase can be seen

Conclusions

- TBR has been shown to increase the predicted temperature of a 1.3μm dilute nitride EEL by up to 0.5K

- A small decrease in optical power is also predicted

- Impact of TBR increased by
  - More interfaces
  - Materials with large acoustic mismatch (GaN/SiC HFETs)
  - Interface defects (nitrogen plasma damage)
  - Increased heat flux

- Need for more ***more accurate*** TBR values
  - Ideally from experiment
  - Better numerical models for calculation of TBR are also needed

- For the first time the impact of TBR has been considered within a full electro-optical-thermal laser simulation tool

Other devices structures where TBR has an impact

- **Structures with relatively thick layers (L≈ Λ)**
  - Long wavelength VCSELs mirrors
    - e.g. 1.3μm structures for dilute nitride VCSELs
    - 30-60 periods
    - Possible increase of up to 5K
    - Carrier heat flux reduces impact of TBR

- **Devices with large acoustic mismatch**
  - GaN/sapphire, GaN/SiC and GaN/AlN
    - Heterostructure field-effect transistors (HFETs)

- **Structures with layer thicknesses that are much smaller than the phonon m.p.f. (L « Λ)**
  - Short wavelength VCSELs
  - Quantum cascade lasers
    - High temperature sensitivity