Rensselaer

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CONSEJO SUPERIOR DE INVESTIGACIONES CIENTÍFICAS

IMM

Time dependent simulations of thermoelectric thin films and nanowires for direct determination of their efficiency with COMSOL Multi-physics®.

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FINDER

Funcional Nanoscale Devices for Energy REcovery

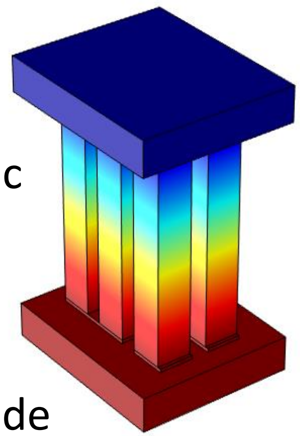
COMSOL CONFERENCE ROTTERDAM 2013

I. Introduction

Thermoelectric materials transform heat into electricity, and vice-versa.

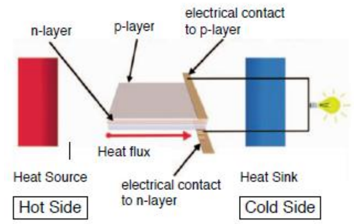
Cold side

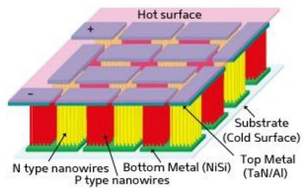
Thermoelectric pellets



Hot side

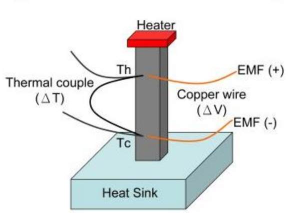
Nano-structuration increases efficiency of thermoelectric materials.



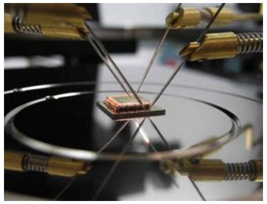


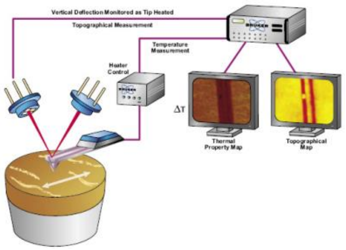
- ZT determination: *Measurement of individual properties.*

S = Seebeck coefficient.
σ = Electrical conductivity.
k = Thermal conductivity.



$$ZT = \frac{S^2\sigma}{k}T$$





Harman technique

Direct ZT determination

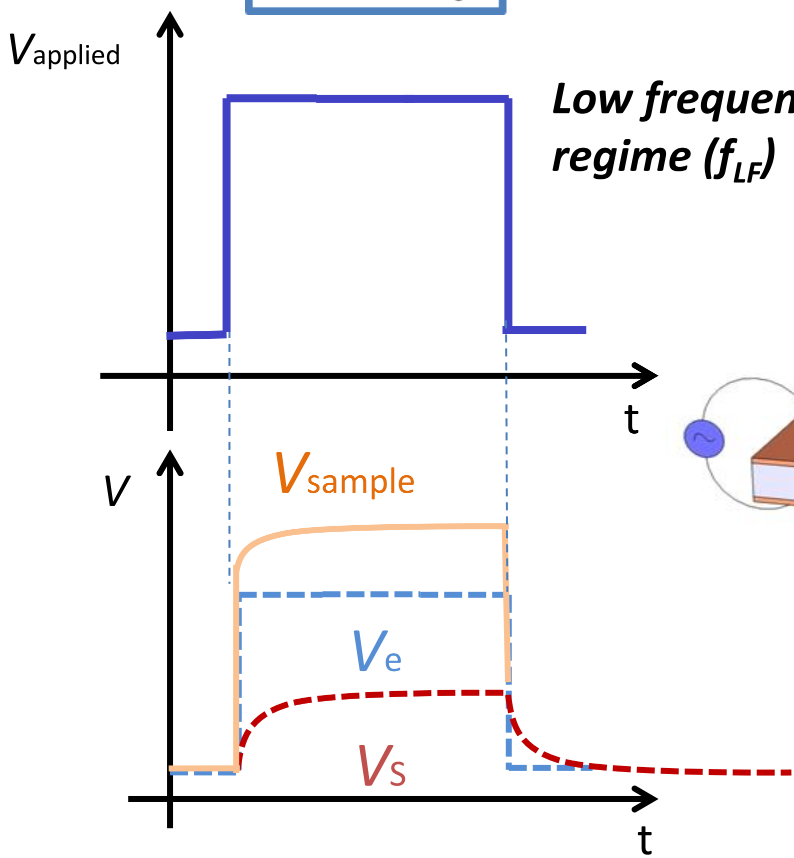
Traditional

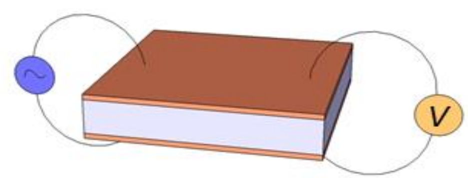
$$ZT = \frac{V_s}{V_e}$$

Modified

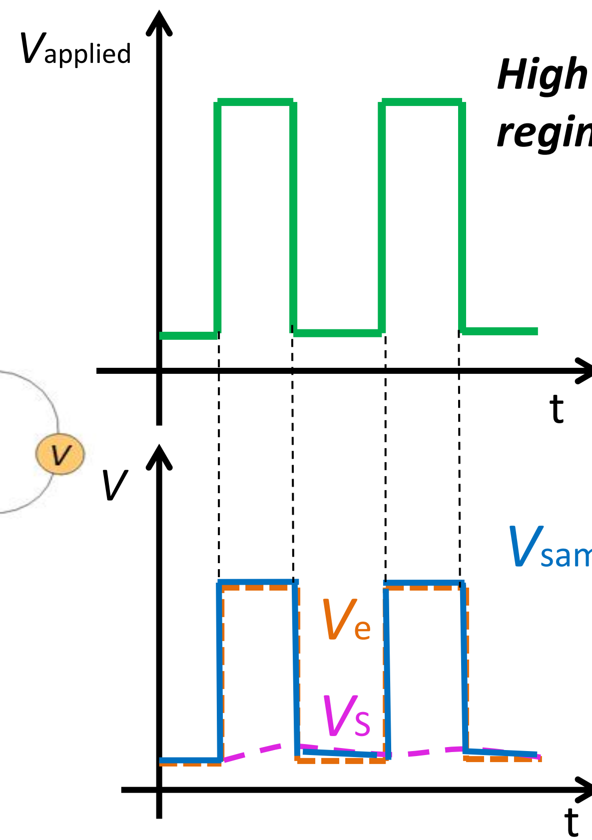
$$ZT = \frac{V_{LF}}{V_{HF}} - 1$$

Low frequency regime (f_{LF})





High frequency regime (f_{HF})



II. COMSOL Model.

Thermoelectric equations

Field equation

$$\rho C \frac{\partial T}{\partial t} + \nabla \cdot \boldsymbol{q} = \boldsymbol{\phi}$$

$$\nabla \cdot \left(\boldsymbol{J} + \frac{\partial \boldsymbol{D}}{\partial t} \right) = 0$$

$$\boldsymbol{E} = -\nabla \varphi$$

Constitutive equations

$$\boldsymbol{q} = [\Pi] \cdot \boldsymbol{J} - [k] \cdot \nabla T$$

$$\boldsymbol{J} = [\sigma] \cdot (\boldsymbol{E} - [S] \cdot \nabla T)$$

$$\boldsymbol{D} = -[\varepsilon] \cdot \boldsymbol{E}$$

ρ = density
σ = electrical conductivity
S = Seebeck coeficient
$[\Pi]=T\cdot S$ = Peltier coefficient
ε = dielectric permitivity
C = specific heat capacity
T = absolute temperature
$\boldsymbol{\varphi}$ = heat generation rate
$\boldsymbol{J}$ = current density vector
$\boldsymbol{E}$ = electric field vector

Coupled-Field equation

$$\rho C \frac{\partial T}{\partial t} - \vec{\nabla}\left((\sigma\alpha^2 T + \lambda)\vec{\nabla} T\right) - \vec{\nabla}\left(\sigma\alpha T \vec{\nabla} V\right) = \sigma((\vec{\nabla} V)^2 + \sigma \vec{\nabla} T \vec{\nabla} V)$$

$$\vec{\nabla}\left(\sigma\alpha\vec{\nabla} T\right) + \vec{\nabla}\left(\sigma\vec{\nabla} V\right) = -\vec{\nabla}\left([\varepsilon]\vec{\nabla}\frac{\partial V}{\partial t}\right)$$

(Antonova et al., Finite elements for thermoelectric device analysis in ANSYS, ICT (2005))

Δu PDE (c)

Match equations with PDE of COMSOL module

Convection effects with Heat Transfer COMSOL module

Conjugate Heat Transfer

Heat convective coefficient: *h = 10-100 W/Km^2*

Box of air:

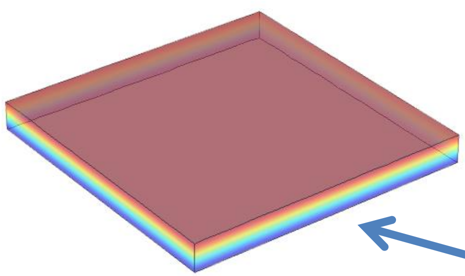
- Heat equation for fluids.
- Effects of gravity for air.

II. COMSOL modeling

- Geometry:

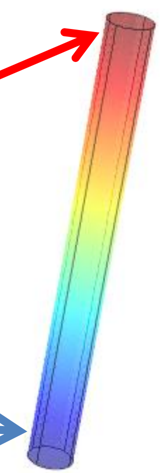
Thin Films

Nanowires



Boundary conditions:

- *Top side temperature and voltage evolve freely.*
- *Bottom side fixed at 293.15 K (heat sink) and grounded (V=0).*



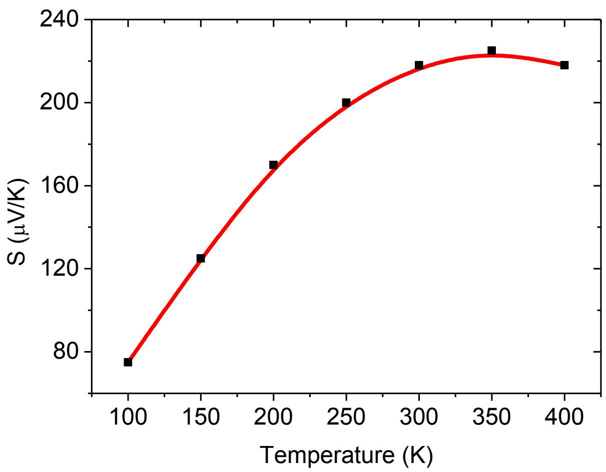
- Variable thickness.
- With and without electrodes and electrical wire.

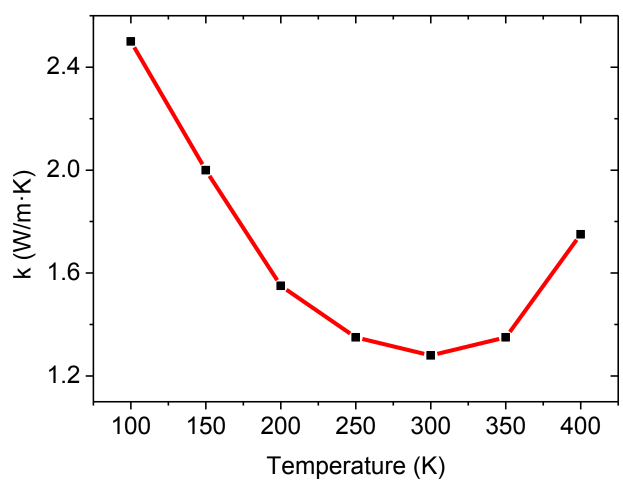
- Variable diameter.
- Length 20µm.

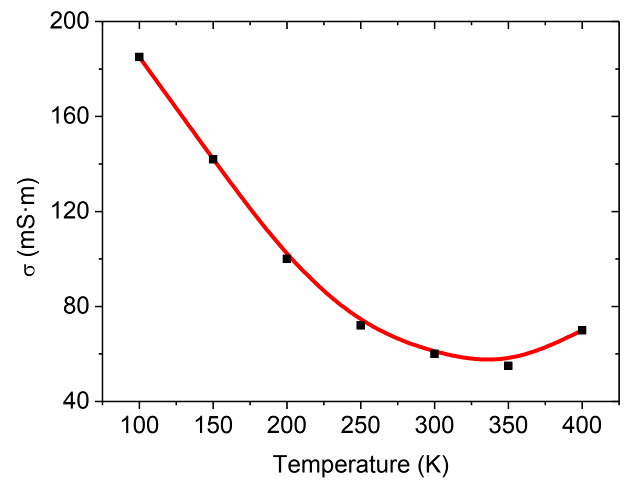
Thermoelectric properties

- Material: p-type Bi_2Te_3
- *S(T)*, *σ(T)* and *k(T)*

T (K)	S (µV/K)	k (W/K·m)	σ (mS·m)
100	75	2.5	185
150	125	2	142
200	170	1.55	100
250	200	1.35	72
300	218	1.28	60
350	225	1.35	55
400	218	1.75	70



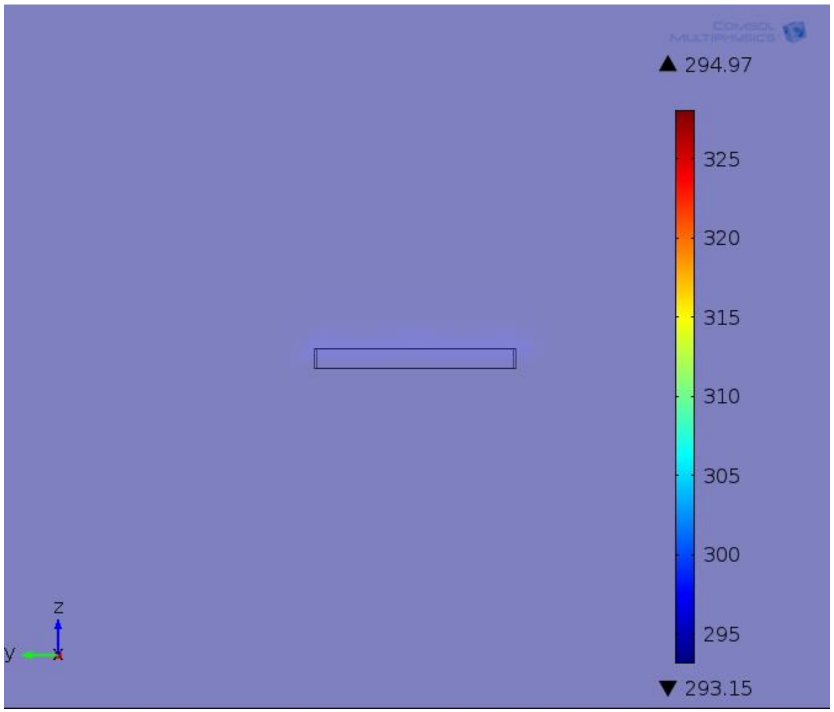


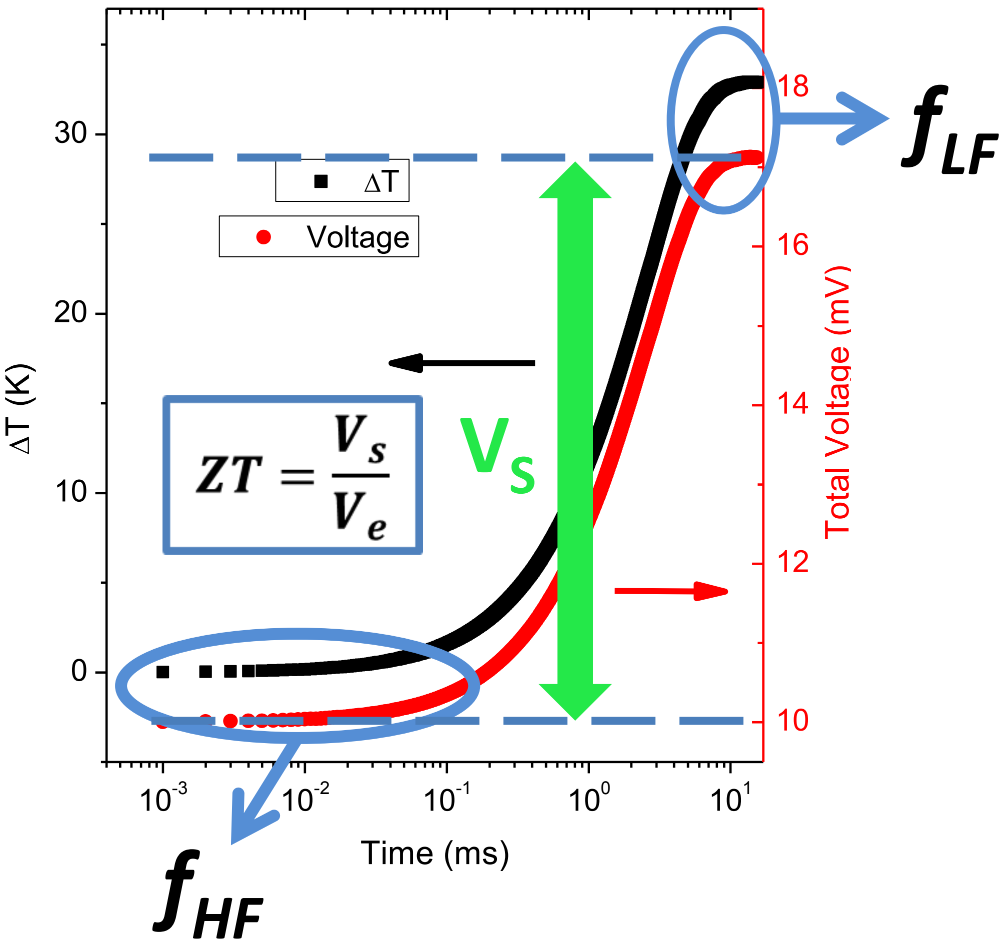


Seifert, W., Ueltzen, M., Müller, E.; One Dimensional Modelling of Thermoelectric Cooling; phys.stat.sol. (a) 194, No.1, pp 277 – 290; 2002

III. Results: Films.

- *Sample Temperature* and *voltage* evolution during *10mV, 0.1 s, pulse*.





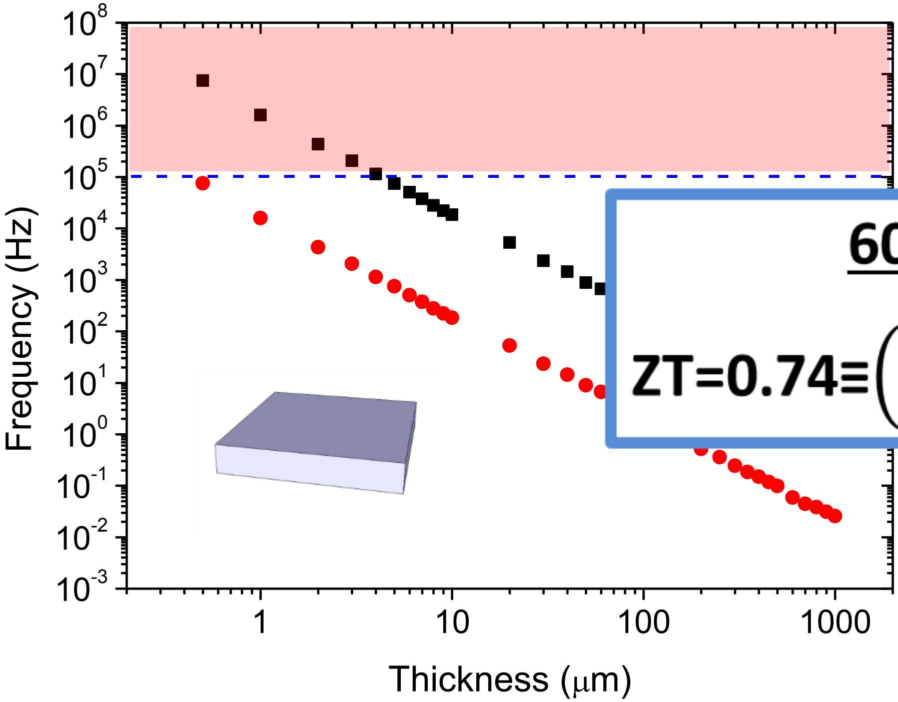
Example: 60µm film

Ideal Conditions

Dimension vs Frequency

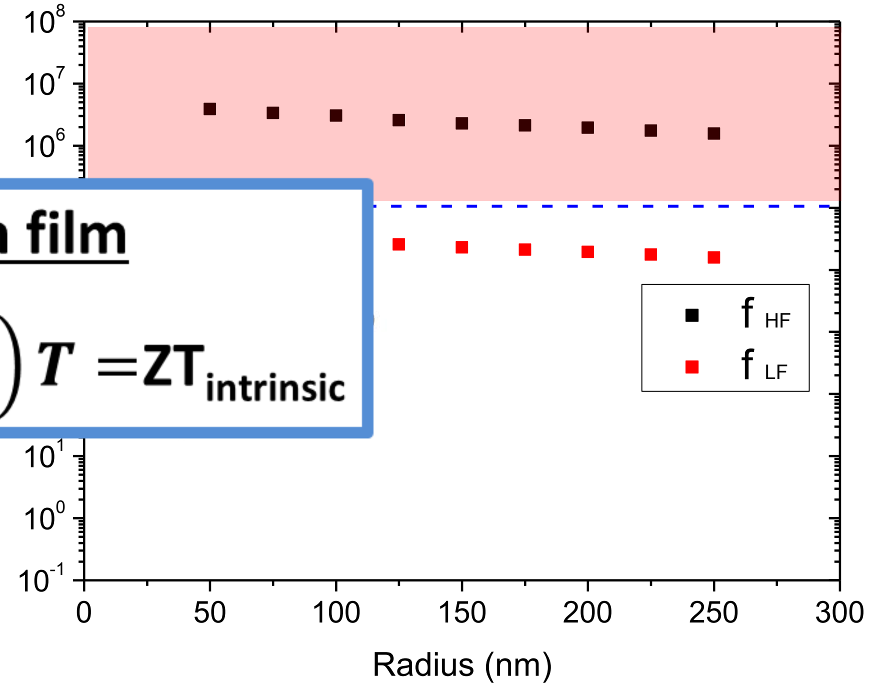
Thin films

High (f_{HF}) and low (f_{LF}) frequencies needed for experimental Harman determination of ZT



Nanowires

f_{HF} in nanowires is extremely high to be measured with typical experimental devices.



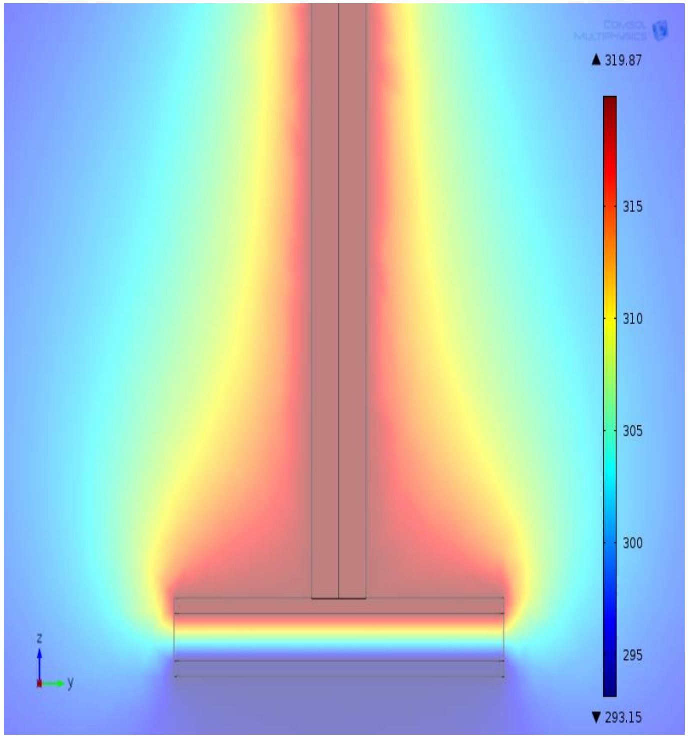
60µm film

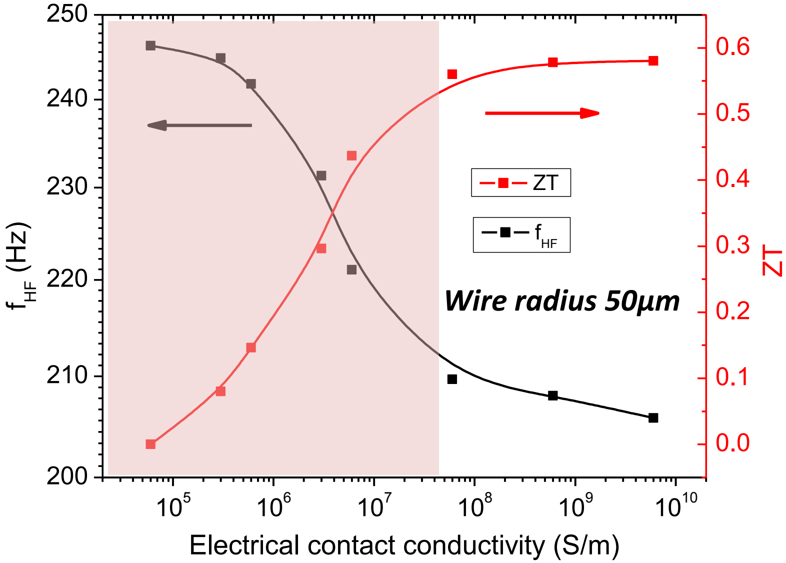
$$ZT=0.74\equiv\left(\frac{\sigma S^2}{k}\right)T = ZT_{intrinsic}$$

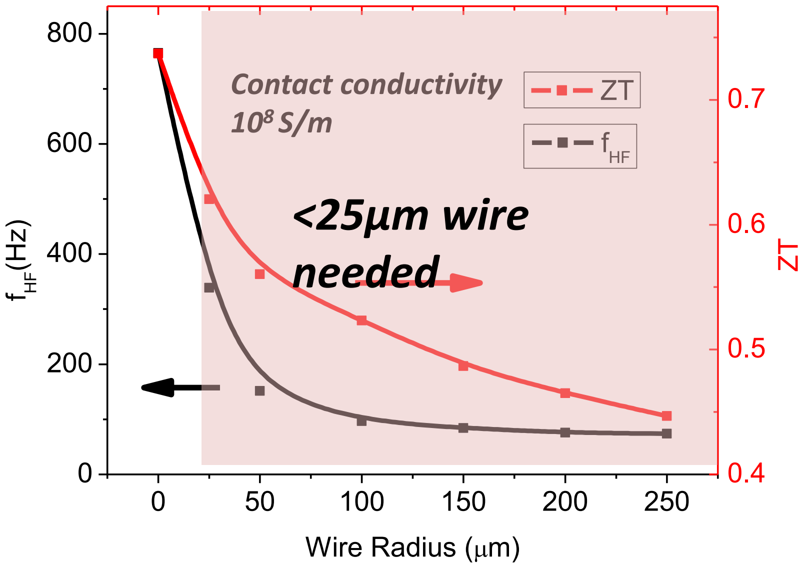
Vacuum and atmospheric conditions show similar results of ZT and f_{HF}.

Influence of electrical contacts

Under the presence of contact resistances and electrical wire.





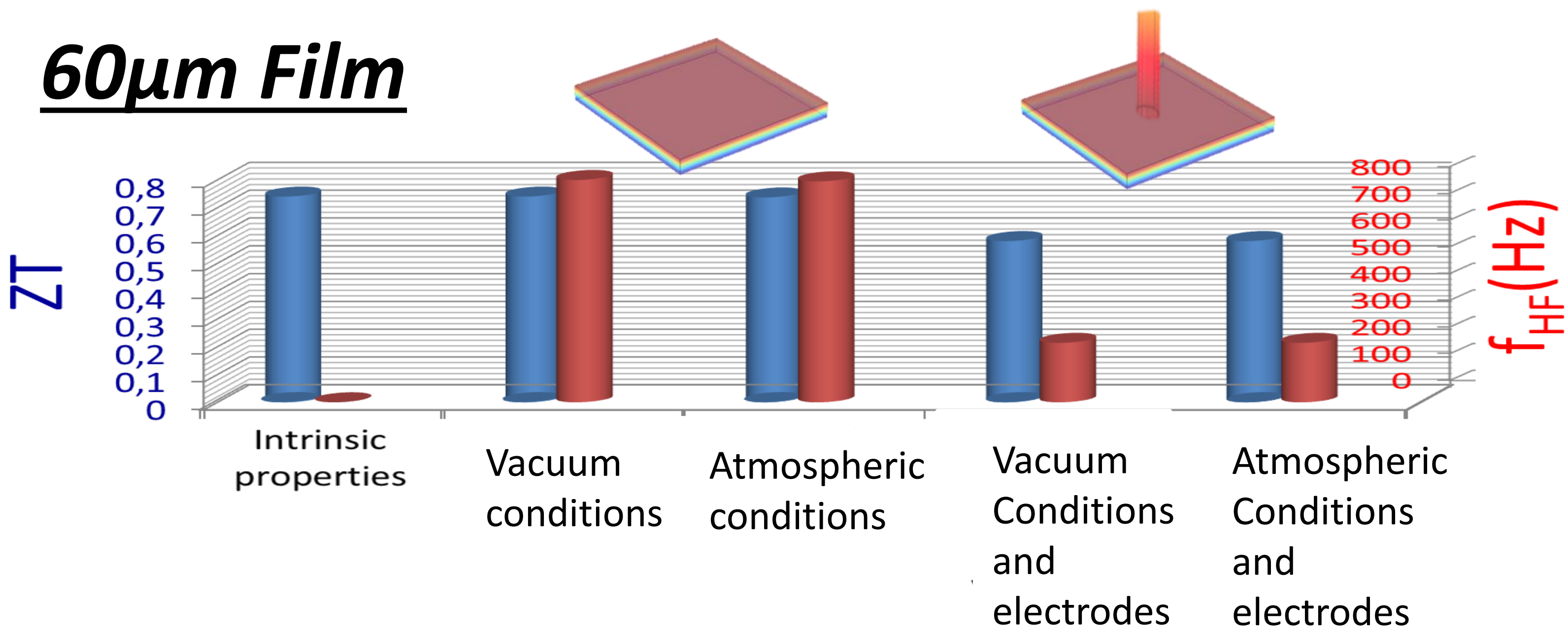


f_{HF} and ZT are modified depending on the electrical contact resistance and wire diameter

Conclusions

- *Development of thermoelectric COMSOL module* for time dependent simulations.
- *Elucidation of experimental conditions* to measure nanostructures with Harman technique.

60μm Film



Thank you for your attention!