Cooling and Seebeck effects in Double-Barrier Semiconductor Heterostructures

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Thematic day « Beyond Fourier »

The 9th of September 2022

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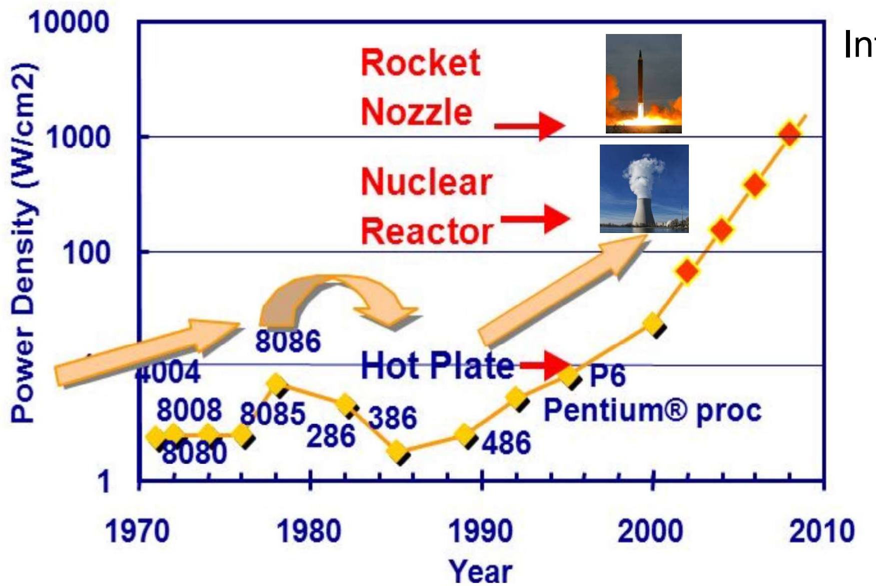
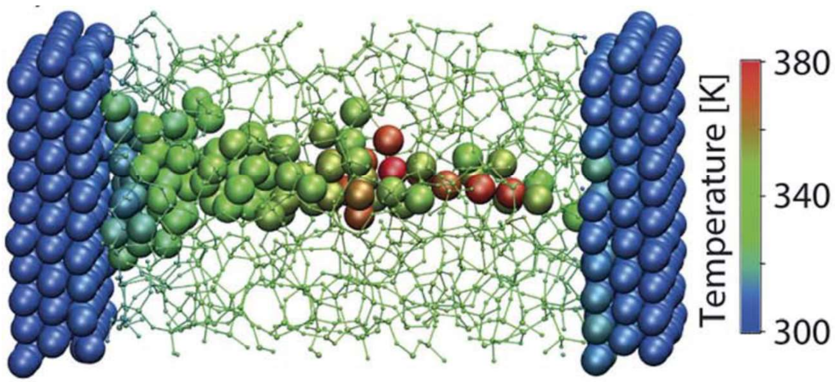
Cooling at the nanoscale

➢ **Self-heating: scientific and industrial issues**



Intel, 2004



CBRAM

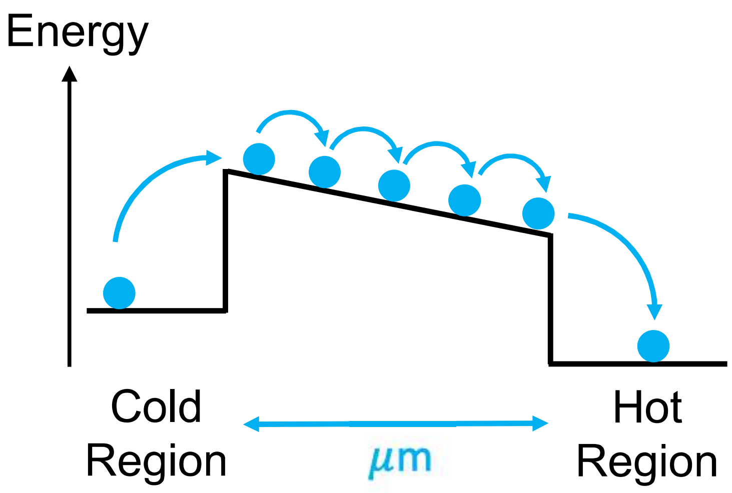
Nanoscale Adv., **2,** 2648 (2020)
M. Luisier, ETH Zurich

➢ Significant reduction of lifetimes and performances.

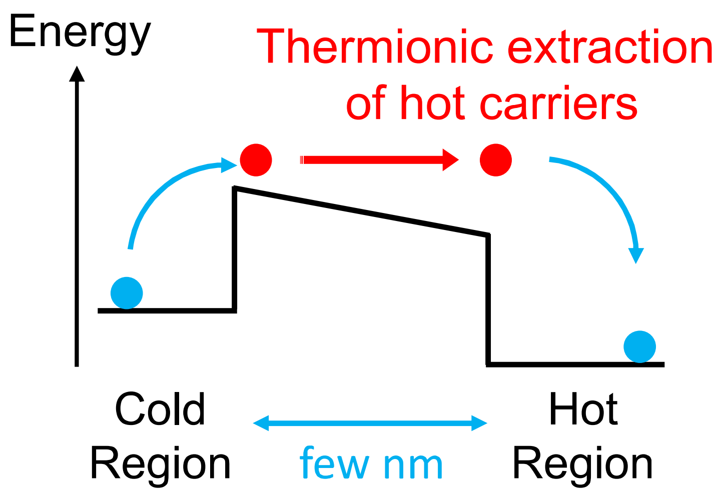
➢ "Bulk" refrigeration is extremely power consuming**.**

Urgent need of local source of cooling

Thermionic cooling*



Thermoelectric Peltier effect



Thermionic cooling

- Devices working in non-equilibrium regime.

Non-equilibrium ➜ Highest cooling power!

- Exploratory field: strong theoretical support.

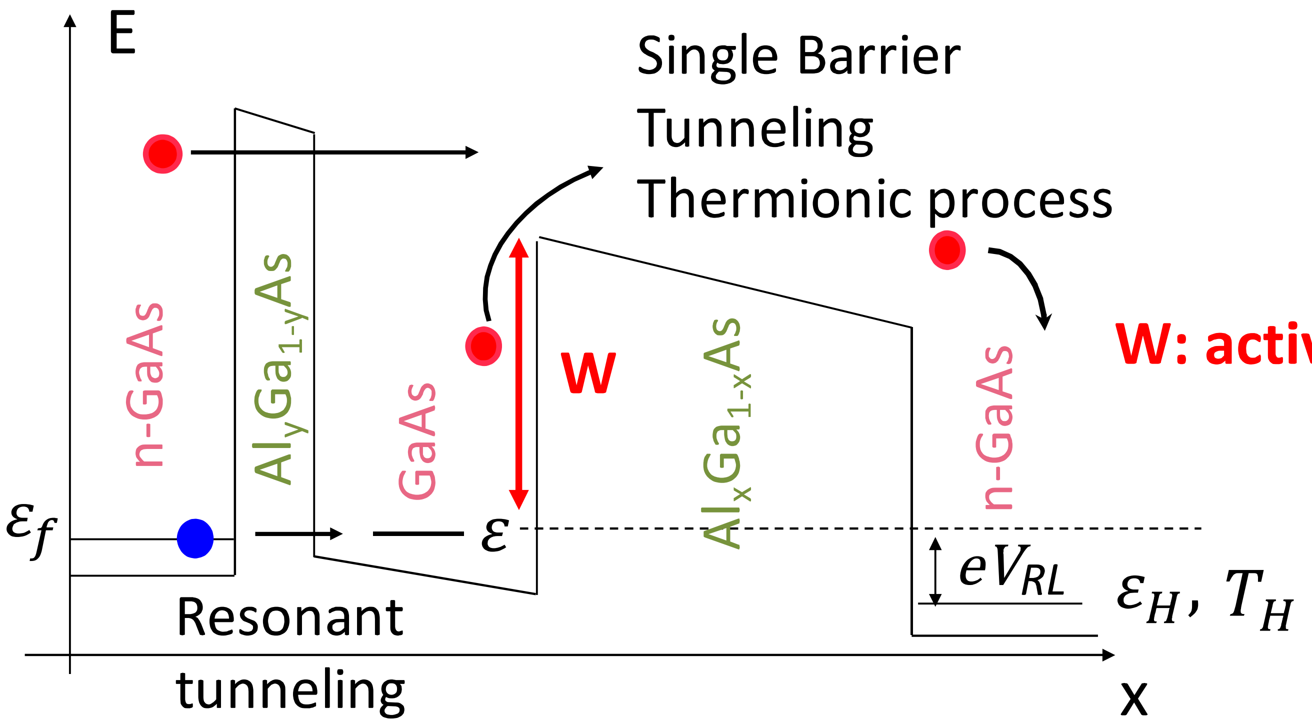
Goal: use nano-structures to improve cooling efficiency.

*G. D. Mahan, *J. Appl. Phys.*, **76**, 4362 (1994).

*G. D. Mahan and L. M. Woods, *Phys. Rev. Lett.*, **80**, 4016 (1998).

Original thermionic cooling devices

- Coupling localized state and tunneling barrier*:



- Main idea: injecting cold electrons and extracting hot electrons.

- Investigate the concept of local temperature at the nanoscale.

*K. A. Chao, M. Larsson, and A. G. Mal'shukov, *Appl. Phys. Lett.*, **87**, 022103 (2005).

Simulations Requirements

Coupling of electron and heat transport

Electron transport

Treatment of quantum effects and non-equilibrium phenomena

Heat transport

- Electron → Non-Equilibrium Green's Function (NEGF) 👌
  - Effective mass approach, k.p, tight-binding, ab initio…
- Heat → Non-Equilibrium Green's Function (NEGF) 😅

Much less documented topic:
Harmonic (ballistic): N. Mingo and L. Yang, *Phys. Rev. B* **68**, 245406 (2003).

NEGF for phonon

- NEGF for electrons: Schrödinger equation

$$(E\mathbf{I} - \mathbf{H})\overline{\psi} = \bar{0} \quad \Rightarrow \quad \left[G^R(E)\right]$$

- NEGF for phonons: dynamical equation

$$\omega^2 \mathrm{M} + \Phi_{nm}^{ij} \bar{R} = \bar{O} \quad \text{with} \quad \Phi_{nm}^{ij} = \frac{\partial^2 V^{harm}}{\partial R_n^i \, \partial R_m^j}$$

Vibration frequency (ω^2) · Mass of the atoms (matrix) (M) · 2^{nd} order FC (Φ_{nm}^{ij}) · Displacement of the atoms (R_n^i)

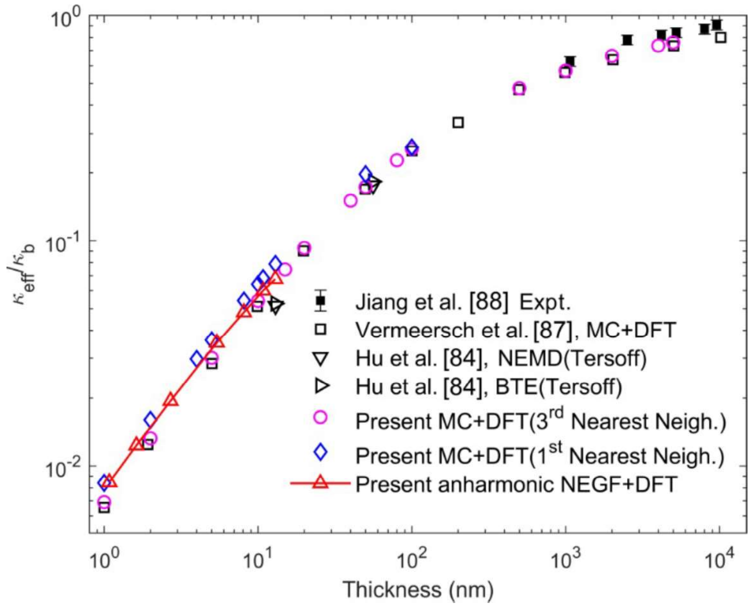
Retarded Green's function $$\mathbf{G}^{\mathrm{R}}(\omega) = [\omega^2 \mathbf{I} - \mathbf{\Phi} - \mathbf{\Sigma}^{\mathrm{R}}(\omega)]^{-1}$$

- Anharmonic: N. Mingo, *Phys. Rev. B* **74**, 125402 (2006). (junctions)
J. S. Wang, N. Zeng, J. Wang, and C. K. Gan, *Phys. Rev. E* **75**, 061128 (2007).
M. Luisier, *Phys. Rev. B* **86**, 245407 (2012). (nanowires)
K. Miao *et al., Appl. Phys. Lett*. **108**, 113107 (2016). (Büttiker Probes)
J. H. Dai and Z. T. Tian, *Phys. Rev. B* **101**, 041301 (2020). (interfaces)
R. Rhyner and M. Luisier, *Phys. Rev. B* **89**, 235311 (2014). (NEGF coupling e-/ph!!)

NEGF for phonon

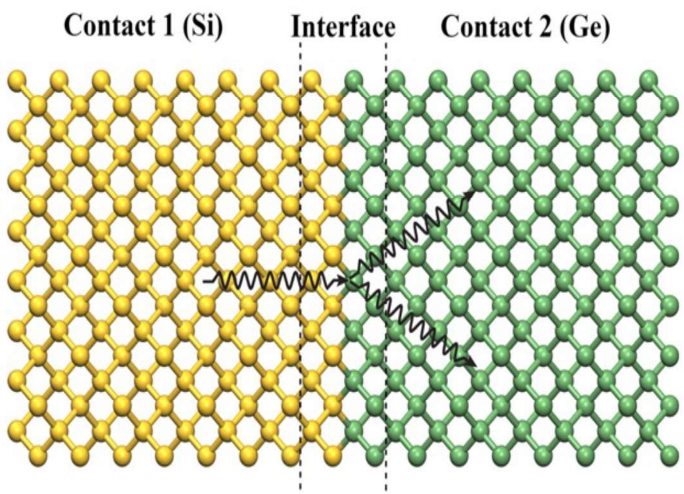
➢ Anharmonic phonon NEGF development: additional issues

Thermal conductivity Si film



Y. Guo, *et al., Phys. Rev. B*, **102**, 195412 (2020).

Si/Ge interface



Y. Guo, *et al., Phys. Rev. B* **103** (17), 174306 (2021).

➢ Anharmonicity:

1) Non-local treatment of the phonon-phonon self-energies!
2) 4^{th} order force constant might be needed…

→ NEGF for phonons can be only applied to rather small (tens of nanometers) systems.

Alternative approach:

NEGF for electrons
+
Heat equation

→ M. Bescond *et al. J. Phys.: Condens. Matter* **30**, 064005 (2018).

LIMMS Laboratory for Integrated Micro-Mechatronic Systems LIMMS/CNRS-IIS UMI 2820 · cnrs · im2np Institut Matériaux Microélectronique Nanosciences de Provence · Aix*Marseille université initiative d'excellence · Institute of Industrial Science The University of Tokyo

NEGF + Heat equation

- **Non-equilibrium Green's function coupled to heat equation***

NEGF equations for electrons

$$G^r_{k_t} = \left[(E-V)I - H_{k_t} - \Sigma^r_{L,k_t} - \Sigma^r_{R,k_t} - \Sigma^r_{S,k_t}\right]^{-1}$$

Poisson equation

$$\nabla.(\epsilon\nabla V) = -\rho\left[G^{\lessgtr}\right]$$

Heat equation

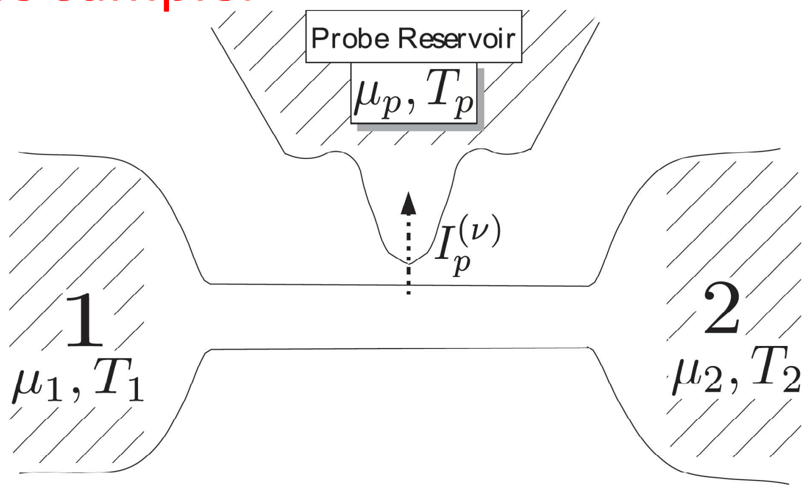
$$\left[-\frac{\partial}{\partial x}\left[\kappa_{\text{th}}(x)\frac{\partial}{\partial x}T_{AC}(x)\right]\right]_j = Q_j$$

- Most of physical properties: current, electron density, LDOS, local phonon temperatures, cooling power, efficiency…
- But… We are in a strong non-equilibrium regime… $T_{AC} \neq T_{POP} \neq T_e$
- Temperature of electrons in the active region???

Electronic temperature: virtual probe technique

- System out of equilibrium:
  Electronic and lattice temperatures usually not coincide.
- Accurate electronic temperature measurement (i.e. that follows the thermodynamic laws) requires simultaneously local voltage measurement.[1,2]
- Technique: vanish net charge current ($I_p^{(0)}$) **and** net heat current ($I_p^{(1)}$) into the probe.
  --> probe in local equilibrium with the sample.

$$I_p^{(\nu)} = 0, \quad \nu \in \{0, 1\}$$

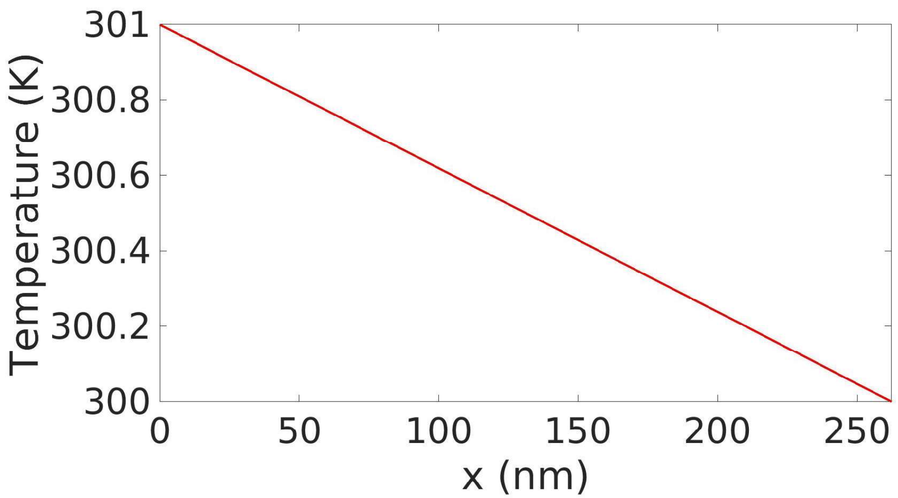


[1] C. A. Stafford, *Phys. Rev. B* **93**, 245403 (2016).
[2] A. Shastry and C. A. Stafford, *Phys. Rev. B* **94**, 155433 (2016).

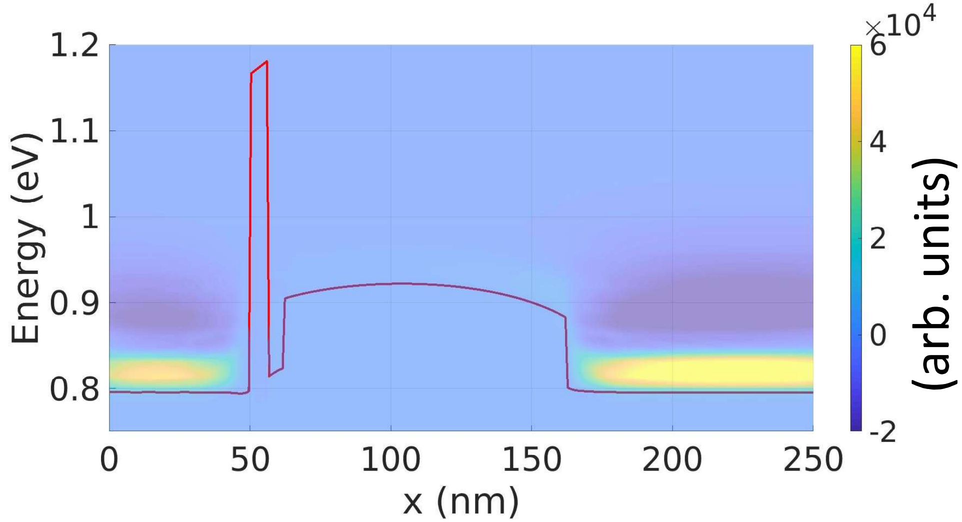
Thermoelectric properties

Lattice temperature gradient

ΔT=1 K



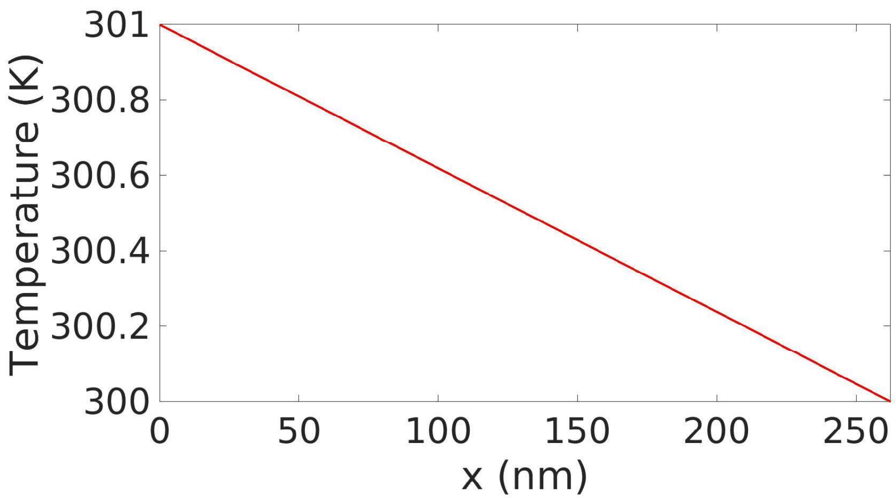
Current spectrum



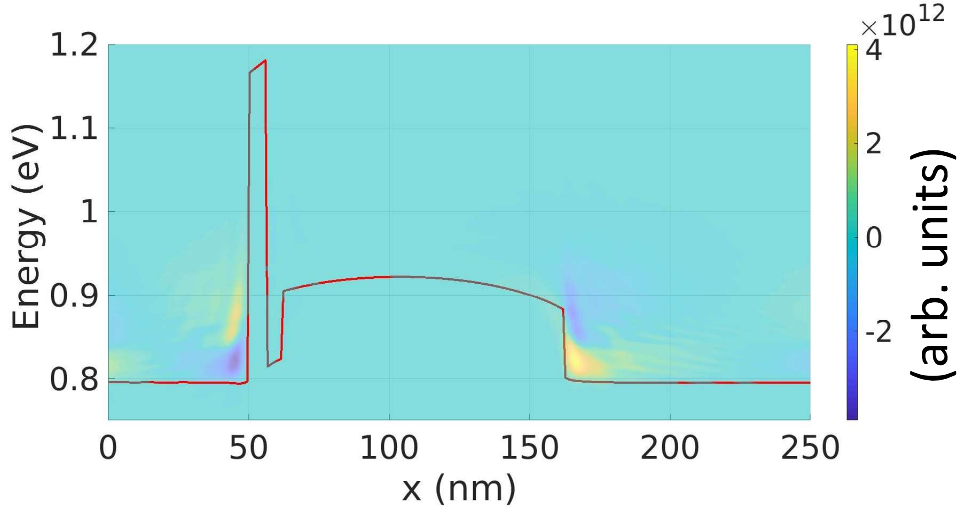
- Two current components in the access regions.
- At the barrier: phonon emission/absorption and back flow towards the contacts

Lattice temperature gradient

ΔT=1 K



Derivative of energy current



- Two current components in the access regions.
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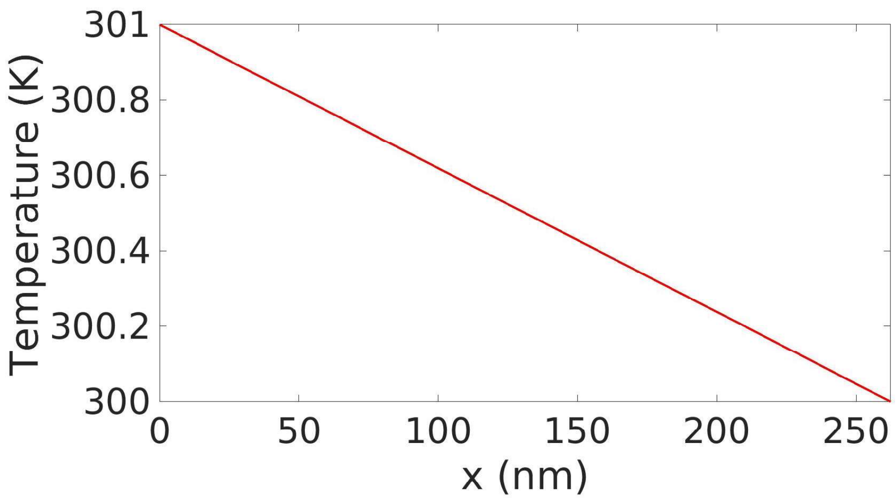
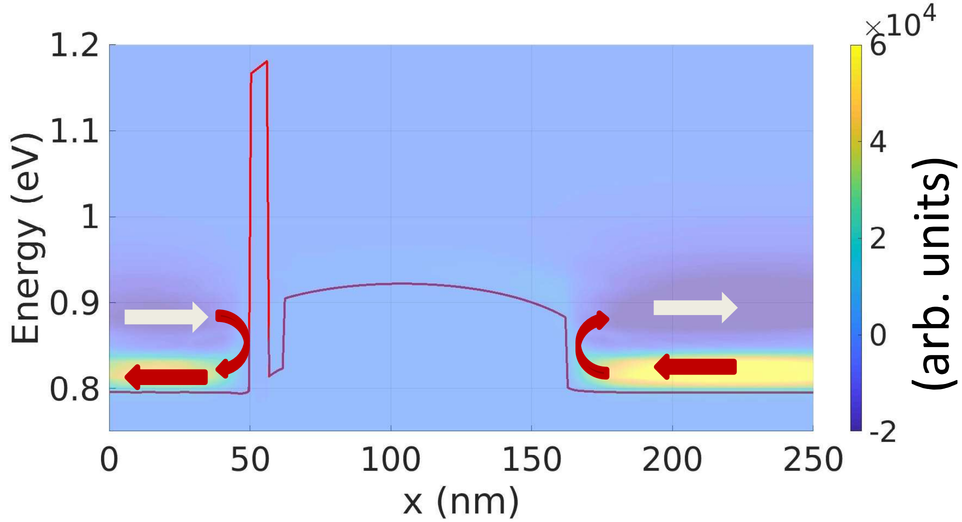
Lattice temperature gradient

ΔT=1 K



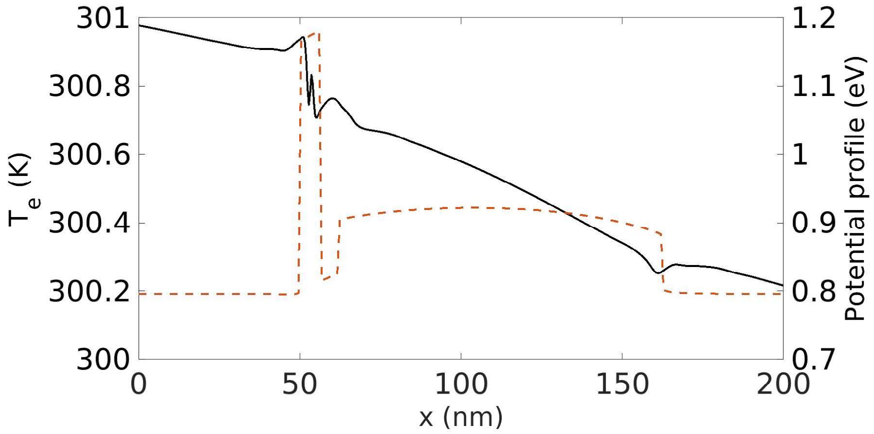
Current spectrum

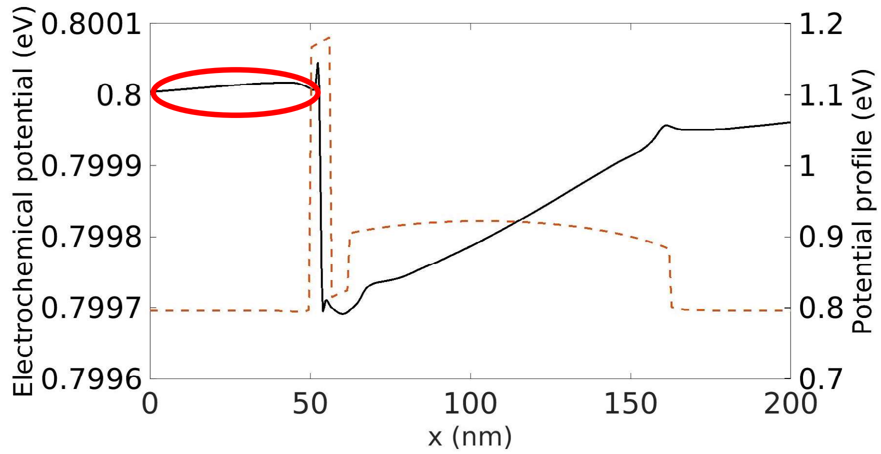


- Two current components in the access regions.
- At the barrier: phonon emission/absorption and back flow towards the contacts

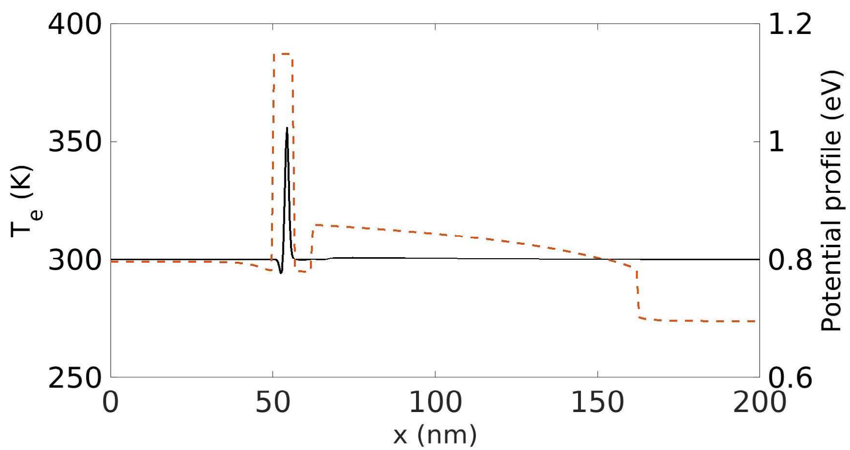
Electron temperature and Chemical potential

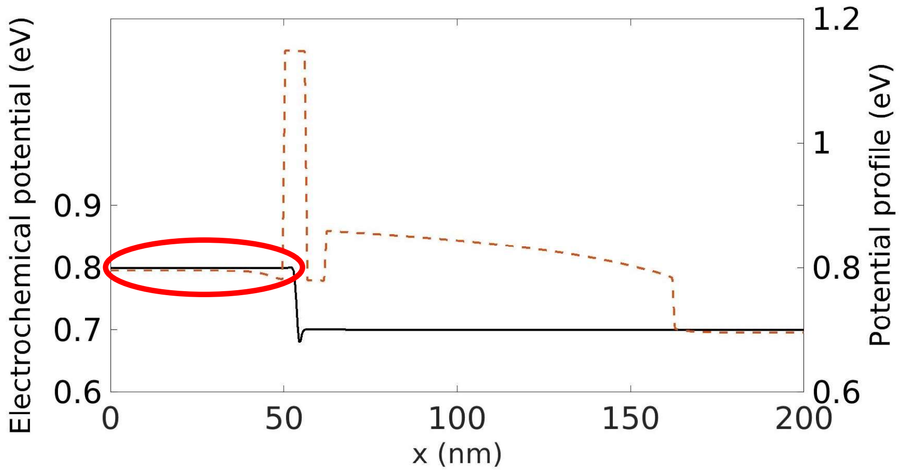
ΔT=1 K, ΔV=0 V





ΔT=0 K, ΔV=0.1 V

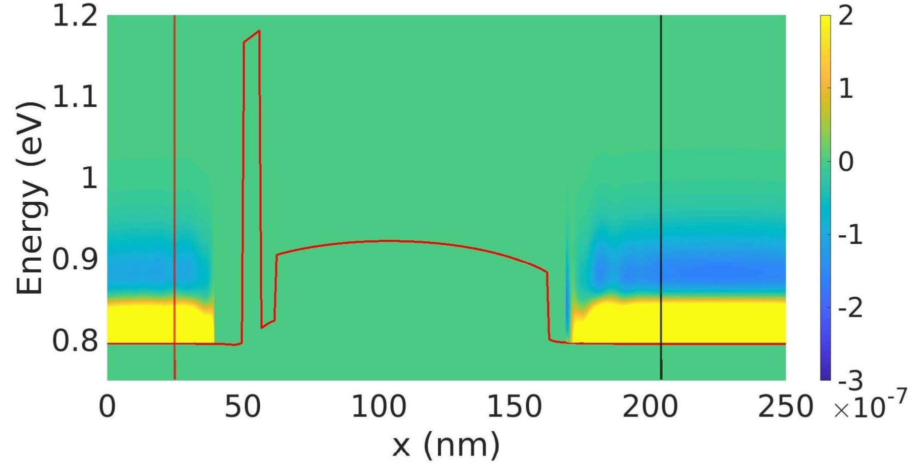




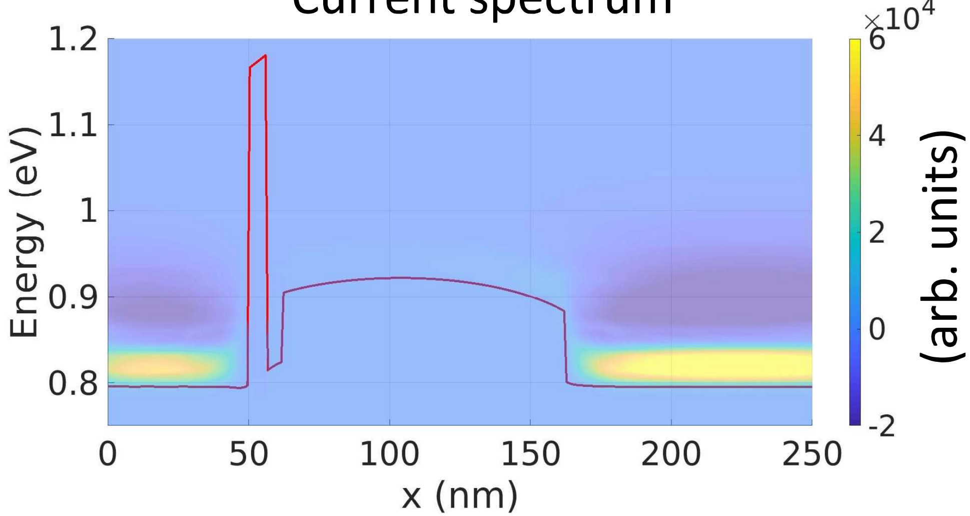
Difference of the Fermi-Dirac distributions

ΔT=1 K, ΔV=0 V

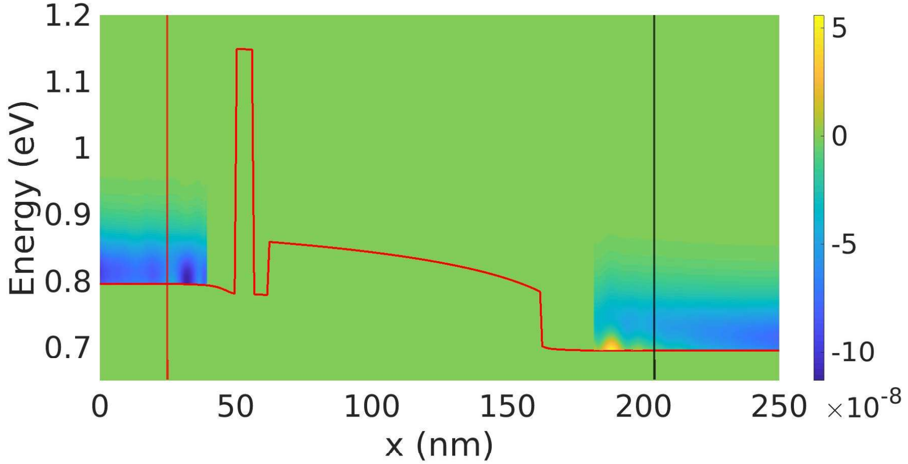
Δf_{FD}

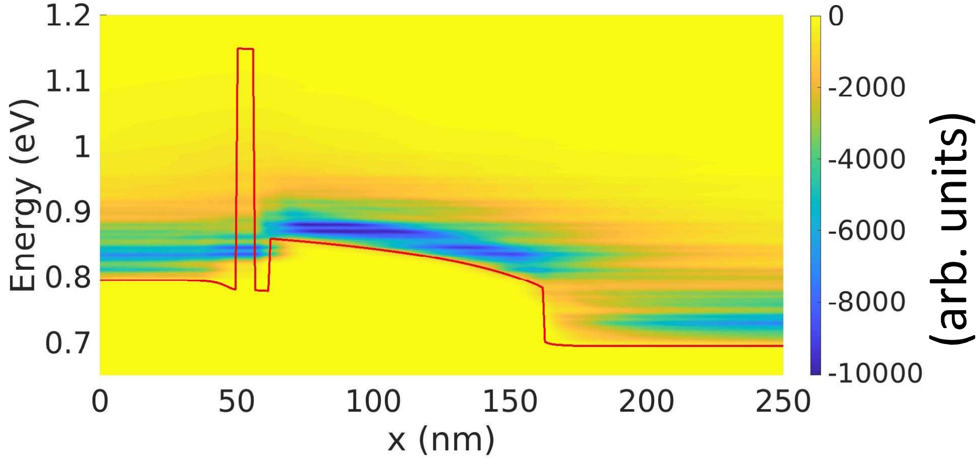


Current spectrum



ΔT=0 K, ΔV=0.1 V

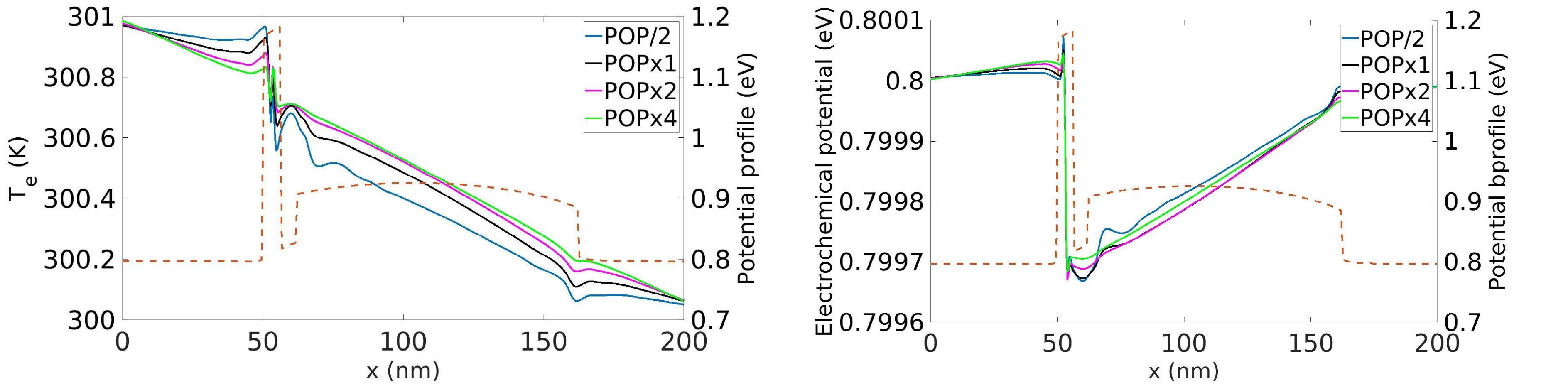




Origin of the reverse current component

- Reverse current: due to the variation of μ in the device.
- Increase of μ required to maintain the electron density with a ΔT_e.

Impact of the electron-phonon coupling



- Increasing coupling: T_e follow $T_{Lattice}$

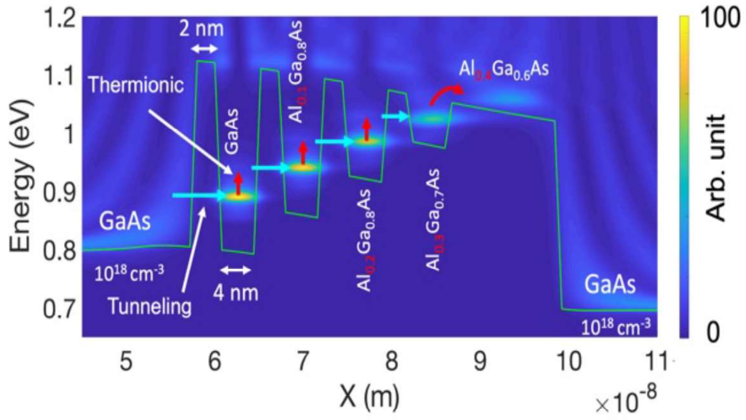
➡ Larger T_e decrease

➡ Larger μ increase

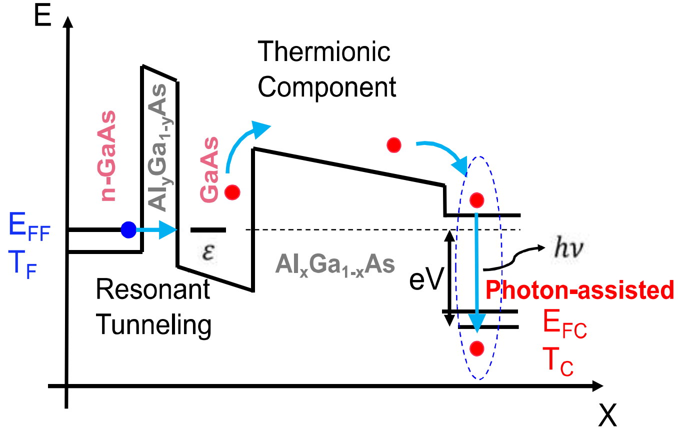
Conclusion

- **Coupling NEGF and heat equation:** good insight of the physical properties of the thermoelectric systems (good agreement with experiment).

- **Conception and optimization of devices**



Quantum cascade cooler



Opto-thermionic pumping

Novel generation of cooling devices

ANR GELATO (Oct. 2021- Apr.2025)

LIMMS, CNRS, IIS-University of Tokyo:

- Pr. Kazuhiko Hirakawa

Dr. Chloé Salhani
Post-doc

Mr. Xiangyu Zhu
PhD student

NQS group, IM2NP, CNRS, Aix-Marseille University:

Pr. N. Cavassilas

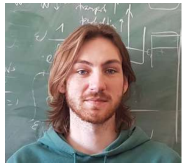
Dr. F. Michelini
(Assoc. Pr.)

Dr. A.-M. Daré
(Assoc. Pr.)

Prof. M. Lannoo
(Emeritus)

Celine Belabbas (Intern)

Dr. A. Crépieux
(Assoc. Pr. at CPT)



Mr. G. Etesse
(PhD student)

Thank you!