Thermally-Excited Nonequilibrium States Between Electrons and Phonons for Energy Conversion

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Phonon Transport

Superlattices

Nanocomposites

Boltzmann Eq. Approach

Monte Carlo Simulation

Molecular Dynamics

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Thermoelectric Materials

ONR MURI (K.L. Wang, Dresselhaus)

NASA (Z.F. Ren/J.-P. Fleurial/M.S. Dresselhaus)

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Motivation

- It is relatively easy to electrically drive electron and phonon out of equilibrium: hot and cold electrons.
- Can we drive electrons and phonons out of equilibrium by a temperature difference?

Cold Electrons in Thermoelectrics

Hot Electrons in MOSFET
Potential-Step Amplified Thermal Electric Energy Converter (PANTEC)

Region 1  Region 2

Potential Interface

Forward Structure

Reverse Structure

G. Chen
J. Appl. Phys.
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Sharp Interface:
1. Electron Mean Free Path > Space Charge Region
2. Single Carrier Transport
Interface Transport

- Charge Balance
- Energy Balance

- Interface Seebeck Effect

\[ S_i \approx \frac{E_{f1} - E_{f2}}{e(T_{e1} - T_{e2})} = -\frac{\kappa_B}{e} \left( 2 + \frac{E_{c1} - E_{f2}}{\kappa_B T_{e1}} \right) \]

Interface Seebeck Voltage = \( S_i (T_{e1} - T_{e2}) \)

Mahan et al., JAP (1998)
Amplification of Temperature Discontinuity

\[ (T_{e1} - T_{e2})_f \propto -\frac{k_{e2}}{J_{R,f}} \frac{dT_{e2}}{dx} \]

Amplification Factor

\[ (T_{e1} - T_{e2})_f \sim e^{\Delta / (\kappa_B T_e)} \Lambda e_2 \frac{dT_{e2}}{dx} \]

No Amplification

\[ (T_{e1} - T_{e2})_r \propto -\frac{k_{e2}}{J_{R,r}} \frac{dT_{e2}}{dx} \]

\[ (T_{e1} - T_{e2})_f \sim \Lambda e_2 \frac{dT_{e2}}{dx} \]
Two-Temperature Modeling Results

\[ \Delta \frac{1}{k_B T} = 8.3 \]

\[ \mu = 20,000 \text{ cm}^2/\text{Vs}; \quad m^* = 0.014 m_e; \quad G = 10^{10} \text{ W/m}^3\text{K} \]

\[ k_p = 1 \text{ W/mK}; \quad n_2 = 3.18 \times 10^{17} \text{ cm}^{-3}; \quad n_1 = 5.8 \times 10^{16} \text{ cm}^{-3} \]
Open Circuit Voltage

- Forward Structure
- Pure Thermoelectric
- Reverse Structure

$n_2 = 1.3 \times 10^{18} \text{ cm}^{-3}$
$G_2 = 10^{11} \text{ W/m}^3\text{K}$
$\mu = 7700 \text{ V cm/s}$
$d_1 = 0.1 \text{ \mu m}$
$d_2 = 5 \text{ \mu m}$
$K_p = 1 \text{ W/mK}$
PANTEC Refrigerator

COLD SIDE TEMPERATURE (K) vs. CURRENT DENSITY (Am⁻²)

- Bulk
- Dots Reverse Structure

- $n_2 = 3.18 \times 10^{17}$ cm⁻³
- $\mu = 20000$ cm²/Vs
- $K_p = 1$ W/mK
- $d_1 = 1000$ Å
- $d_2 = 5$ μm
Surface-Plasmon Coupled Nonequilibrium Thermoelectric Energy Conversion

Nonequilibrium Thermoelectric Devices

- Explore nonequilibrium between electrons and phonons
- Couple the cooling target with thermoelectric element without direct lattice contact

\[ ZT = \frac{\sigma S^2 T}{k_e + \kappa_p} \]

Surface Plasmon Coupling of Electrons

Model Based on Fluctuation-Dissipation Theorem

Three orders of magnitude increase in energy transfer flux due to surface plasmon resonance

Macroscopic gap

Nanoscale gap

Far-Field

Surface Waves
Two Temperature Model

Electrons
\[
\frac{d}{dx} \left( k_e \frac{dT_e}{dx} \right) - G \left( T_e - T_p \right) + \frac{J_p^2}{\sigma} = 0
\]

Phonons
\[
\frac{d}{dx} \left( k_p \frac{dT_p}{dx} \right) + G \left( T_e - T_p \right) = 0
\]

Electron-Phonon Coupling Factor

Coupling Boundary
\[
q_{Load} = q_{sp} \left( T_1, T_e \bigg|_{x=0} \right) = SjT_e \bigg|_{x=0} - k_e \frac{dT_e}{dx} \bigg|_{x=0}
\]
\[
\frac{dT_p}{dx} = 0
\]
Power Generation Mode

Heat Source $T_1$ → Vacuum Gap → Power Generation $T_p$ → Load $T_2$

- $T_1 = 500$ K
- $G = 10^9$ W/(m$^3$ K)
- $G = 10^{10}$ W/(m$^3$ K)
- $G = 10^{12}$ W/(m$^3$ K)
Refrigeration Mode

Cooling Load $q = 50 \text{ W/cm}^2$

- $G = 10^8 \text{ W/(m}^3\text{K)}$
- $G = 10^{10} \text{ W/(m}^3\text{K)}$
- $G = 10^{12} \text{ W/(m}^3\text{K)}$

- Conventional

Caption:

- $k_e/k = 0.1$
- $Z = 0.002 \text{K}^{-1}$
- $T_H = 300 \text{K}$

Graphs showing:
- Cold End Temperature vs. ThermoElectric Element Length
- COP vs. ThermoElectric Element Length

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Surface Wave Experiments

- Extraordinary transmission
- Near field radiation transfer between parallel plates
- Near field radiation transfer between sphere and plate
Phonon-Polariton Extraordinary Transmission

4 \mu m Period 2 \mu m Holes

\[ T_{\text{with holes}} / T_{\text{without holes}} \]

Wavelength \( \lambda \) (\mu m)

Experimental Data
MEEP Calculation

with Soljacic and Joannopoulos
AFM-Based Near-Field Experiment

- AFM measures deflection of cantilever with sub-Å accuracy
- Deflection is generally due to forces between tip and sample
- With a bimetallic cantilever, thermal changes also cause deflections
Initial Experimental Results

- Conductance (W/K^-1) vs. Gap (nm)
- Experimental data
- Near-field theory (two sphere)
- Classical radiative transfer

Graph showing conductance values in the range of $10^{-10}$ to $10^{-8}$ and gap in nanometers from $10^2$ to $10^5$.辅信号 (V) range from -0.3 to -0.8.
How Large is G?

\[ G = \frac{12\sqrt{2}}{\pi^{3/2}} \frac{nm^{5/2} Z_A^2}{\rho \hbar^4 T_e} \left[ \kappa_B T_e \right]^{3/2} \sim 10^{-12} n \left( \frac{m}{m_o} \right)^{5/2} \]

For \( \rho = 5000 \text{ kg/m}^3, Z_A = 4 \text{ eV}, T_e = 300 \text{ K} \)

\[ G \sim n \frac{\kappa_B T}{\tau} \frac{m}{M} = n \frac{e\kappa_B T}{\mu M} \sim 0.4 \times 10^{-12} n \]

For \( \mu = 10000 \text{ cm}^2/\text{Vs}, M \sim 2000 \text{ m} \)
**Hot carrier cooling in III-V**

LO phonon generation and decay limit thermalization

\[ Q \sim n_e \cdot E_p / \tau_{eff} \]
\[ 1/Q = 1/Q_{gen} + 1/Q_{decay} \]
\[ Q_{gen} \sim n_e \cdot E_p / \tau_{LO} \]
\[ Q_{decay} \sim n_p \cdot E_p / \tau_{LA} \]

Carriers at 600K:
- Bulk: \( Q_{decay} \sim 10^{16} \text{ W/m}^3 \)
- MQW: \( Q_{decay} \sim 10^{14} \text{ W/m}^3 \)

From J.F. Guillemoles
Thank you!

Questions?