The impact of thermal boundary resistance in opto-electronic devices


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

e-mail: eexrm1@nottingham.ac.uk
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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 980nm 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

- This effect is mainly due to phonon scattering/reflections at material interfaces
- TBR first observed by Kapitza (1941)²

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Consider a superlattice with a period $L$, where $\Lambda$ is the average phonon mean free path ($\approx 20\text{nm}$)

**One can distinguish two regimes:**

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

2) $L \ll \Lambda$  \hspace{1cm} 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 ($m^2 K/W$): 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$[1] \approx 7 - 8 \times 10^{-8}$

Discretization scheme for inclusion of TBR

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

\[ \rho L C_L \frac{\partial T}{\partial t} = \nabla \cdot (k \nabla T) + H \]

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

\[
\frac{\partial T}{\partial x} \bigg|_{1/2}^3 = k_1 = k_2 \frac{\partial T}{\partial x} \bigg|_{-1/2}^4
\]

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

\[
T^{3}_{1/2} - T^{4}_{-1/2} = R k_1 \left( \frac{\partial T}{\partial x} \right)^3_{1/2}
\]

- Adapted from a scheme to model discontinuities Quasi-TE modes of semiconductor waveguides\(^{1,2}\)

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Example 1: Structures with multiple layers

Thermal profile of through a DBR mirror structure of 30 periods

Thermal conductivity as a function of layers

Zoomed in interface
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 \(1 \times 10^{23} \text{ m}^{-3}\) 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
  - \((0\text{-}2\text{nd moments of B.T.E.} \rightarrow \text{Hydrodynamic transport model})\)
- Possion's equation
Example 2: Electron and lattice heat flux within a semiconductor wire

- Discrete step in lattice temperature, gradual decrease in electron temperature
Example 3: TBR in high-power edge-emitting lasers

- QW material: $\text{In}_x\text{Ga}_{1-x}\text{As}$
- 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

- TBR introduced at each epitaxial interface
- Typical applications
  - Pumping EDFAs @ 980nm
Electro-thermal Model
- Bipolar 2D Drift Diffusion (DD) model 0\textsuperscript{th} and 1\textsuperscript{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\textsuperscript{nd} moment of BTE

Optical Model
- Photon rate equation
- Valance band structure calculated using 4x4 band \textit{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

- An increase of up to 0.3K is observed in the QW
- Injection current of 1.4A resulting in 1.2W of output power
• Up to half a degree difference in peak temperature of device
• Small temperature differences are important for accurate models
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

- 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

Difference in QW temperatures due to TBR
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 into account when layer thickness smaller than phonon mean free path.

- **Electron heat/Lattice heat/TBR interaction**
  - Abrupt step in lattice temperature observed
  - Slow variation in carrier temperature over TBR

- **High power 980nm ridge waveguide lasers**
  - As bias current is increased -> more heat generation -> more heat flux -> TBR has a larger impact
  - TBR affects lattice temperatures more than $e^-, h^+, LO$-phonon temperatures.
  - Including TBR increases the predicted temperature of 980nm EELs by up to 0.3K
  - By including TBR 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