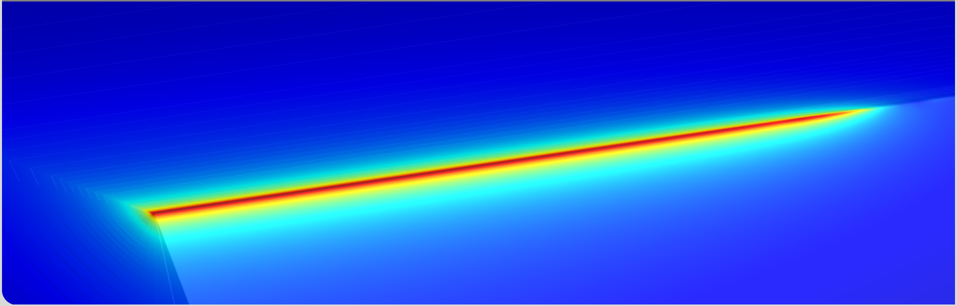
Numerical analysis of the 3ω-method

Comsol Conference, Stuttgart

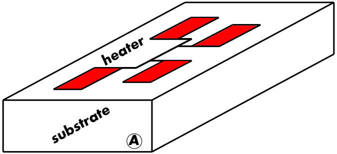
Manuel Feuchter, Marc Kamlah | October 26, 2011

Institute for Applied Materials (IAM)



Outline

Introduction



Concept of the 3ω-method :

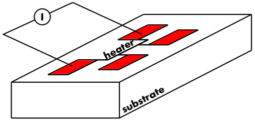
- The 3ω-method is an ac technique to determine the thermal conductivity of an amorphous solid.
- The 3ω-measurement is performed on a thin electrical conducting metal strip (heater) deopsited on the sample surface.
- Literature: [Cahill & Pohl 1987], [Cahill 1990], [Lee & Cahill 1997], [Kim & Feldman 1999], [Borca-Tasciuc 2001], [Chen 2004], [Olson 2005]...

Why do we work on the 3ω-method ?

- Involved in DFG SPP 1386 - Understanding size and interface dependent anisotropic thermal conduction in correlated multilayer structures.
- Goal: Minimize thermal conductivity in nanostructured thermoelectric materials.
- Reliable measurement technique is required.

Functionality of 3ω-method

Alternating current

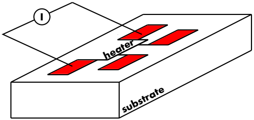


$..\cos\omega..$

| I | ω |

Functionality of 3ω-method

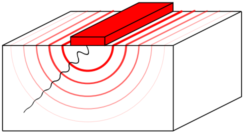
Alternating current



$..\cos\omega..$

| I ω |

Joule heating
$P = R \cdot I^2$

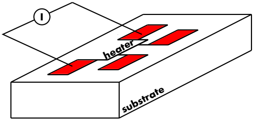


$\cos^2 = ..\cos 2\omega..$

| P 2ω |

Functionality of 3ω-method

Alternating current



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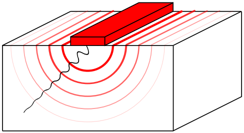


$\cos^2 = ..\cos 2\omega..$

P 2ω

Temperature amplitude ΔT

Analytic solution

Resistance oscillation

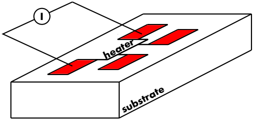
FE-Simulation

R =

R_0 + ΔR 2ω

Functionality of 3ω-method

Alternating current

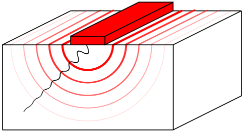


$..\cos\omega..$

$\boxed{I \quad \omega}$

Joule heating

$P = R \cdot I^2$



$\cos^2 = ..\cos 2\omega..$

$\boxed{P \quad 2\omega}$

Temperature amplitude ΔT

Analytic solution

Resistance oscillation

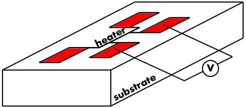
FE-Simulation

$\boxed{R} =$

$\boxed{R_0} + \boxed{\Delta R \quad 2\omega}$

Modulated voltage

$U = I \cdot R$



$\cos\omega \cdot \cos 2\omega =$

$\cos\omega \cdot \cos 3\omega$

$\boxed{\omega \quad 3\omega}$

Functionality of 3ω-method

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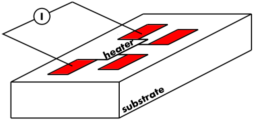
Alternating current



..cos ω..

$I \quad \omega$

Joule heating

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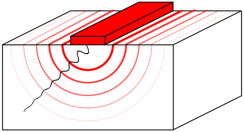

$\cos^2 = ..\cos 2\omega..$

$P \quad 2\omega$

Temperature amplitude ΔT

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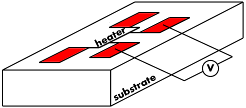
$R =$

$R_0 + \Delta R \quad 2\omega$

Modulated voltage

$U = I \cdot R$



$\cos\omega \cdot \cos 2\omega =$

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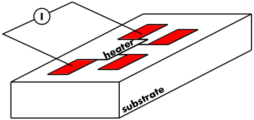
$U \quad \omega \quad 3\omega$

Functionality of 3ω-method

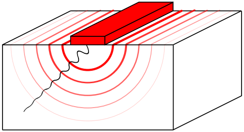
Alternating current



..cos ω..

I ω

Joule heating
$P = R \cdot I^2$



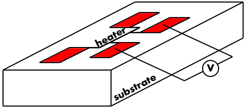
$\cos^2 = ..\cos 2\omega..$

P 2ω

Temperature amplitude ΔT
Analytic solution
Resistance oscillation
FE-Simulation

$R = R_0 + \Delta R \; 2\omega$

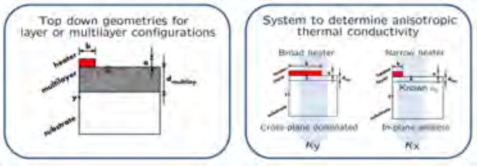
Modulated voltage
$U = I \cdot R$



$\cos\omega \cdot \cos 2\omega =$
$\cos\omega \cdot \cos 3\omega$

U ω 3ω

Geometry configurations

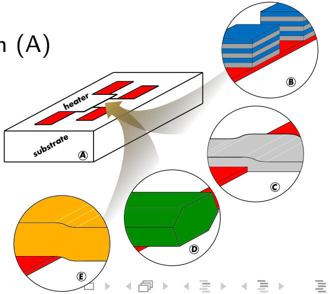


Classic geometry configuration:

- Heater is placed on top of (multi)layer-substrate systems.
- Analytic solutions are available.

Inverse geometry configuration:

- New possibilities to determine the thermal conductivity of nanostructured materials.
- Always the same heater-substrate platform (A) as sample holder.
  - Known system properties.
  - Optimum reproducibility.
- No analytic solutions are available.



Strategy for nanostructured materials

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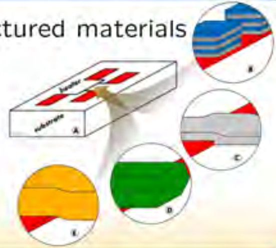
Nanostructured materials



Measurements on investigated materials

Input:
P/I at certain f_c applied on produced sample

Observed:
ΔT

Finite Element Simulations

to create a data basis for various influence factors on ΔT

Input parameters:
P/I, f_c, a, b, d_{lay}, $\kappa_{lay\perp}$, $\kappa_{lay||}$, κ_{subs}

Output parameter:
ΔT

Neural Network

used to solve the inverse problem
to obtain κ from ΔT

Input:
ΔT from measurement

Output:
emergent κ

Finite Element Simulations
COMSOL Multiphysics

- Heat conduction equation has to be solved in the time domain.
- Mathematic interface is used in the general form of the partial differential equation (PDEg).

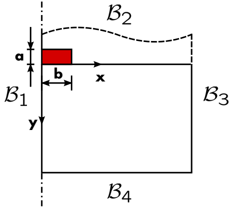
Example for 2d:

$$Q = [\varrho_0 \cdot (1 + \alpha \cdot (T - T_0))]/(A) \cdot I_0^2 \cdot \frac{1}{2} \cdot (1 + \cos(2\omega t))$$

$$\frac{\partial^2 T_h}{\partial x^2} + \frac{\partial^2 T_h}{\partial y^2} - \frac{1}{D_h}\frac{\partial T_h}{\partial t} + \frac{Q}{\kappa_h} = 0\,,$$

$$\frac{\partial^2 T_s}{\partial x^2} + \frac{\partial^2 T_s}{\partial y^2} - \frac{1}{D_s}\frac{\partial T_s}{\partial t} = 0\,,$$

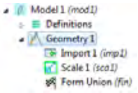
$$\kappa_{m_x}\frac{\partial^2 T_m}{\partial x^2} + \kappa_{m_y}\frac{\partial^2 T_m}{\partial y^2} - \rho_m c_{p_m}\frac{\partial T_m}{\partial t} = 0$$

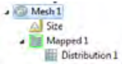


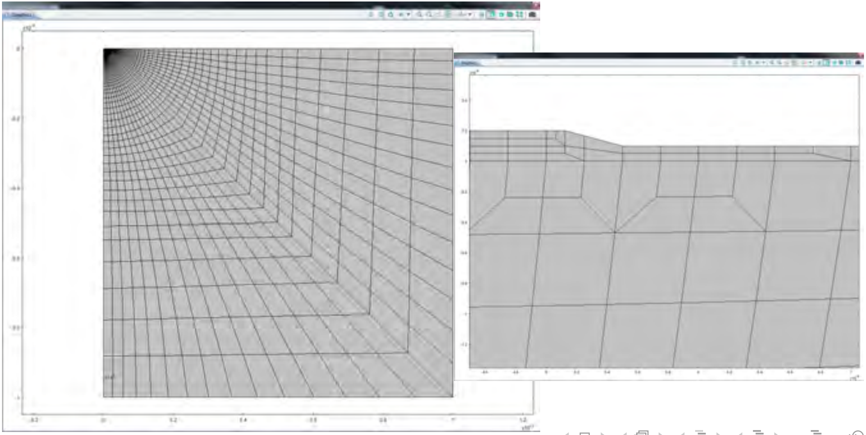
$$\kappa_n \frac{\partial T_s}{\partial n} - h_{bc} \cdot (T - T_0) = 0$$

Geometry import to generate mesh

Example for 2d:



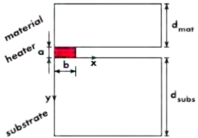


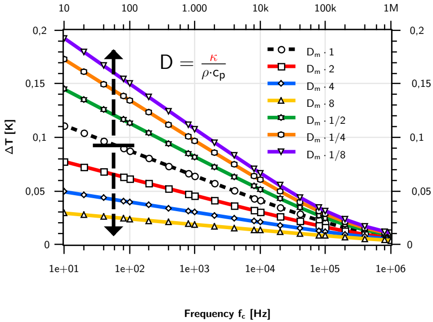


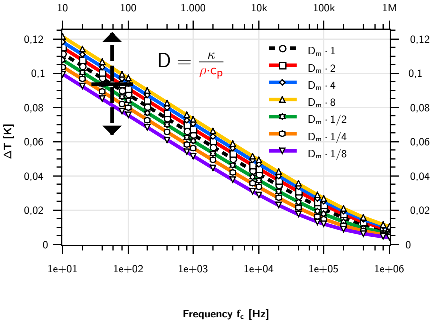
Examples

Placed material on top, ideal system:

- Two times substrate, contact just over heater.
  - To study the influence of material parameters on the temperature amplitude.



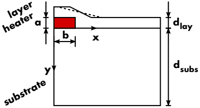


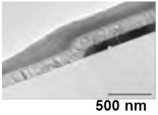


Examples

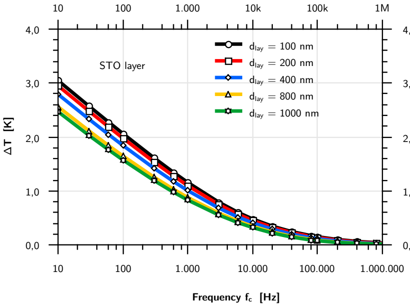
Thin layer on top:

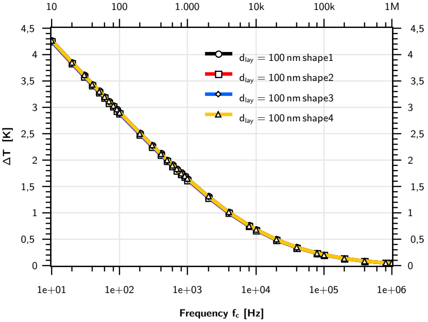
- Bad conducting substrate for a sensitivity in ΔT .
- Contour shape analysis.





By S. Wiedigen, project partner





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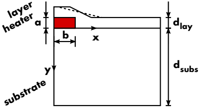

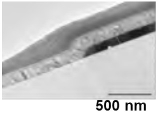

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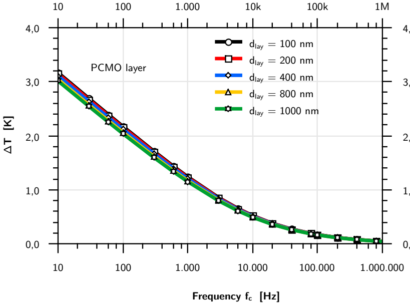
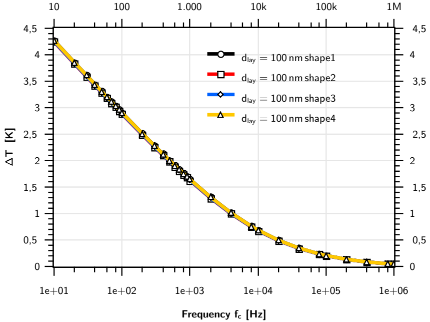
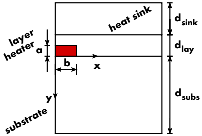


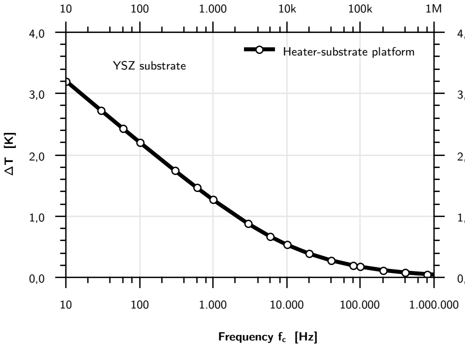


How to enhance the sensitivity for change in κ_{lay}?

Application of heat sink:

- Heat sink: Good thermal conducting to attract heat.
- Full covering heat sink.





Examples

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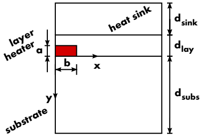

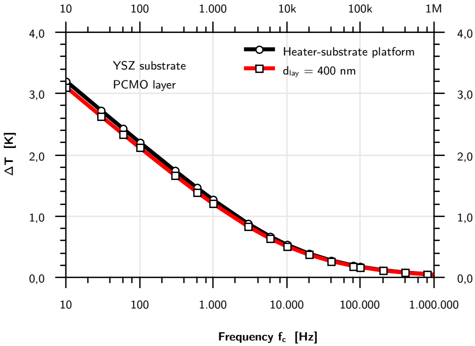

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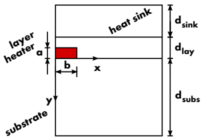
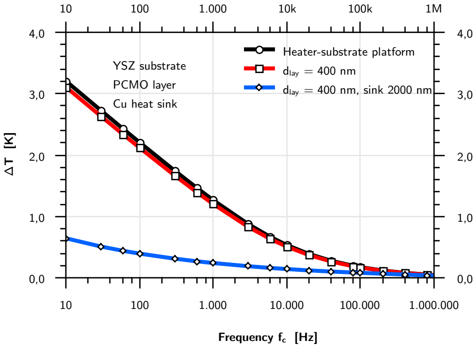
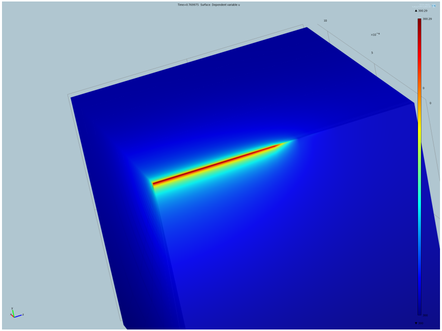




- Heat flow analysis for 3d structures.
- Multiphysical coupling with respect to mechanical and dielectric properties.
- Bottom electrode configurations with additional heaters to measure Seebeck cross-plane.



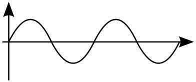
Acknowledgement:

- DFG for funding.
- Project partners from the University of Göttingen,
  Institute for material physics
  Group of C. Jooss and C. Volkert
- Supervisor M. Kamlah

THANK YOU FOR YOUR ATTENTION!

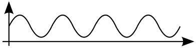
Attachment

Alternating current



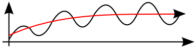
$$I = I_0 \cos(\omega t)$$

Joule heating



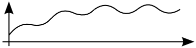
$$P_{JH} = \frac{P_0}{2}(1 + \cos(2\omega t))$$

Temperature oscillation



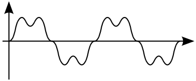
$$\Delta T(t) = \Delta T \cos(2\omega t + \varphi)$$

Resistance oscillation



$$R = R_0 + \Delta R \cos(2\omega t + \varphi)$$

Modulated voltage



$$U = I \cdot R$$

$$U = I_0 R_0 \cos(\omega t) + \frac{I_0 \Delta R}{2}(\cos(3\omega t + \varphi) + \cos(\omega t + \varphi))$$