The impact of thermal boundary resistance in opto-electronic devices

R. MacKenzie[1]*, J.J. Lim, S. Bull, S. Sujecki and E.C. Larkins*

School of Electrical and Electronic Engineering, University of Nottingham,
University Park, Nottingham, NG7 2RD, United Kingdom

e-mail[1]: eexrm1@nottingham.ac.uk

Acknowledgments

The University of Nottingham

R. MacKenzie gratefully acknowledges the support of the **Engineering and Physical Sciences Research Council** (EPSRC), U.K.

EPSRC Engineering and Physical Sciences Research Council

We gratefully acknowledge the EC IST projects **FAST ACCESS** (IST-004772) and WWW.BRIGHTER.EU (IST-035266).

FAST ACCESS

WWW • BRIGHTER • EU

www.fastaccessproject.eu

www.ist-brighter.eu

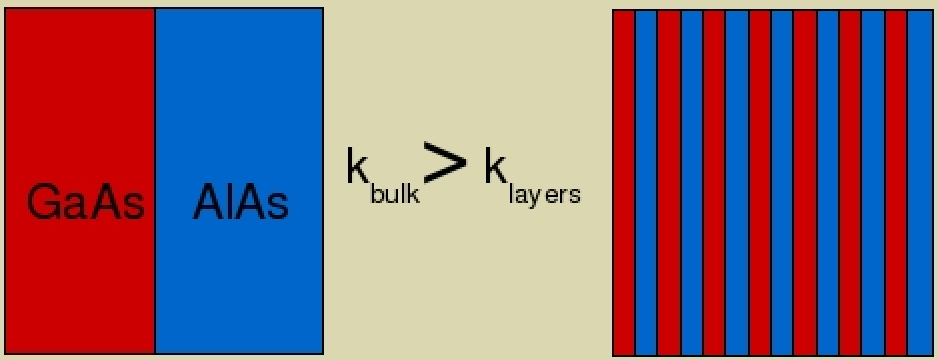
Presentation outline

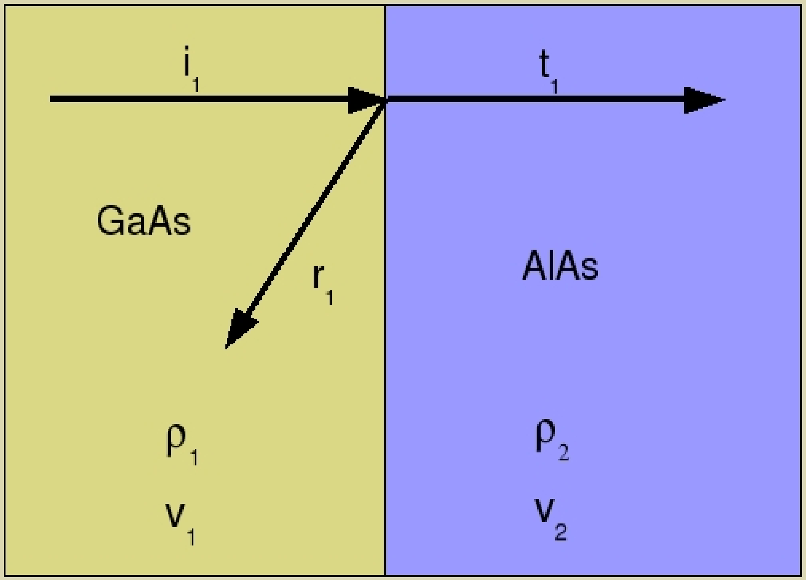
- Heat flow through structures with multiple epitaxial layers
    - Theory of Thermal Boundary Resistance (TBR)
- Examples:
    - Example 1 - Thermal conductivity of a VCSEL mirror
    - Example 2 - Electron/phonon heat flux over a TBR
    - Example 3 - High brightness 975nm edge-emitting laser
        - Full electro-opto-thermal simulations
        - Impact on L-I curves
- 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 = 58.4$m^{-1}K^{-1}$
  - Superlattices thermal conductivity = 5.0$m^{-1}K^{-1}$





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 (≈20nm)

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**

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
- Layer thickness
- Exhaustive experimental characterization of the effect is not complete
  - Still no real consensus on microscopic models for TBR
- Diffuse Mismatch Model (DMM) is used in this work
  - Has shown some agreement with experiment
- Typical values *(m^2K/W)* : *GaAs/AlGaAs* $\approx 1.2 \times 10^{-9}$, *GaN/Si*[1] $\approx 7 \times 10^{-8}$, *GaN/SiC*[1] $\approx 1.2 \times 10^{-7}$, *AlN/Si*[1] $\approx 7-8 \times 10^{-8}$

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

Discretization scheme for inclusion of TBR

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

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

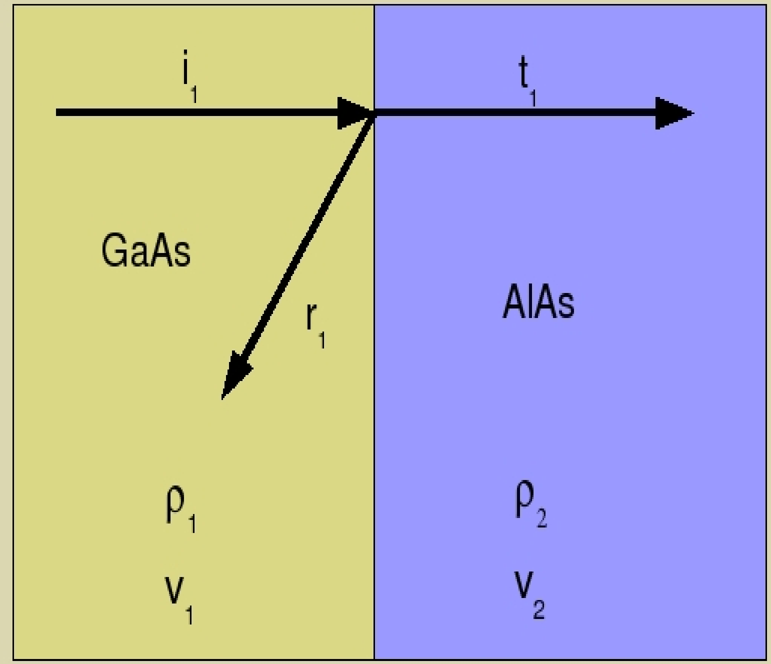
- However, because of abrupt thermal resistances at epitaxial interfaces one must solve:

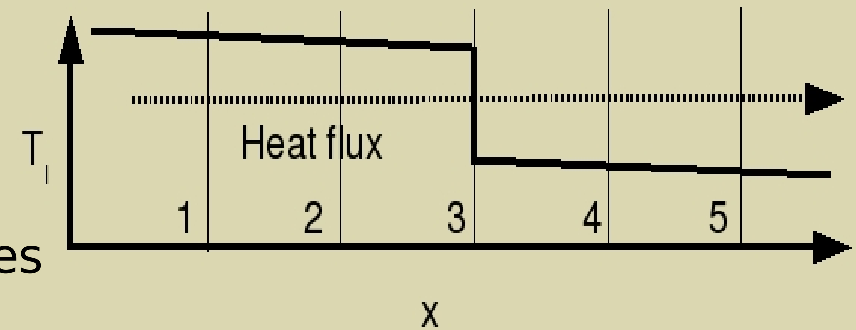
(1) $$\left(\frac{\partial T}{\partial x} \right)^3_{r+1/2} k_1 = k_2 \left(\frac{\partial T}{\partial x} \right)^4_{r+1/2}$$

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

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

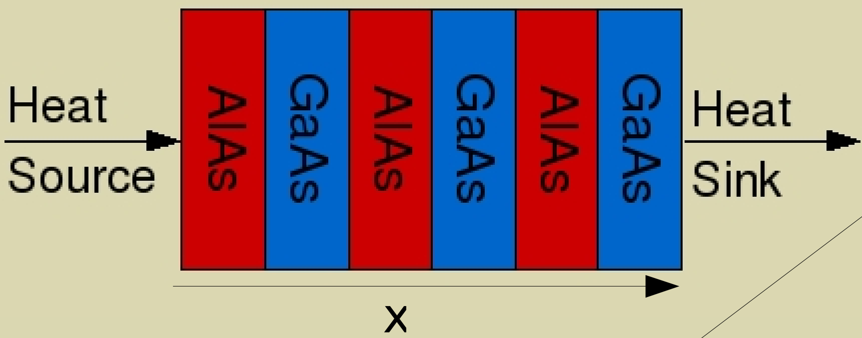
- Adapted[1] from a scheme to model discontinuities Quasi-TE modes of semiconductor waveguides[2]

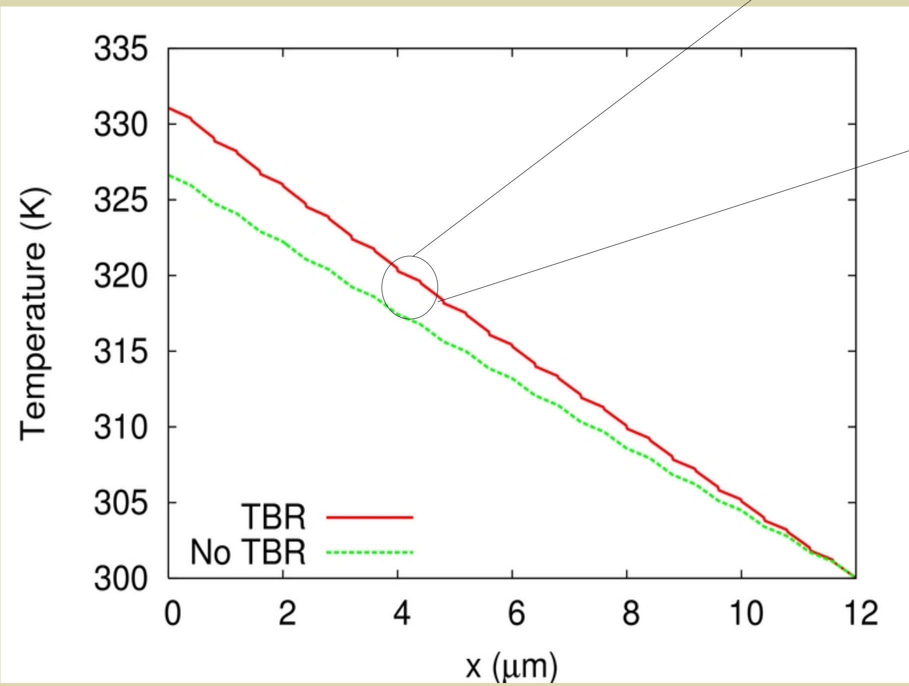




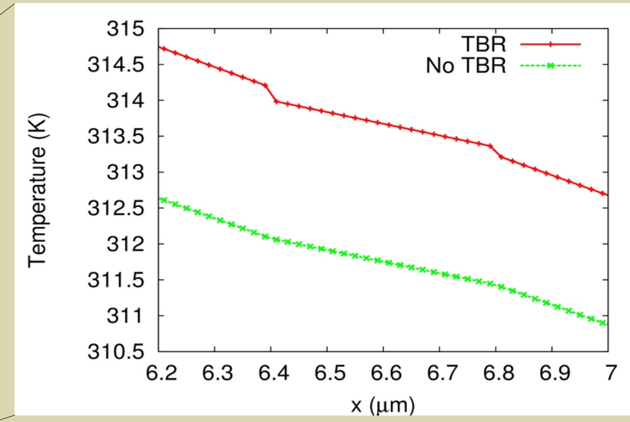
1) R. MacKenzie *et.al.* Phys. Stat.Sol. c accepted for publication, 2) M.S. Stern, IEE Proc. Vol. 135, pp. 56-63 (1998)

Example 1:
Structures with multiple layers

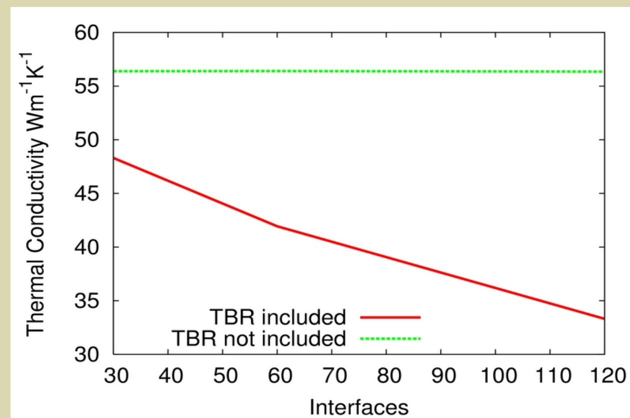




Thermal profile of through a DBR mirror structure of 30 periods



Zoomed in interface

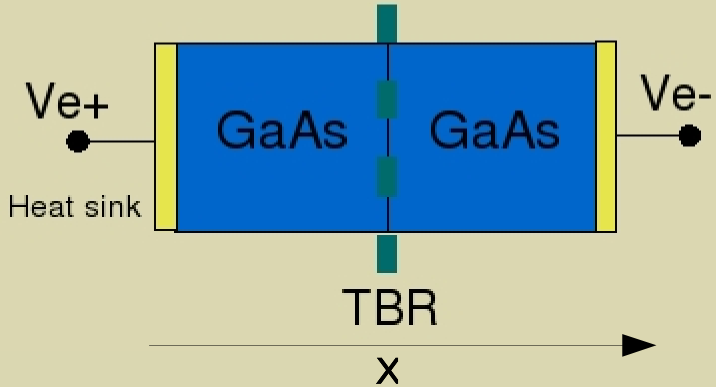


Thermal conductivity as a function of layers

Example 2:
Electron and lattice heat flux within a semiconductor slab

Slab of GaAs with a TBR at the center of it, possibly caused by defects

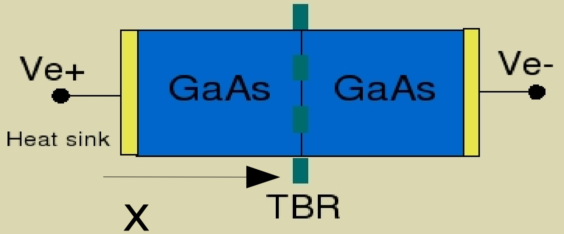
- Doped with $1x10^{23} m^{-3}$ donors
- Apply voltage across device
- Examine interplay of electron heat, lattice heat and TBR

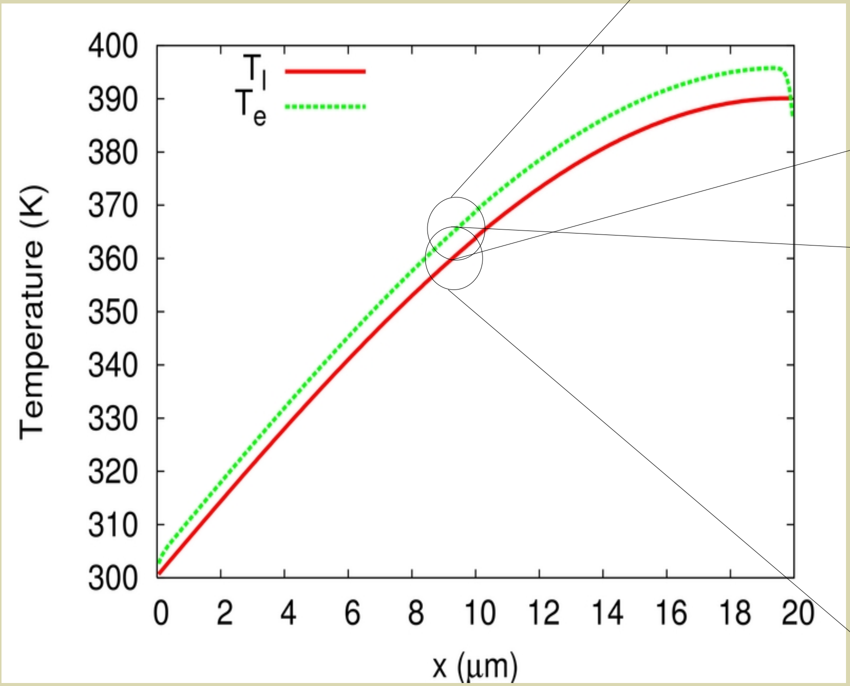


Equations solved:

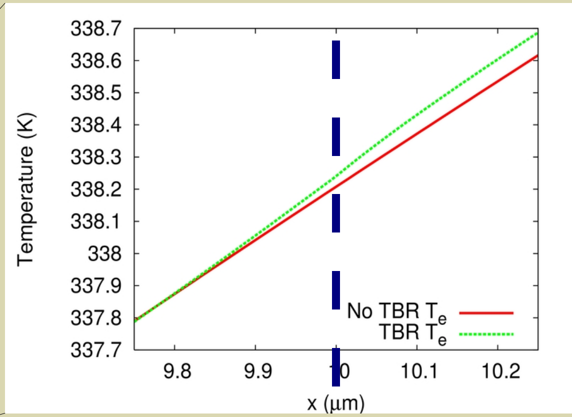
- Lattice heat equation
- Current continuity equation
- Energy balance equation for electrons
  - (0^{th}-2^{nd} moments of B.T.E. -> Hydrodynamic transport model)
- Possion's equation

Example 2:
Electron and lattice heat flux within a semiconductor wire

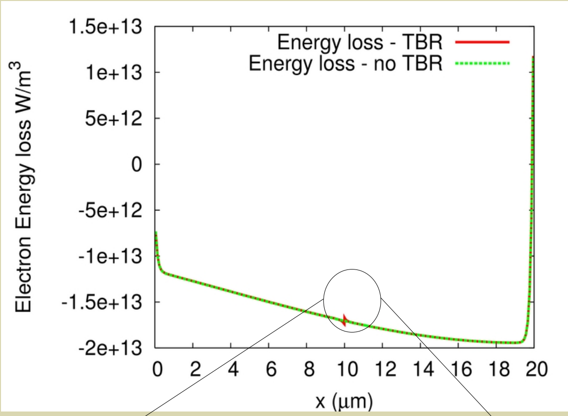




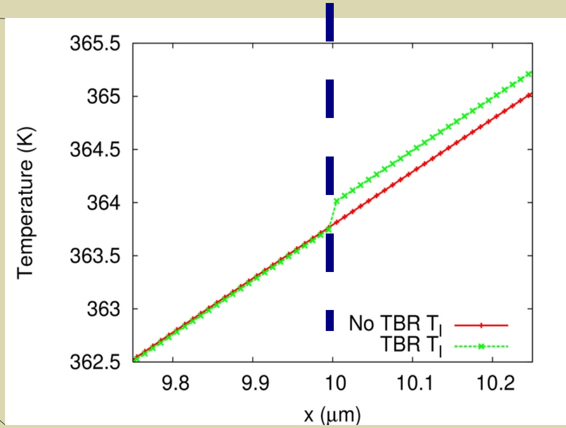
Electron and lattice temperature (without TBR)



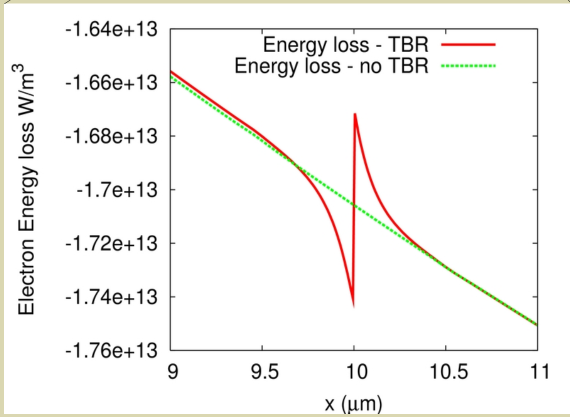
Zoomed in profile of electron temperature



Electron energy loss rate



Zoomed in profile of lattice temperature

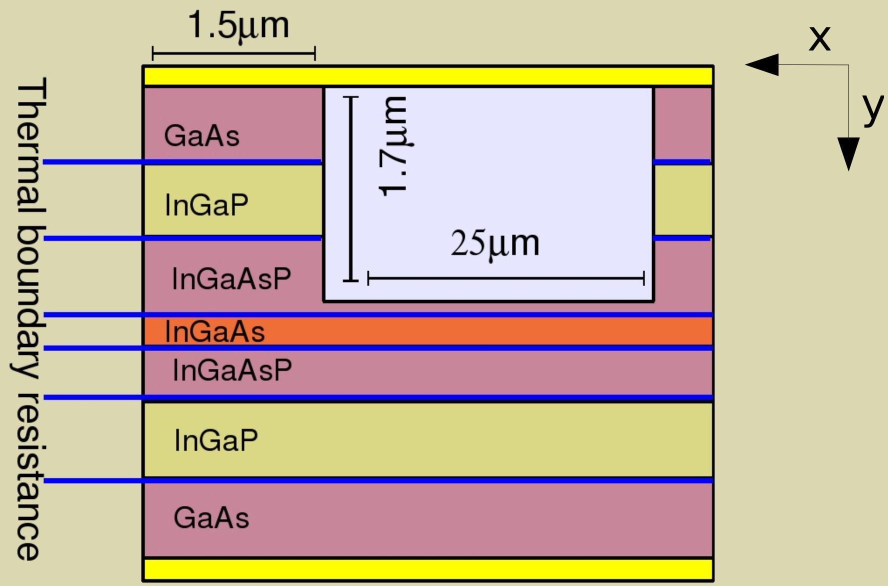


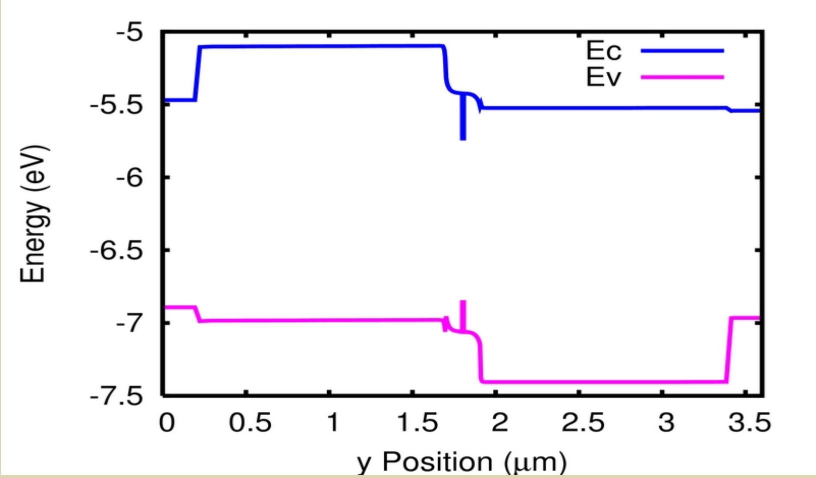
Electron energy loss rate – zoomed in

- Discrete step in lattice temperature, gradual decrease in electron temperature

Example 3:
TBR in high-power edge-emitting lasers

QW material:	$In_xGa_{x-1}As$
Number of QWs:	1
Front facet output power:	P_{out} = 1 – 1.2 W
Device length:	2mm
Back facet coating:	0.90
Front facet coating:	0.03



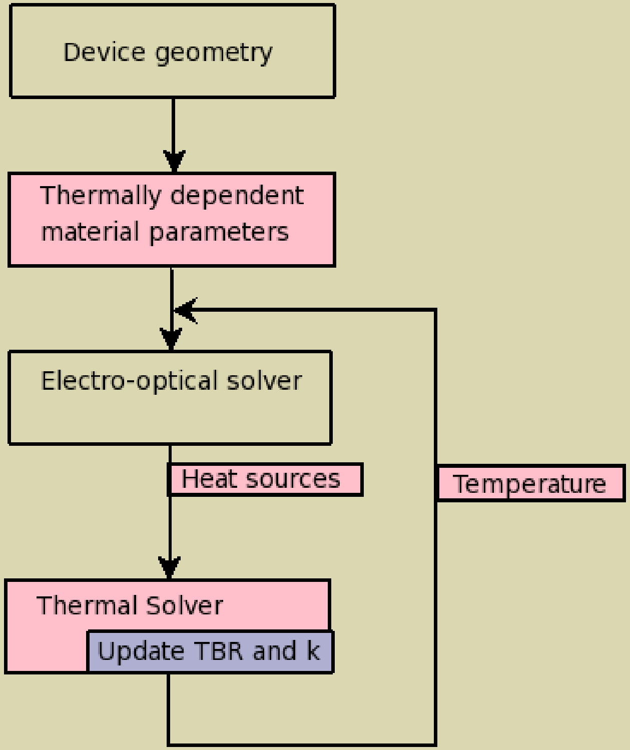


- Half space simulations
- TBR introduced at each epitaxial interface
- Typical applications
  - Pumping EDFAs @ 980nm

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 the QW
- 4 temperature model for the QW
  - Electron, hole, LO-phonon and lattice temperatures
- 2D lattice heat equation
  - Heat sources derived from 2^{nd} moment of BTE



Optical Model

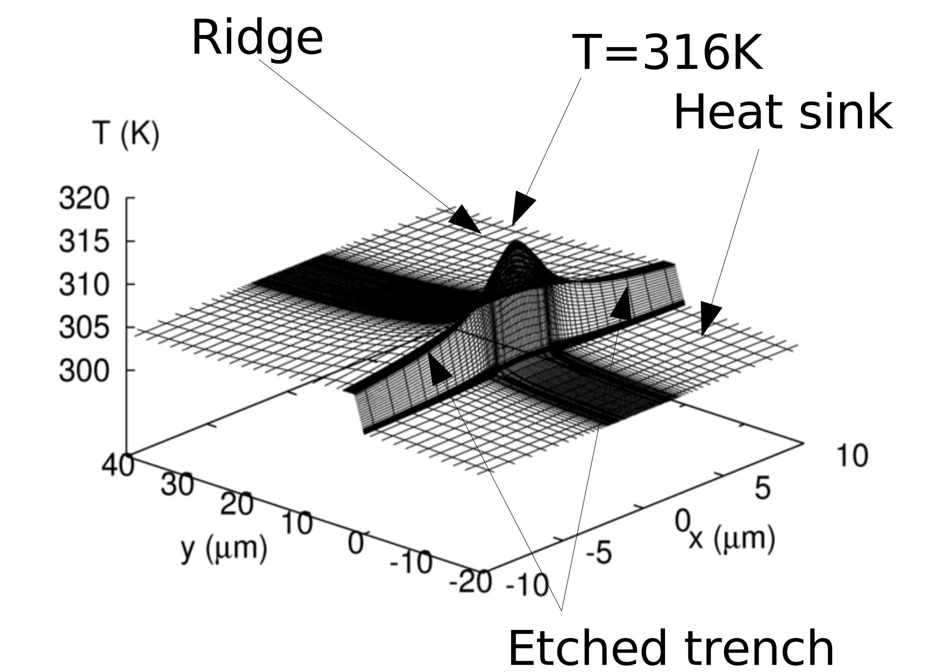
- Photon rate equation
- Valance band structure calculated using 4x4 band ***k.p***
- Parabolic band model for the conduction band
- Fermi's Golden rule used to calculate the stimulated and spontaneous emission rates
- 2D mode solver

All equations solved using Newton's method

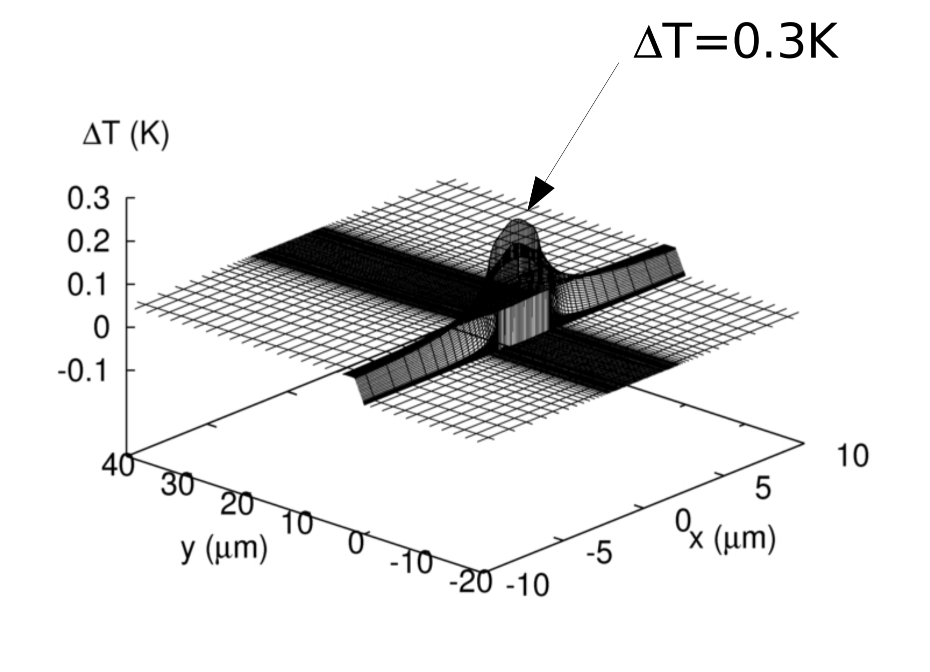
2D thermal profiles and the impact of TBR

The University of Nottingham

2D thermal profile



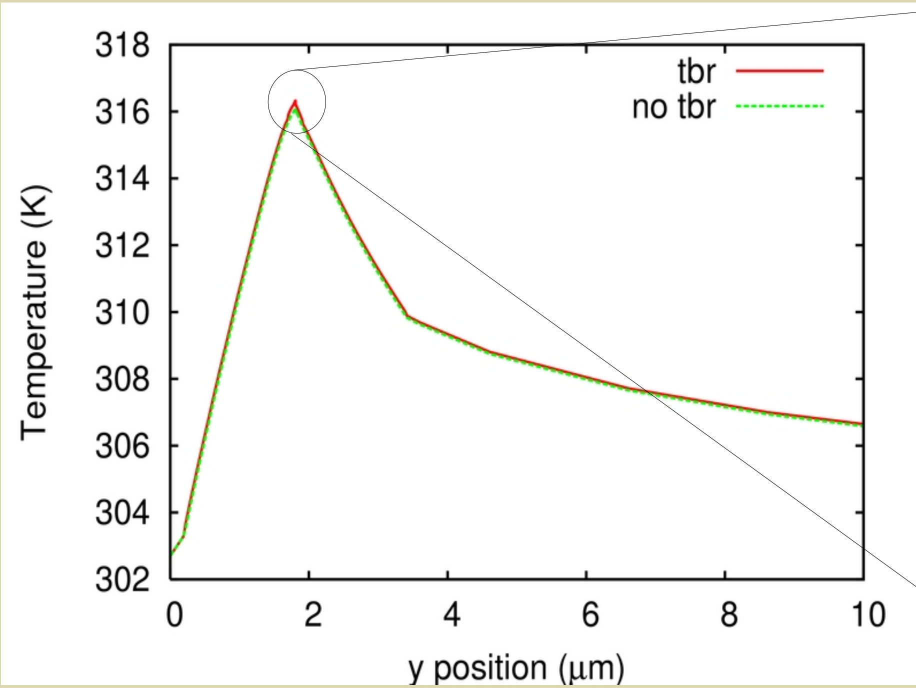
Temperature increase caused by TBR



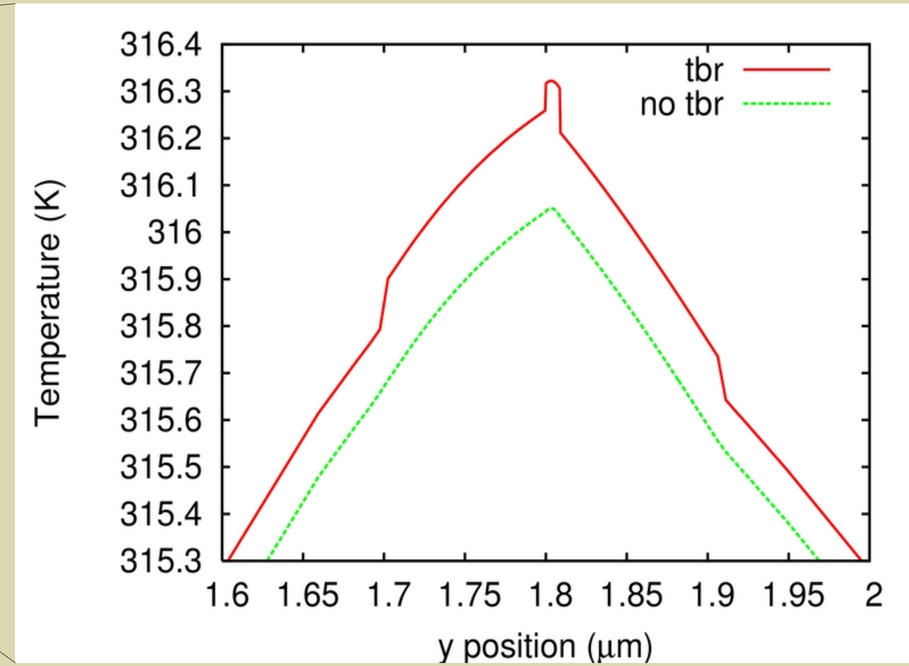
- A sudden increase in the temperature is observed
- An increase of up to 0.3K is observed in the QW

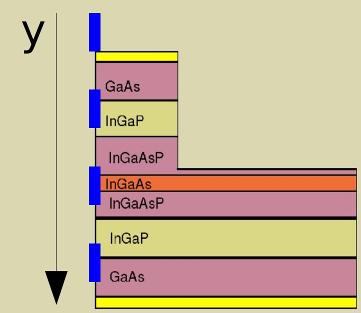
Vertical thermal profile with with and without TBR

Vertical thermal profile



Zoomed in profile

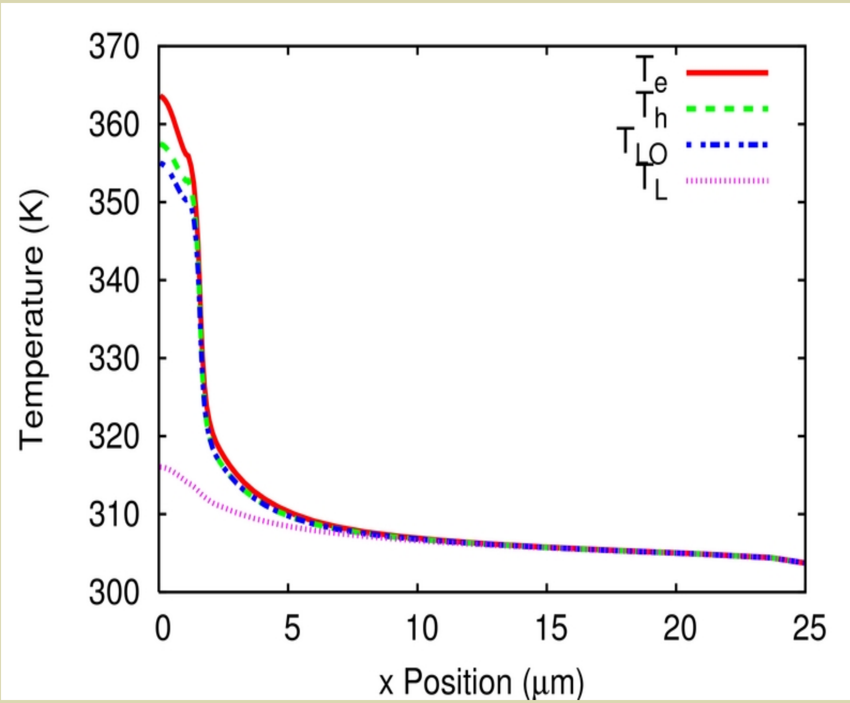




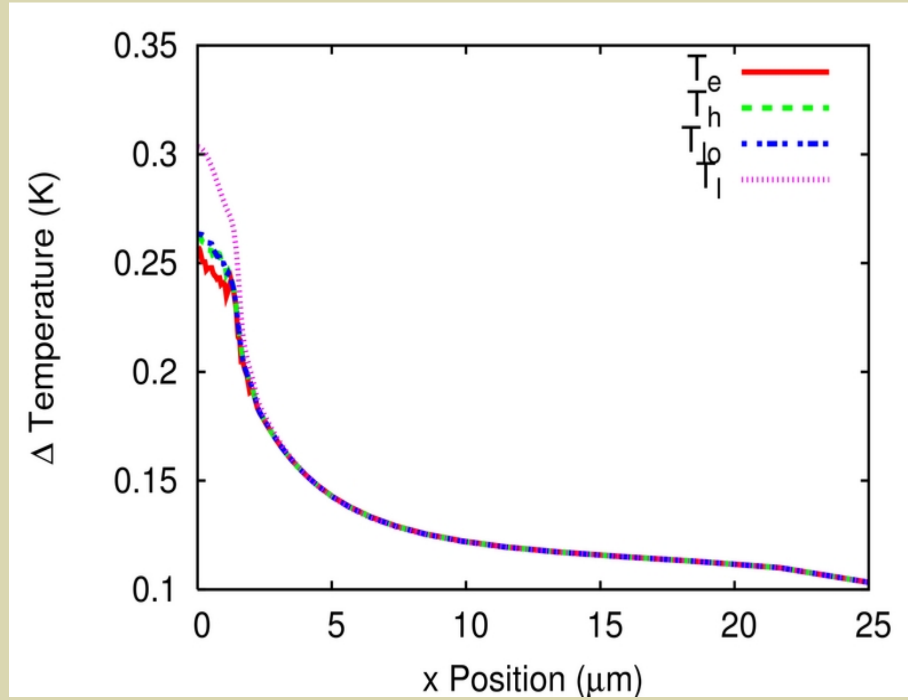
- Up to half a degree difference in peak temperature of device
- Small temperature differences are important for accurate models

Horizontal electron, hole , LO-phonon and lattice temperatures in the QW

Temperature profiles



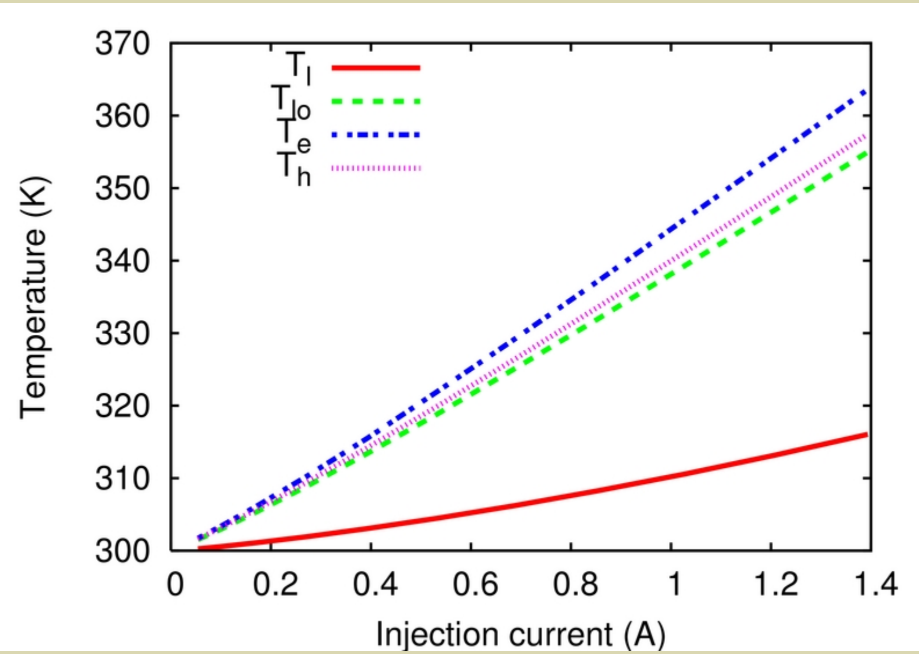
Change in QW temperatures due to TBR



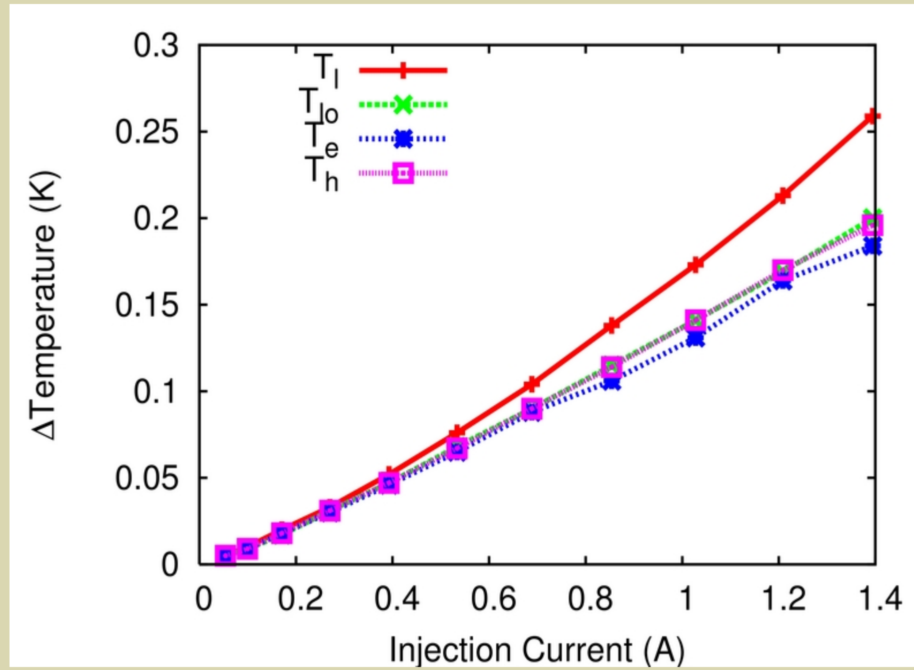
- The lattice temperature is affected most by the TBR
  - Electron, hole and LO-phonon temperatures are dominated by injection current and radiative emission

Impact of TBR on QW temperature

QW Temperatures as a function of injection current



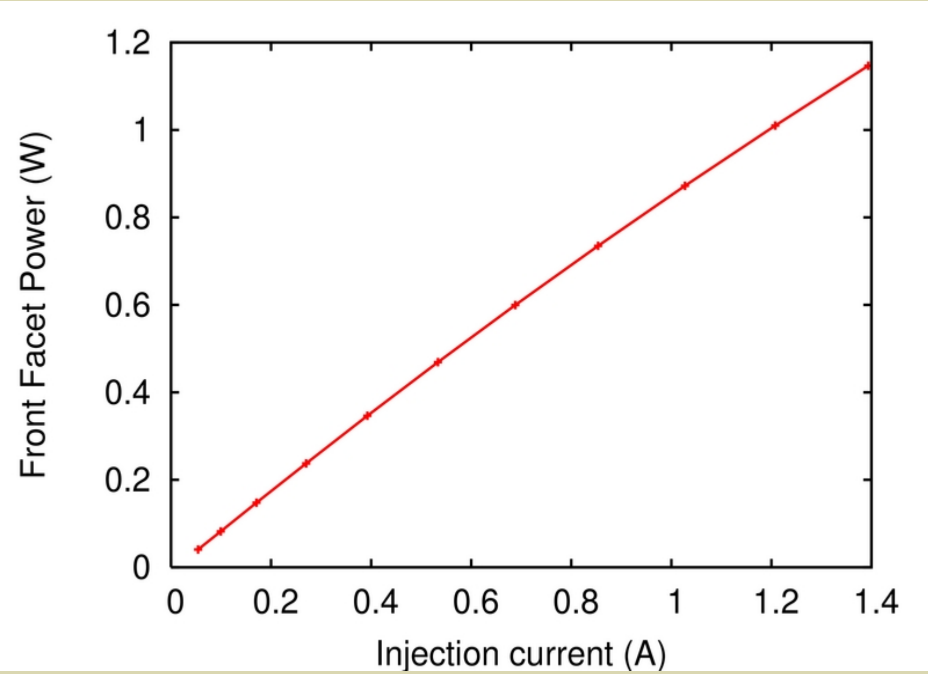
Difference in QW temperatures due to TBR



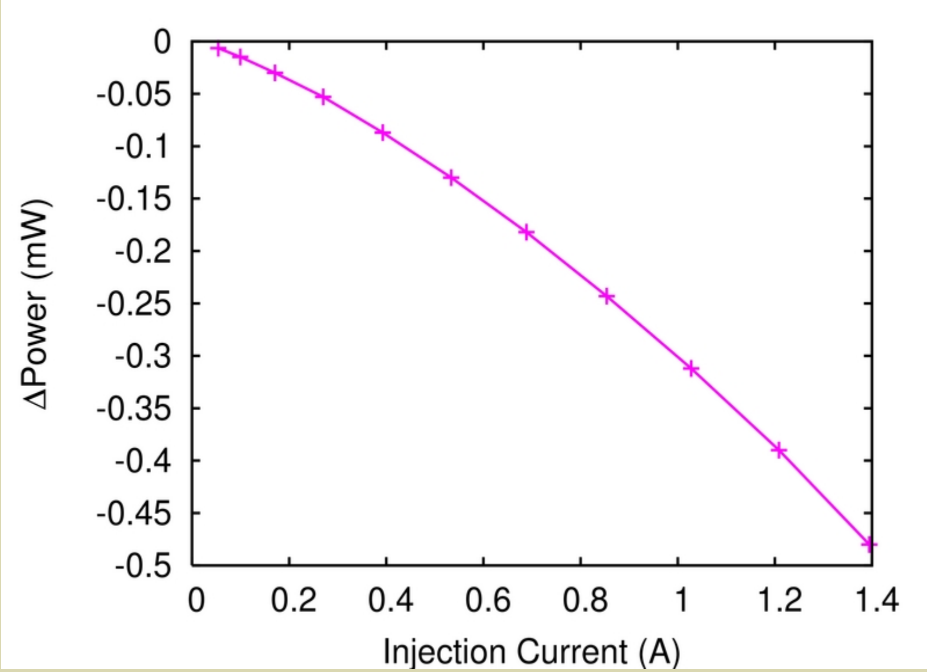
- An increase in QW temperature of up to 0.25K is observed
  - Lattice temperature affected more than that of the electron/hole/LO-phonon populations

Impact of TBR on front facet power

L-I curve for heatsink temperature held at 300K



Impact TBR has on L-I curves



- A decrease of up to 0.5mW in optical power is expected due to TBR

Conclusions

- *Multi layer structures*
  - TBR has a larger impact on multi layer structures
  - However, change in phonon density of states must be taken in to account when layer thickness is comparable to phonon mean free path.
- Electron heat/Lattice heat/TBR interaction
  - Lattice heat affected by TBR / Electron heat not abrupt
- *High power 980nm ridge waveguide lasers*
  - As bias current is increased -> more heat generation -> more heat flux -> TBR has a larger impact
  - Electron/hole/LO-phonon temperatures are not affected as much as lattice temperatures by TBR
  - TBR has been shown to increase the predicted temperature of 980nm EELs by up to 0.3K
  - A 0.5mW decrease in optical power is predicted
- Need for more ***more accurate*** TBR values - Ideally from experiment
  - Better numerical models for calculation of TBR are also needed