



Project No: CZ.02.2.69/0.0/0.0/18_070/0010457

Mezinárodní mobility výzkumných pracovníků MSCA-IF II na ČVUT v Praze
Multi-scale Modelling of Elastocaloric Materials for Integrated Cooling

Využití piezomagnetického a elastokalorického jevu pro chlazení v pevné fázi

Jan Zemen

Konference COMSOL Multiphysics 2021

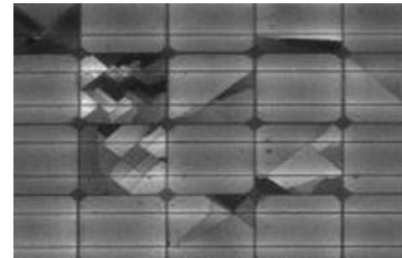
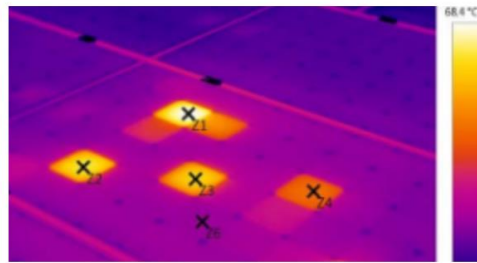
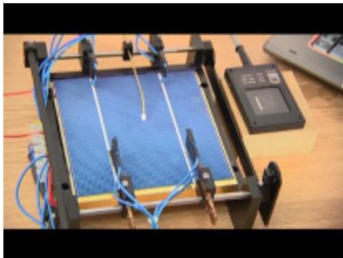
Vinařství U Kapličky, Zaječí

28.5.2021

Katedra elektrotechnologie, ČVUT, FEL

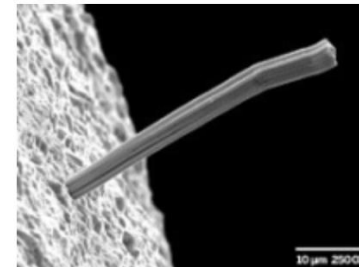
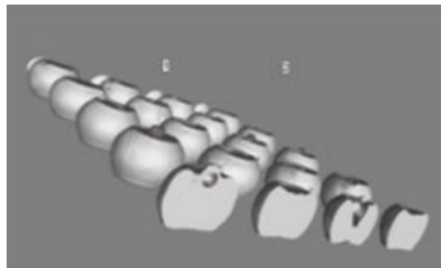
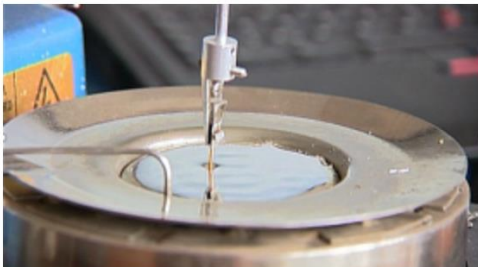
Photovoltaic systems

- Diagnostics of PV cells (cell parameters, LBIV, LBIC,...)
- Thermographic measurement
- Flash test (PASAN)
- PV modules I-V characteristic measurement
- Temperature measurement of PV modules
- Sun irradiation measurement
- Electroluminescence measurement



Conductive joining – soldering or electrically conductive adhesives (ECAs)

- Printed circuit board diagnostics
- Diagnostics of voids in soldered joints, intermetallic layers, whisker and dendritic growth
- Soldering on uncommon substrates: glass, ceramics, silicon, etc.

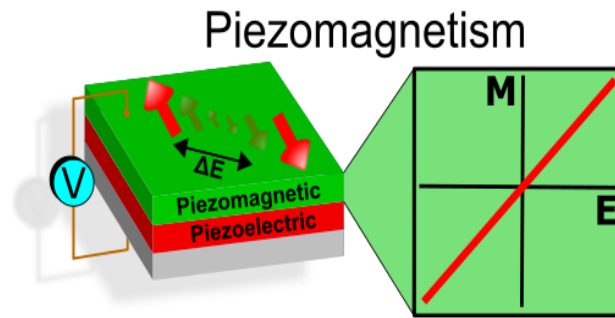
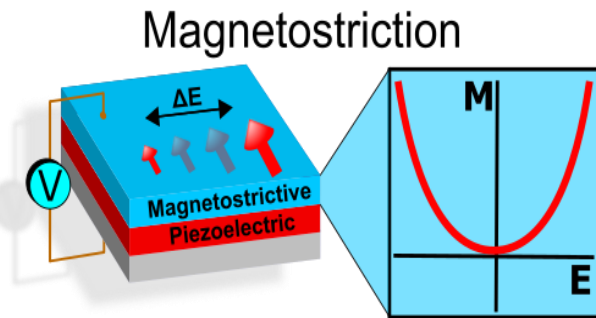
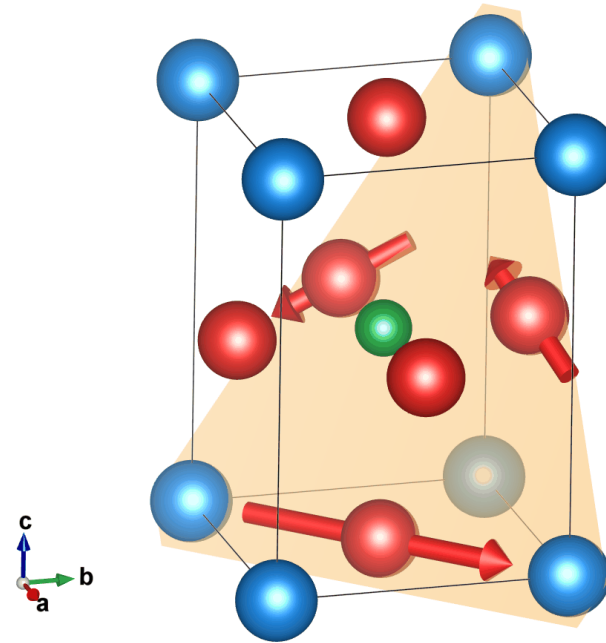
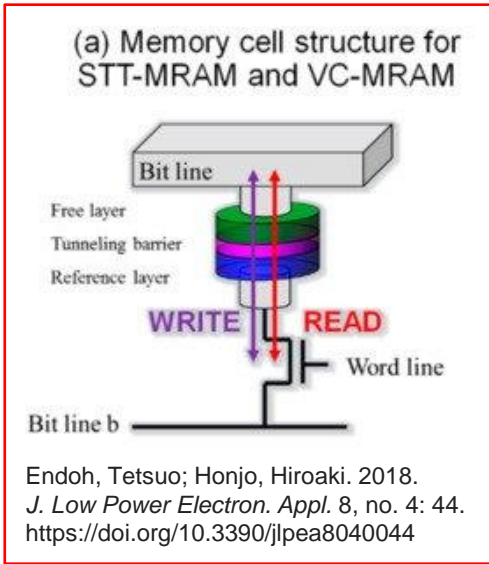


Outline

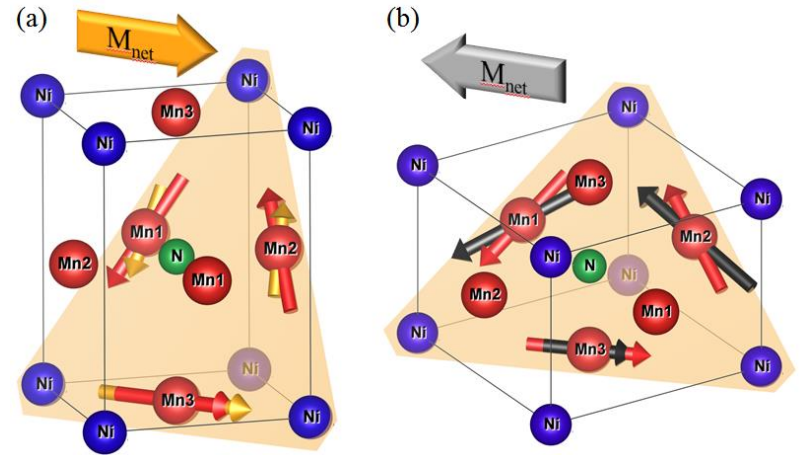
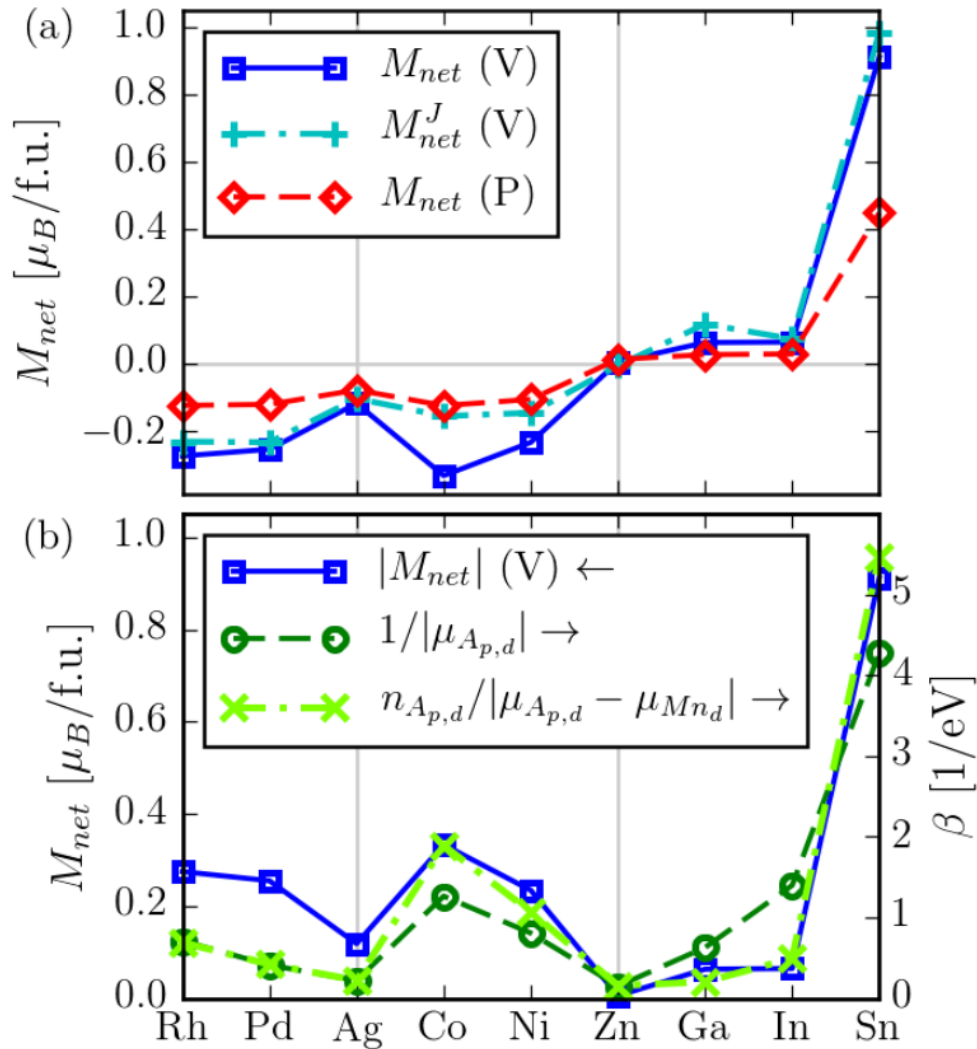
- Piezomagnetický jev
 - mikroskopický původ jevu – lineární závislost magnetizace na strainu
 - FEM model – využití výstupů mikroskopického modelu (SDFT)
- Elastokalorický jev
 - mikroskopický původ jevu – uvolňování latentního tepla
 - FEM model a nutné aproximace
- Shrnutí

Canted triangular antiferromagnetic structure of Mn_3XN

Motivation

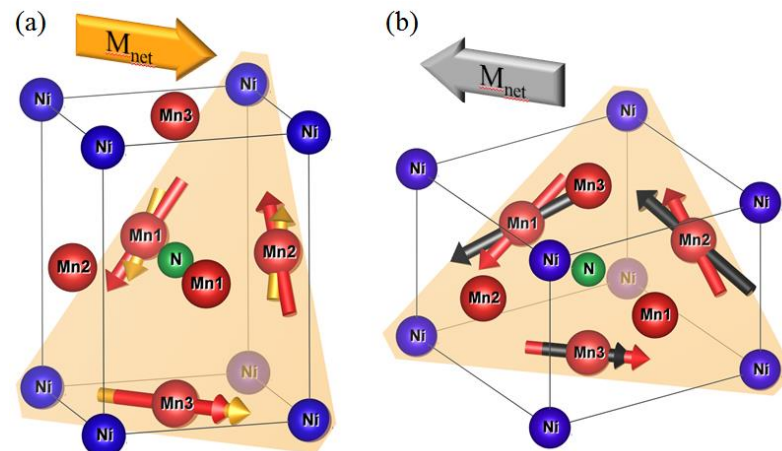
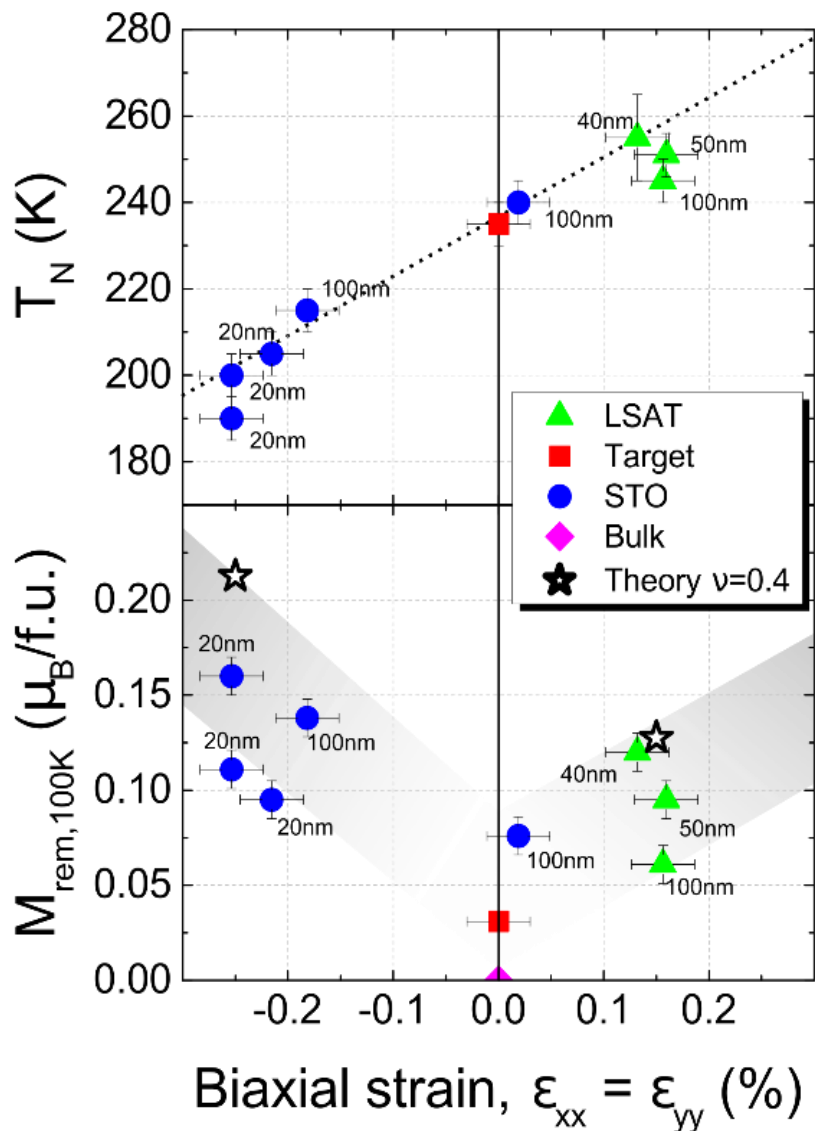


Modeling of piezomagnetism from first principles (SDFT)



Comsol model input:
 Biaxial strain $\sim 1\%$ results in
 Net magnetic field ~ 1 mT

Piezomagnetic effect in Mn_3NiN on different substrates



Giant Piezomagnetism in Mn_3NiN

David Boldrin, Andrei P. Mihai, Bin Zou, Jan Zemen, Ryan Thompson, Ecaterina Ware, Bogdan V. Neamtu, Luis Ghivelder, Bryan Esser, David W. McComb, Peter Petrov, and Lesley F. Cohen

ACS Applied Materials & Interfaces 2018

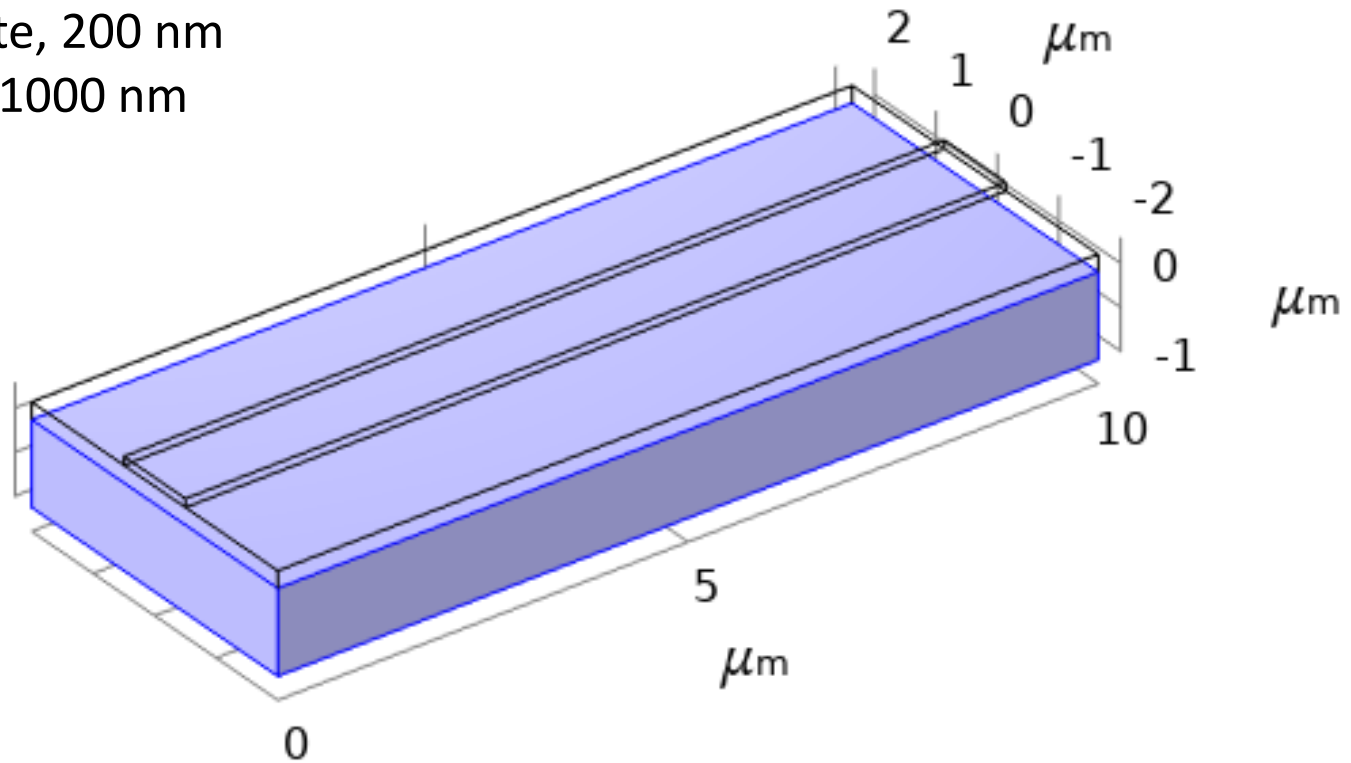
10 (22), 18863-18868

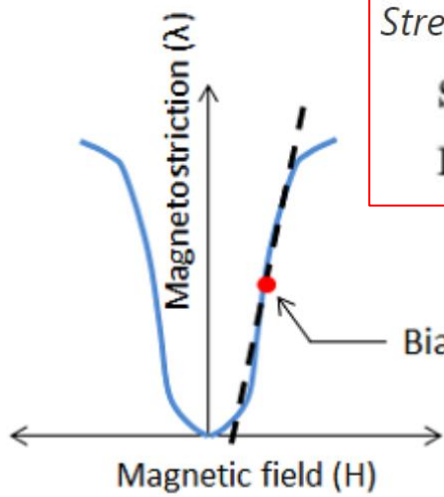
DOI: 10.1021/acsami.8b03112

Device simulated in Comsol



Mn₃NiN bar, 100 nm
MgO substrate, 200 nm
PZT stressor, 1000 nm





Stress-Magnetization

$$S = c_H \epsilon - e_{HS}^T \mathbf{H}$$

$$\mathbf{B} = e_{HS} \epsilon_{el} + \mu_0 \mu_{rS} \mathbf{H}$$

Linearized magnetostriction
or
Ampère's law with strain dependent magnetization

- Component 1 (comp1)
 - Definitions
 - Geometry 1
 - Materials
 - Magnetic Fields (mf)
 - Solid Mechanics (solid)
 - Linear Elastic Material 1
 - Free 1
 - Initial Values 1
 - Fixed Constraint 1
 - Magnetostrictive Material 1**
 - Linear Elastic Material 2
 - External Strain 1
 - External Strain 2
 - External Strain 3
 - External Stress 1
 - Electrostatics (es)
 - Multiphysics
 - Mesh 1
 - Study 1
 - Results
 - Datasets
 - Derived Values
 - Tables
 - Magnetic field
 - Strain
 - Surface 1
 - Arrow Volume 1

Magnetoelastic Properties

Magnetostriction model: Linear

Constitutive relation: Stress-magnetization form

Elasticity matrix, Voigt notation:

c_H User defined

2.77e11	0.58e11	0.58e11	0	0	0
0.58e11	2.77e11	0.58e11	0	0	0
0.58e11	0.58e11	2.77e11	0	0	0
0	0	0	0.57e11	0	0
0	0	0	0	0.57e11	0
0	0	0	0	0	0.57e11

Piezomagnetic coupling matrix, Voigt notation:

e_{HS} User defined

0.01	0.01	-0.01*...	0	0	0
0.01	0.01	-0.01*...	0	0	0
-0.02	-0.02	0.02*0...	0	0	0

Relative permeability: μ_{rS} From material

Density: ρ From material

- Magnetic Fields (mf)
 - Ampère's Law 1
 - Magnetic Insulation 1
 - Initial Values 1
 - Gauge Fixing for A-Field 1
 - Piezomagnetic magnetization**
 - Permeability from material
 - Ampère's Law, Magnetostrictive
 - Magnetic Field 1
 - Magnetic Field 2
- Solid Mechanics (solid)
 - Linear Elastic Material 1
 - Free 1
 - Initial Values 1
 - Piezoelectric Material 1
 - Fixed Constraint 1
 - Magnetostrictive Material 1
- Electrostatics (es)
 - Charge Conservation 1
 - Zero Charge 1
 - Initial Values 1
 - Charge Conservation, Piezoelec
 - Terminal 1

Equation

Material Type: Nonsolid

Coordinate System Selection: Global coordinate system

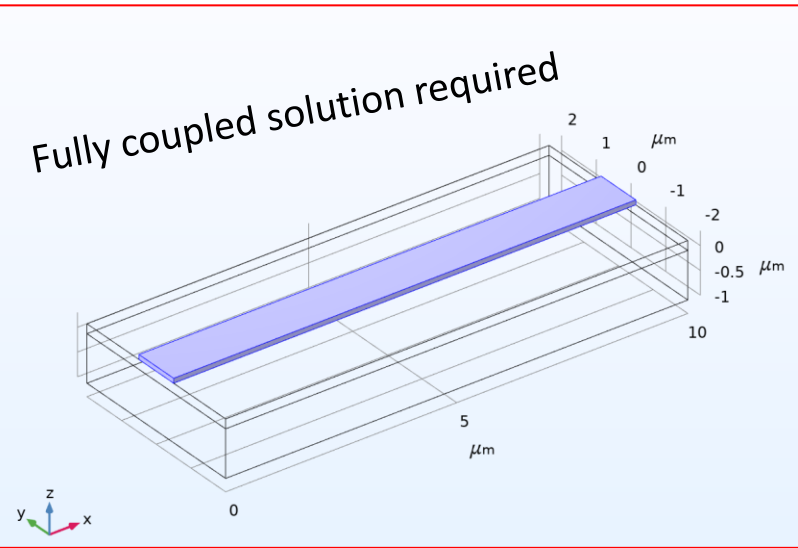
Constitutive Relation B-H: Magnetization

Magnetization model: Magnetization

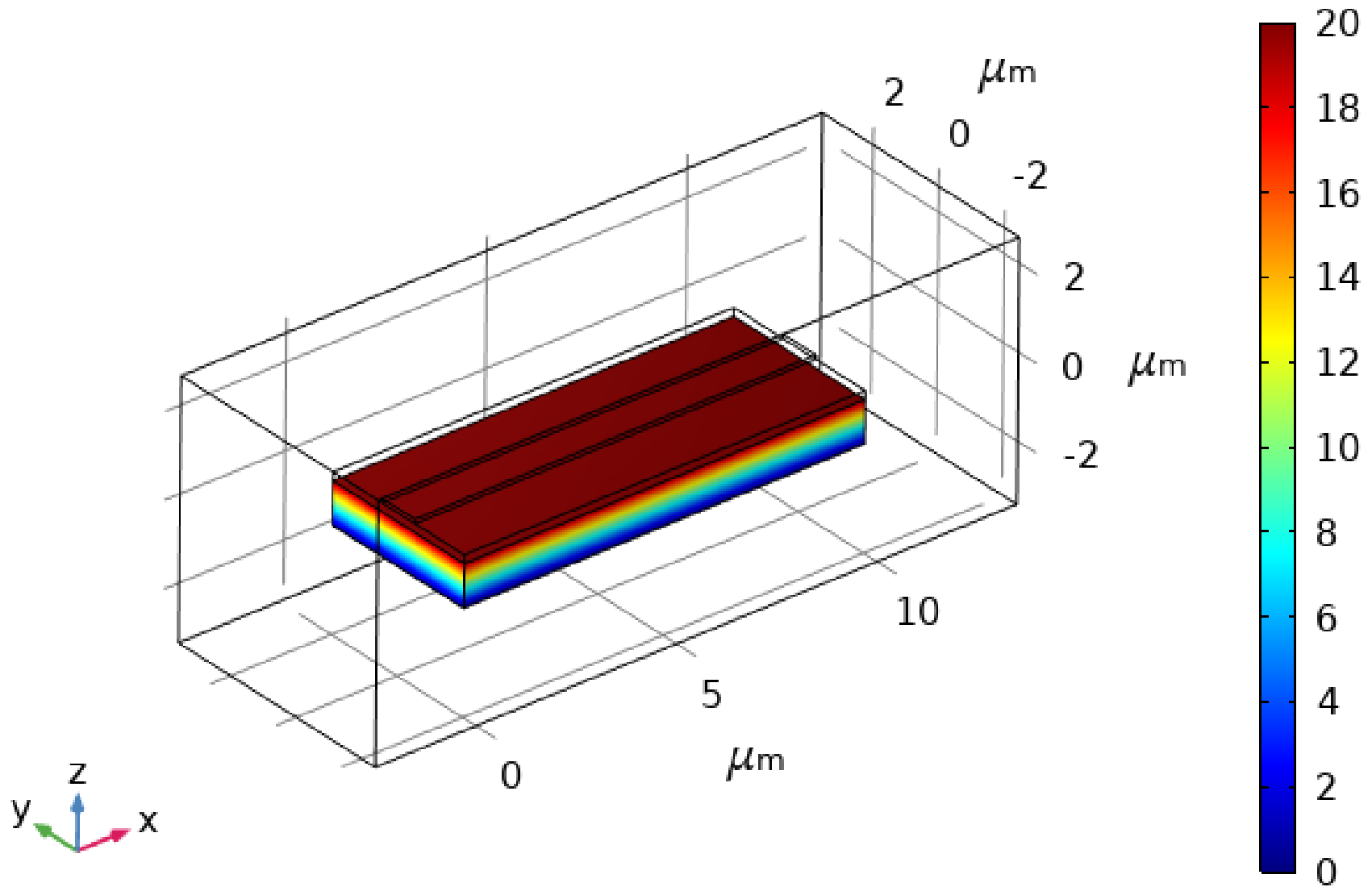
$\mathbf{B} = \mu_0(\mathbf{H} + \mathbf{M})$

Magnetization:

(solid.eXX+solid.eYY)*100*Hinduced	x	
(solid.eXX+solid.eYY)*100*Hinduced	y	A/m
(solid.eXX+solid.eYY)*200*Hinduced	z	



Surface: Electric potential (V)



Meshing

Model Builder

- Multiphysics
 - Piezoelectric Effect 1 (*pze1*)
 - Magnetostriction 1 (*pzm1*)
- Mesh 1
 - Size
 - Mapped 1
 - Distribution 1
 - Distribution 2
 - Mapped 2
 - Distribution 1
 - Distribution 2
 - Swept 1**
 - Distribution 1
 - Free Tetrahedral 1
 - Size 1
 - Free Tetrahedral 2
 - Size 1
- Study 1
 - Step 1: Stationary
 - Step 2: Stationary Magnetic
 - Solver Configurations
- Results
 - Datasets
 - Study 1/Solution 1 (*sol1*)
 - Study 1/Solution Store 1 (*sol2*)
 - Cut Plane 1
 - Cut Line 3D 2

Settings

Swept

Build Selected Build All

Destination faces

Selection: Manual

13

Swept Method

Face meshing method:
Quadrilateral (generate hexahedra)

Sweep path calculation:
Sweep following straight lines

Destination mesh generation:
Determine suitable method

Control Entities

Smooth across removed control entities

Number of iterations:
4

Graphics

Number of elements: 213444

Minimum element quality: 0.1512

Average element quality: 0.6638

Element volume ratio: 9.665E-7

Mesh volume: 576 μm^3

— Domain element statistics

Number of elements: 213444

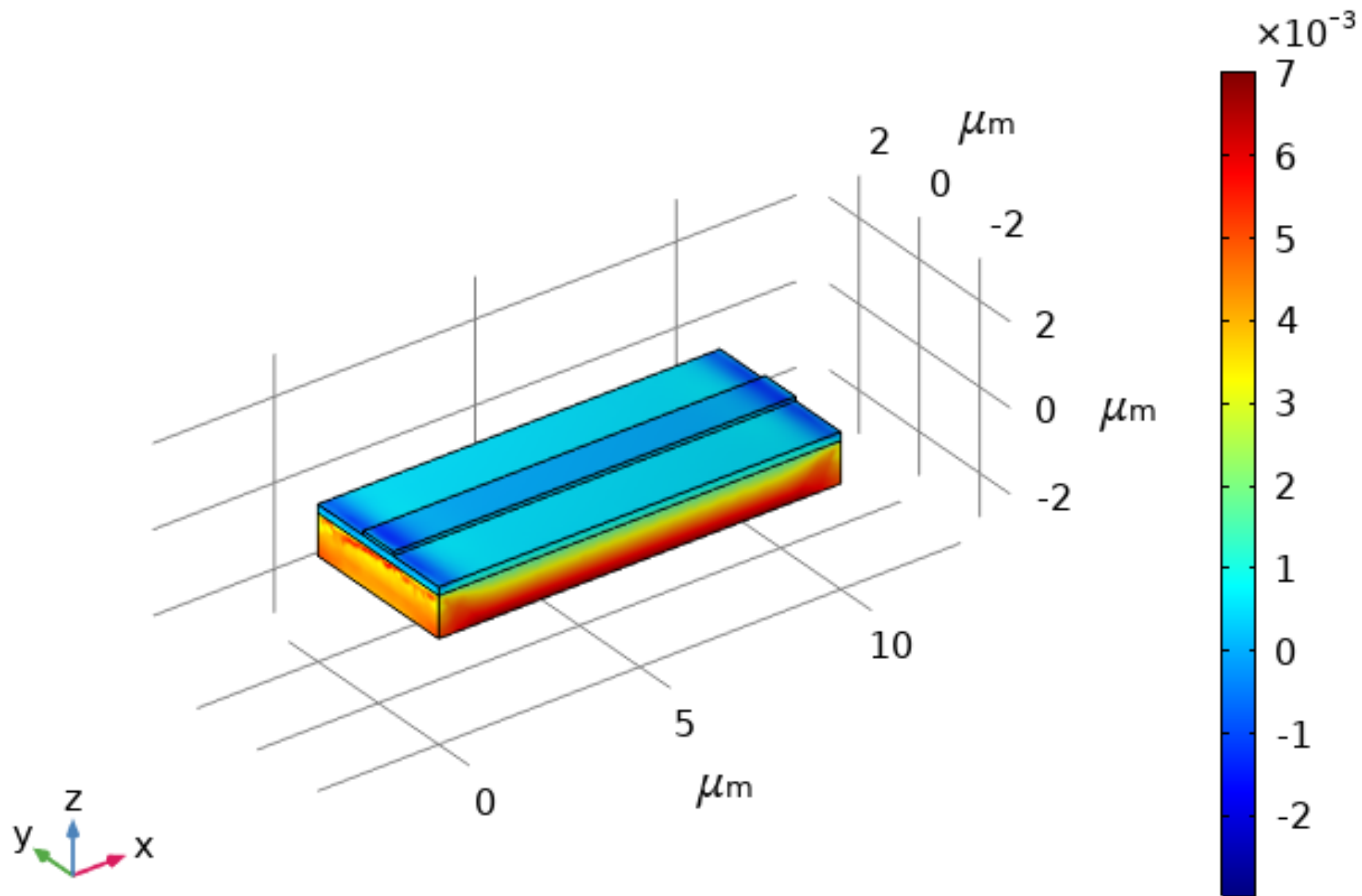
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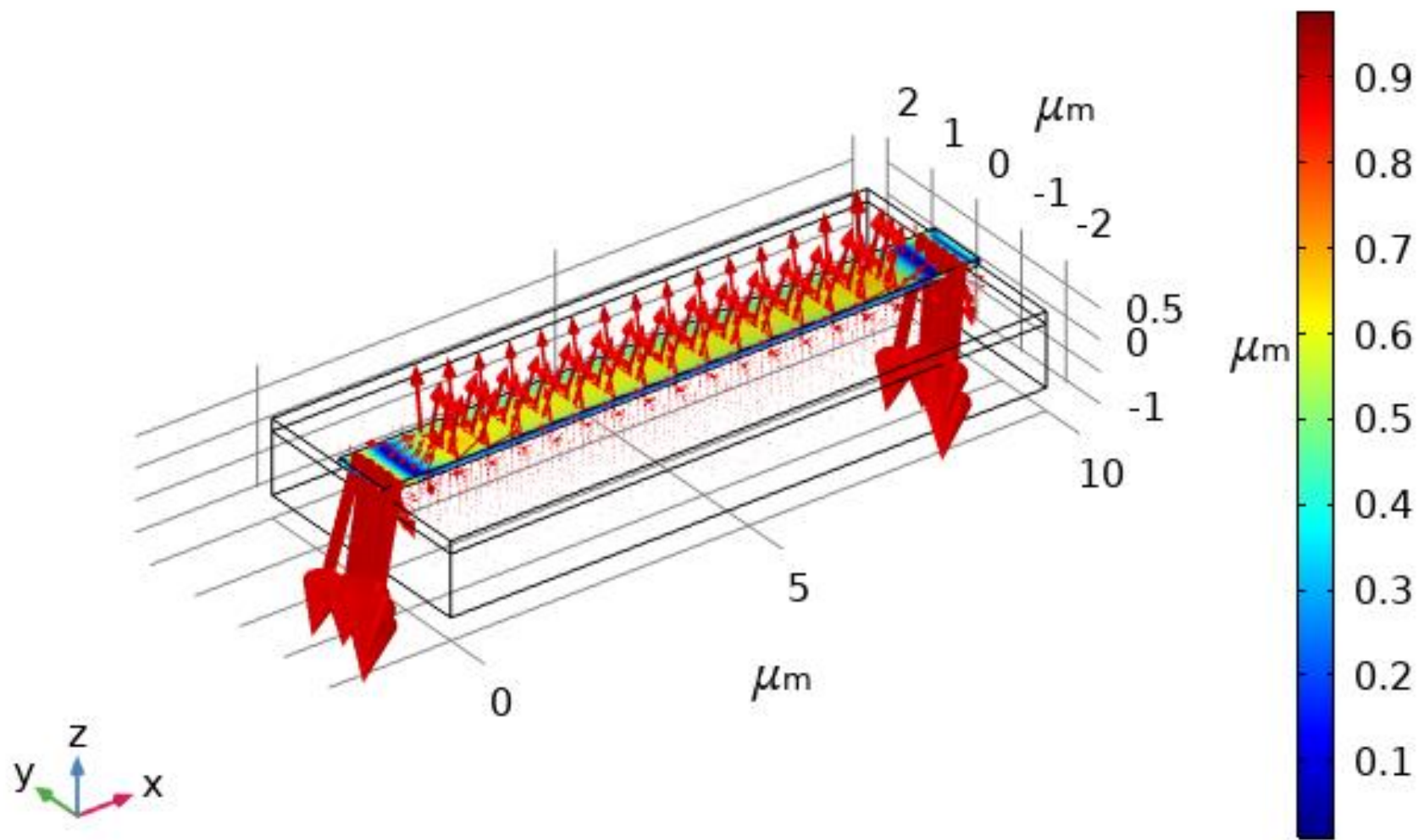
Element volume ratio: 9.665E-7

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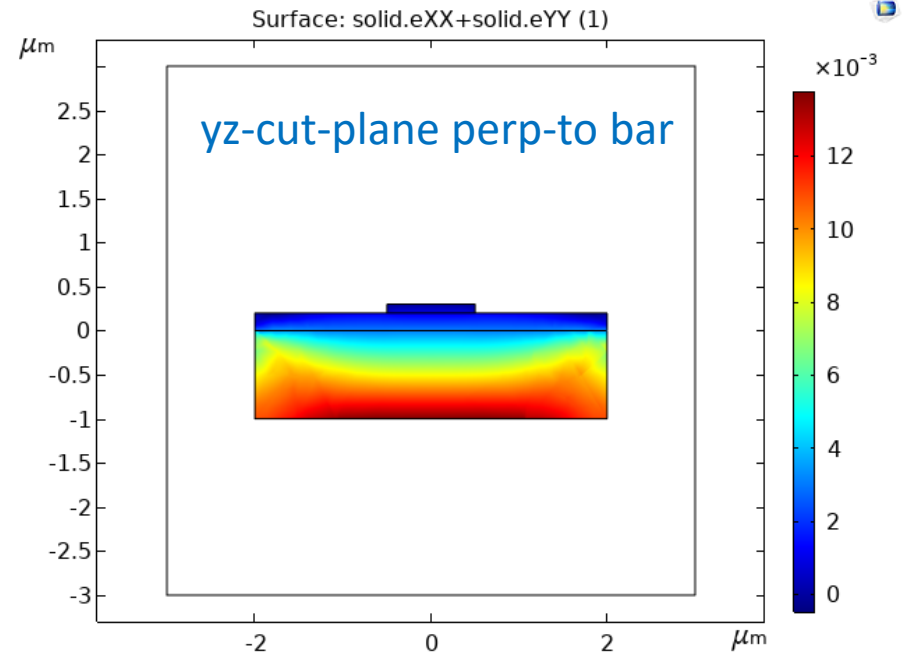
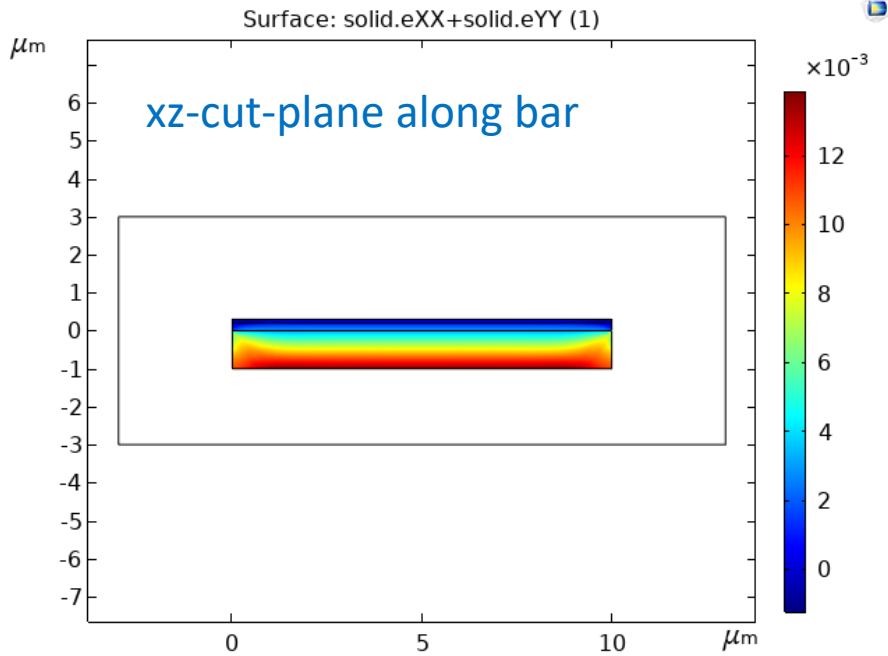
Surface: Strain tensor, XX component (1)



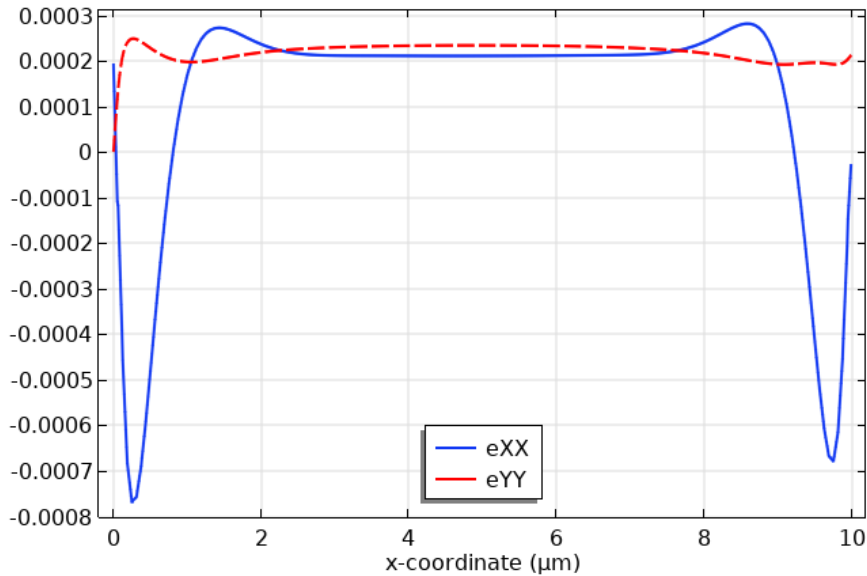
Arrow Volume: Magnetic flux density (spatial frame)
Slice: Magnetic flux density norm (mT)



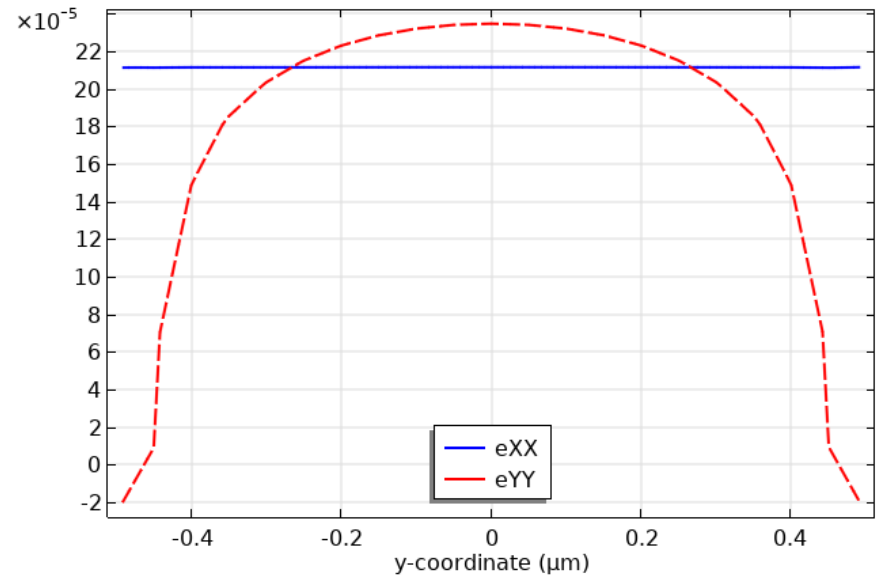
Strain profile



Line Graph: Strain tensor, XX component (1)
Line Graph: Strain tensor, YY component (1)



Line Graph: Strain tensor, XX component (1)
Line Graph: Strain tensor, YY component (1)



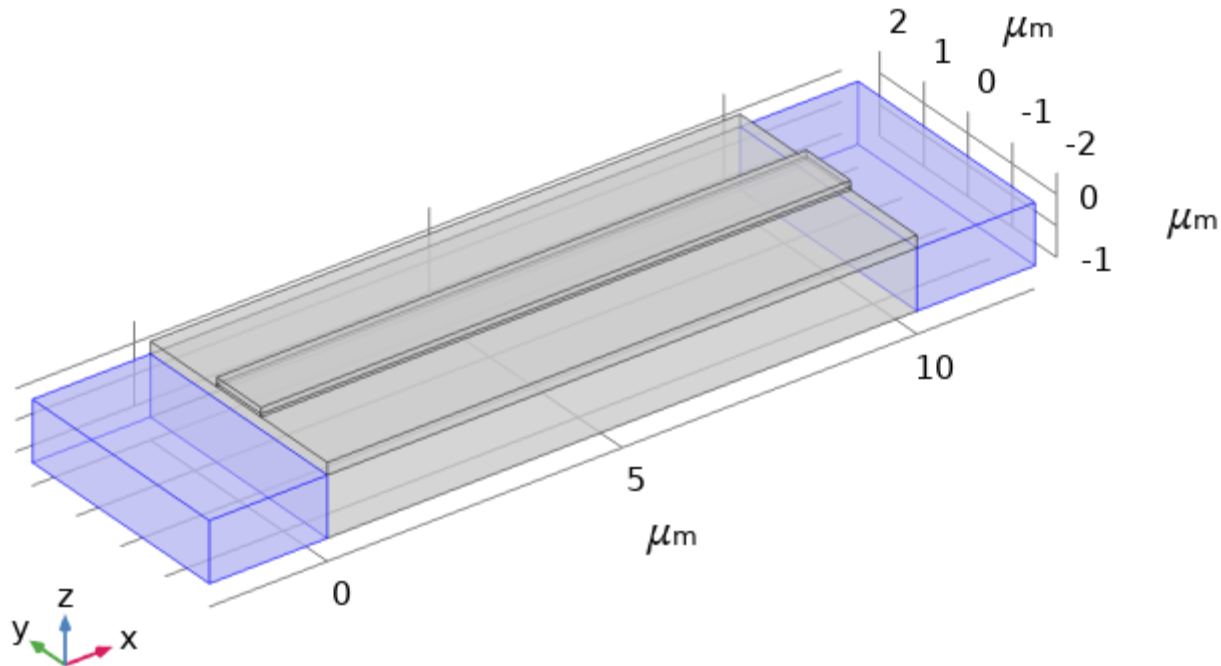
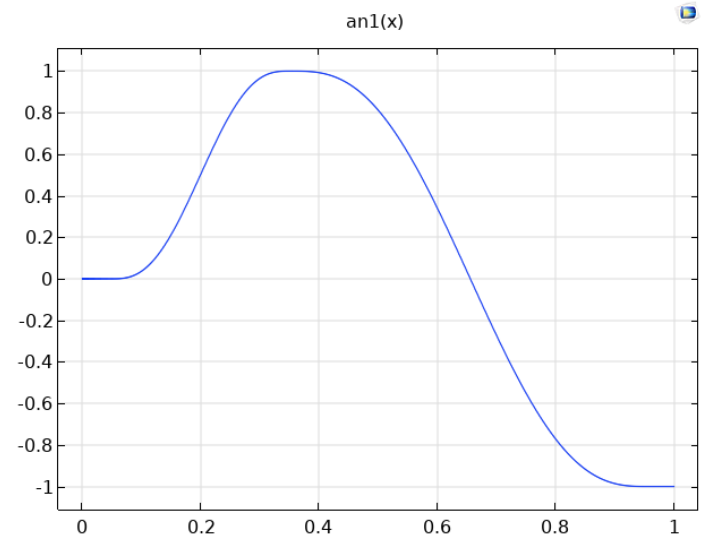
More realistic design with time dependence

External Strain

Strain input:
Strain tensor

Strain tensor:
 ϵ_{ext} User defined

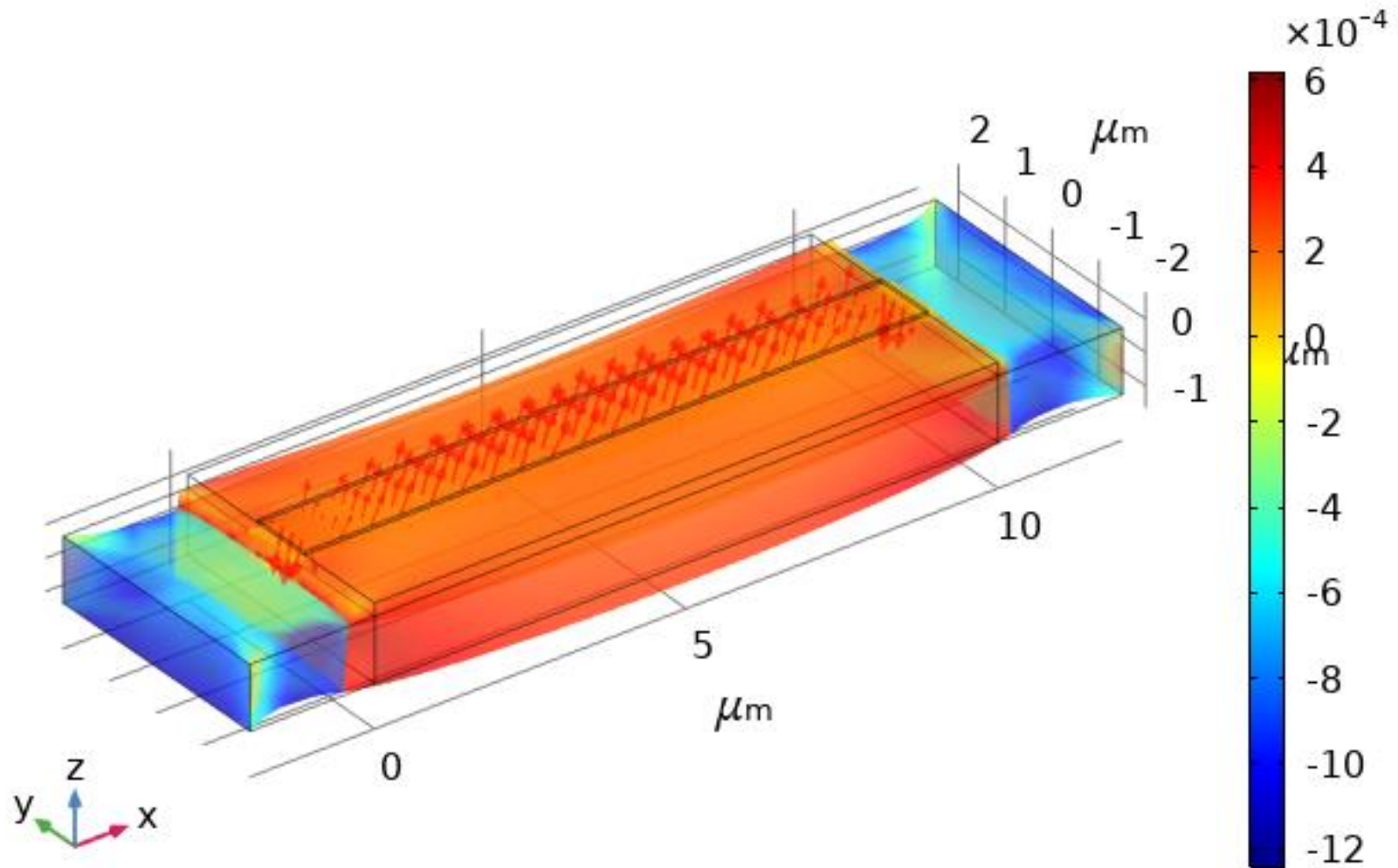
$-0.001 \cdot \text{an1}(t[1/s])$	0	0	1
0	$-0.001 \cdot \text{an1}(t[1/s])$	0	
0	0	0	





Time=0.5 s

Surface: Strain tensor, XX component (1)
Arrow Volume: Magnetic flux density (spatial frame)

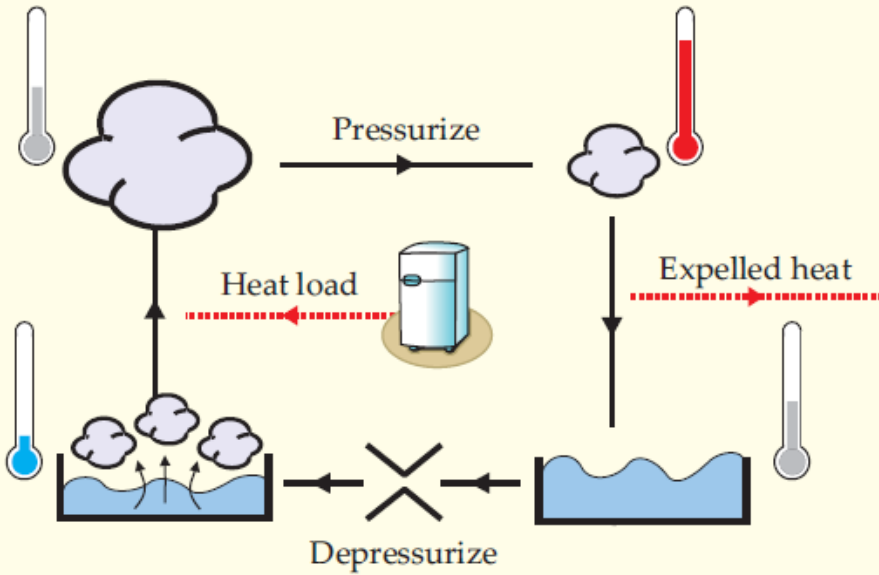


Outline

- Piezomagnetický jev
 - mikroskopický původ jevu – lineární závislost magnetizace na strainu
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Solid state cooling

a Vapor compression cycle



b Ferroic cooling cycle

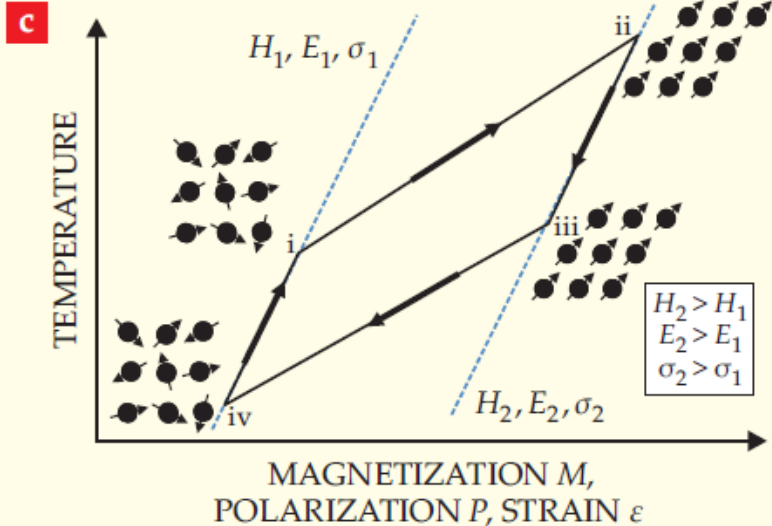
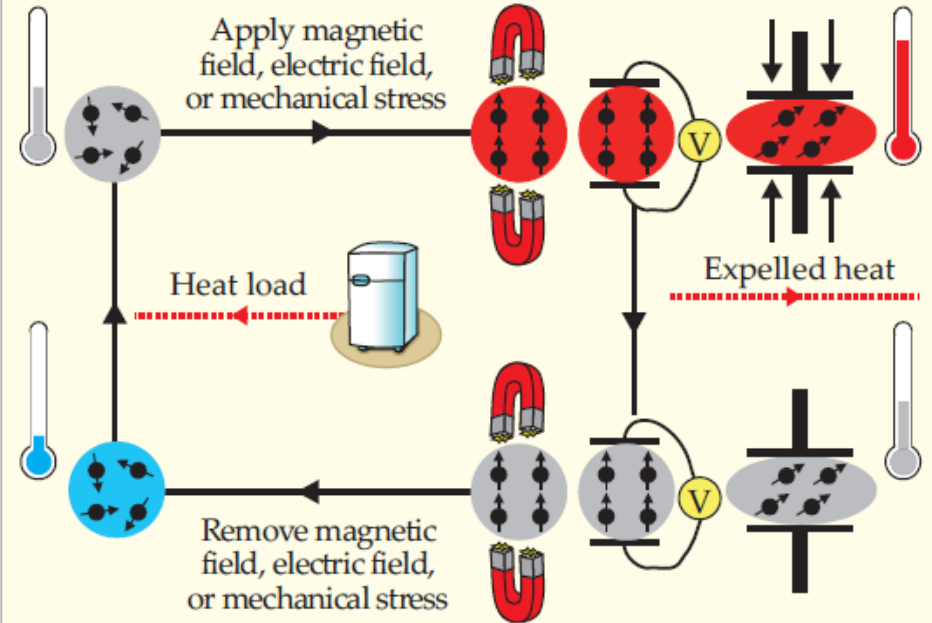


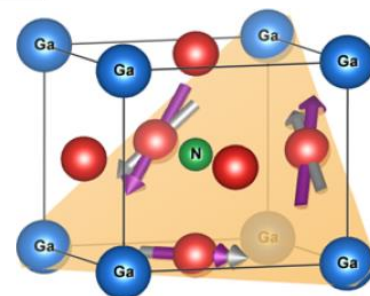
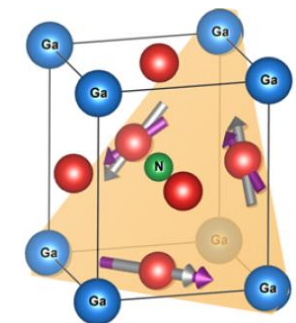
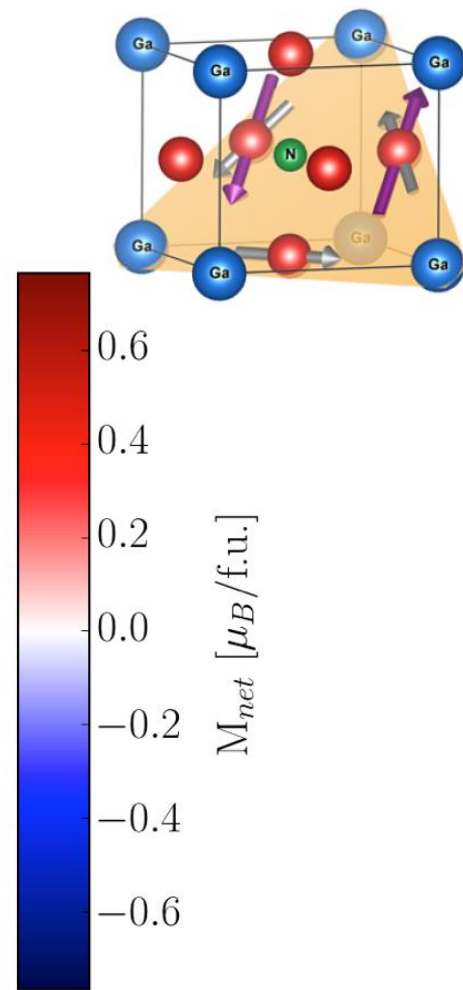
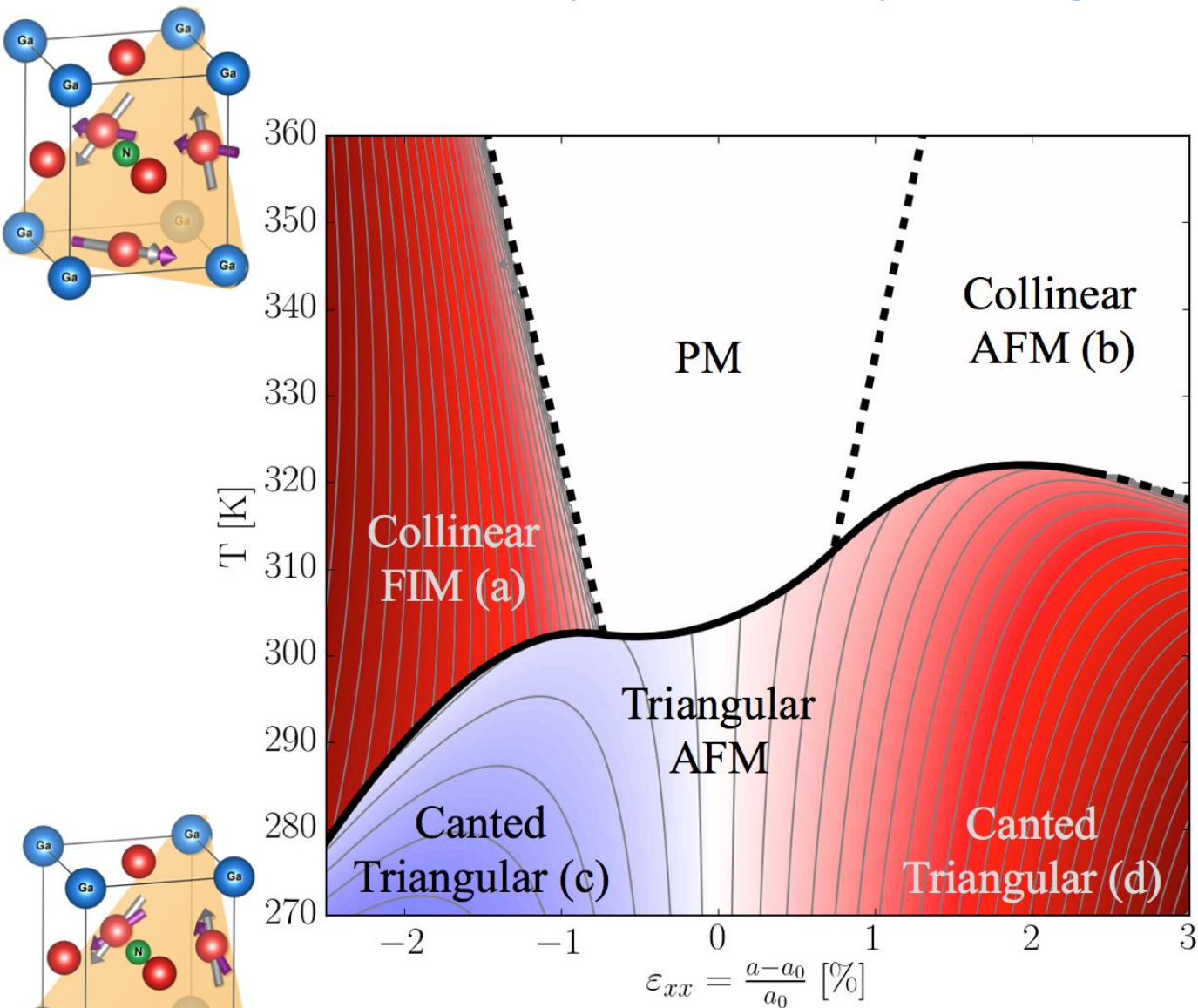
Figure 1. Cooling cycles. (a) The conventional vapor compression cycle uses a liquid–gas phase transition. (b) Caloric-material cooling cycles use magnetic (H), electric (E), or stress (σ) fields to reversibly change the entropy (shown as the vector arrays in gray, red, and blue) of the respective refrigerant material. (c) This temperature–state diagram shows ferroic cooling cycles that utilize a phase transition.

Ichiro Takeuchi, and Karl Sandeman

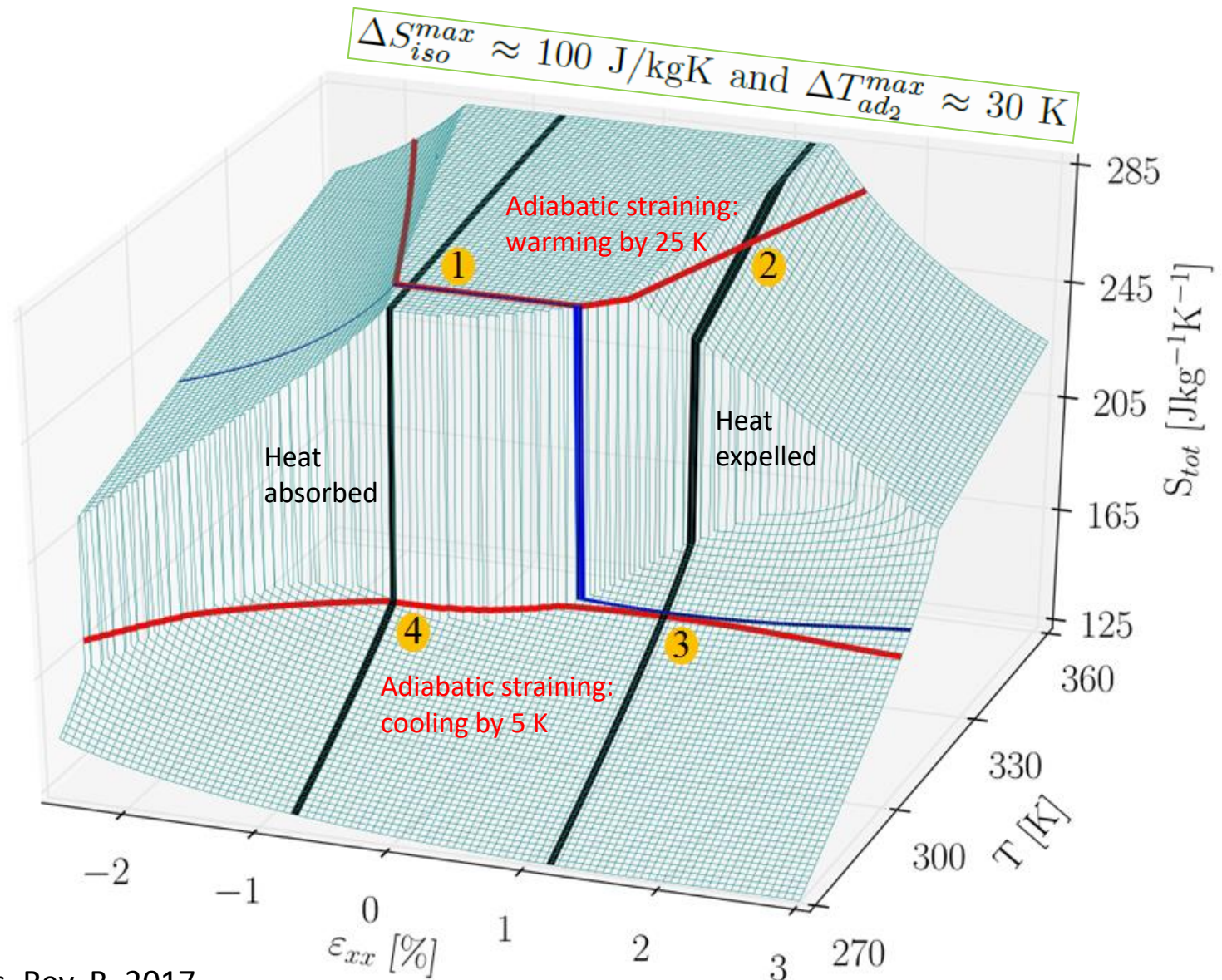
Citation: *Physics Today* **68**, 12, 48 (2015);

View online: <https://doi.org/10.1063/PT.3.3022>

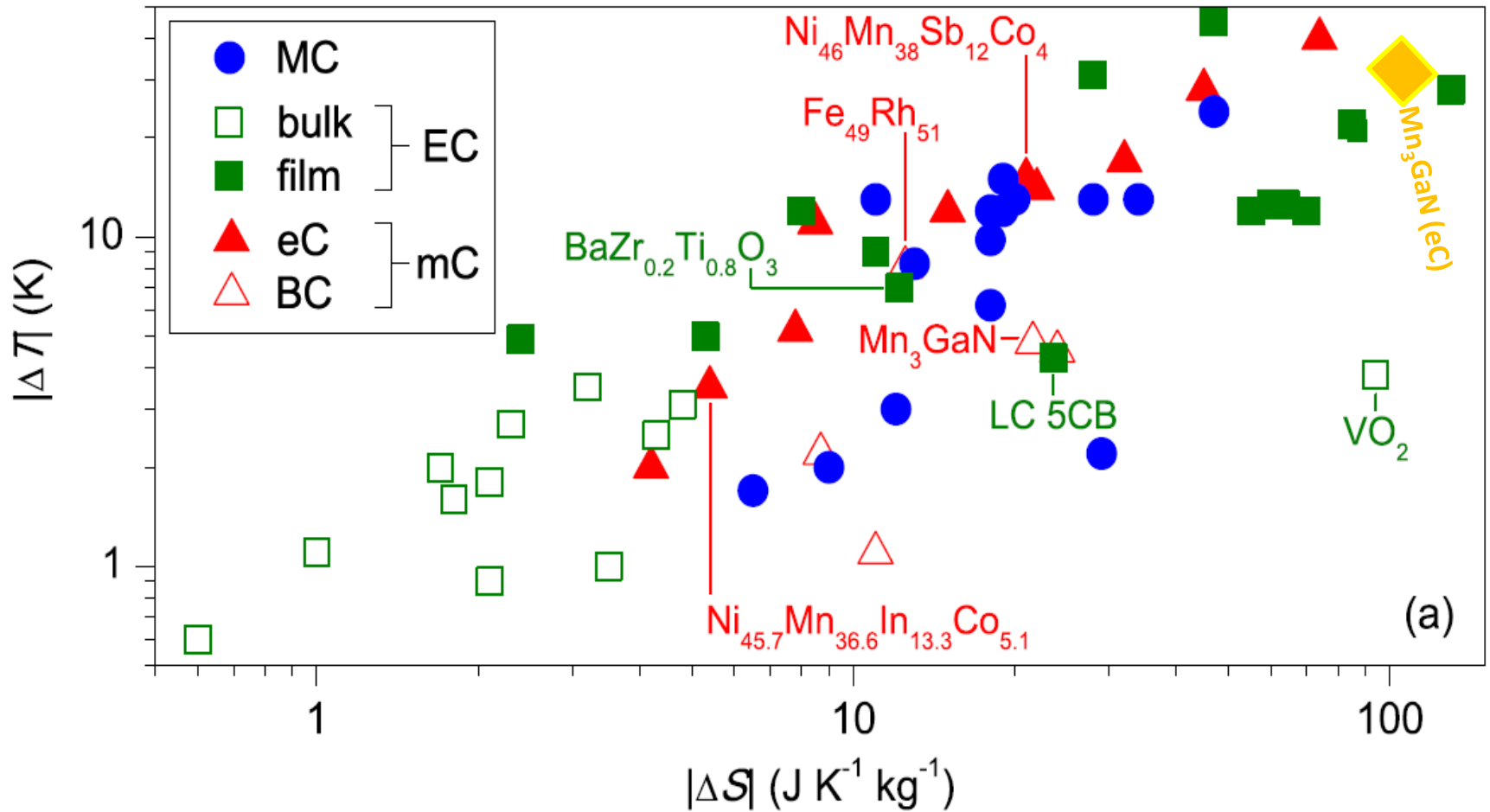
Temperature-strain phase diagram



Elastocaloric cooling cycle – an alternative to magnetocaloric cooling (Rare earth free, driven by a piezo-stressor)



Comparison to other solid-state cooling mechanisms (MagnetoCaloric, ElectroCaloric, mechanoCaloric)



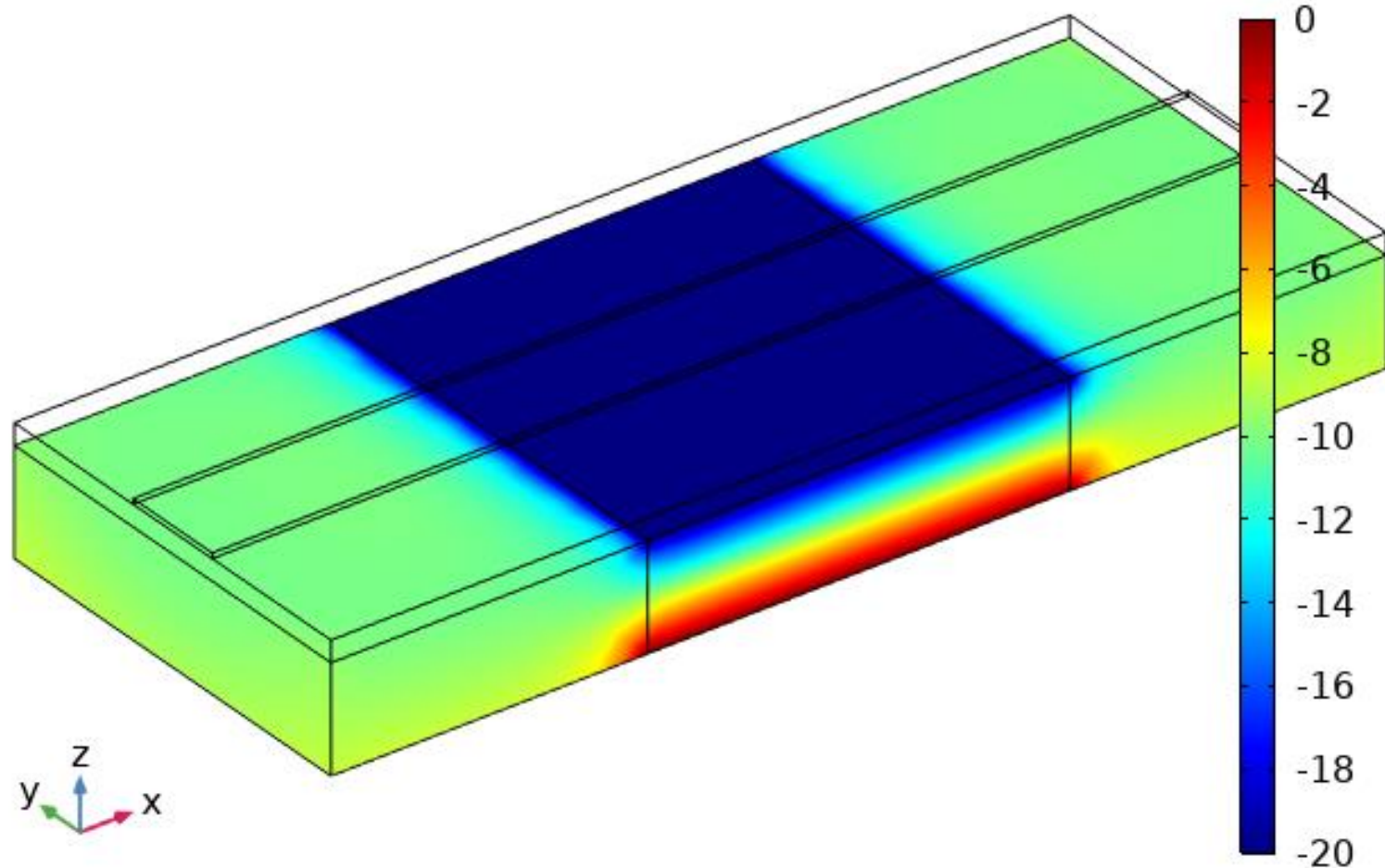
Heat source releasing the latent heat (instead of temperature dependent heat capacity)

The screenshot displays the software interface for a simulation. On the left, a tree view shows the model's structure, including materials like Lead Zirconate Titanate (PZT-5H) and Aluminum (mat16), and physics domains such as Solid Mechanics, Electrostatics, and Heat Transfer in Solids. The 'Heat Source 1' domain is selected. The central panel shows the 'Heat Source' settings for domain 4, with 'General source' selected and a 'User defined' equation for Q_0 . The equation is $QL \cdot \text{rho_MGN} \cdot \text{step3}(T[1/K] \cdot (1 + \text{solid.eXX} \cdot 10000)) - T_{\text{ref}}$ with units W/m^3 . A red arrow points to this equation. The 3D window on the right shows a rectangular block with dimensions in μm : length 5, width 2, and height 1. A blue highlighted region represents the heat source. The coordinate system (x, y, z) is shown at the bottom left of the 3D view.

$QL \sim$ latent heat released or absorbed at phase transition

Time=1 s

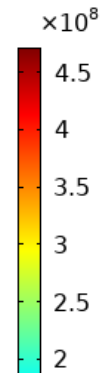
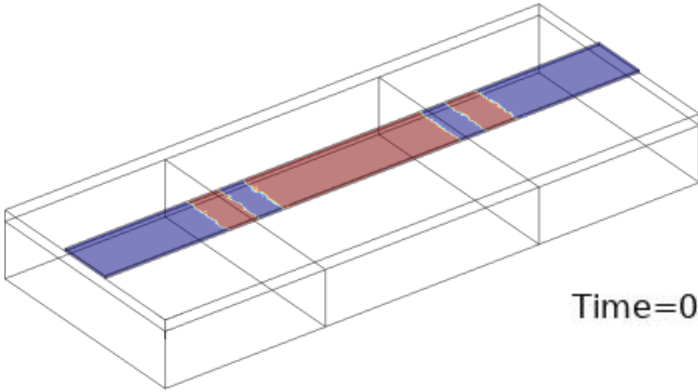
Surface: Electric potential (V)



Stressor is activated locally (not along the whole bar as in previous case)

Time=0.5 s

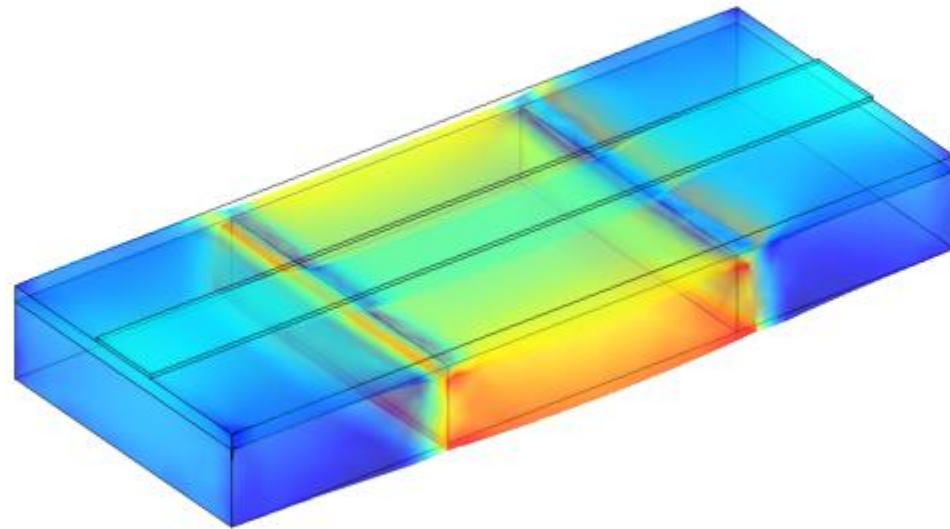
Slice: Total heat source (W/m³)



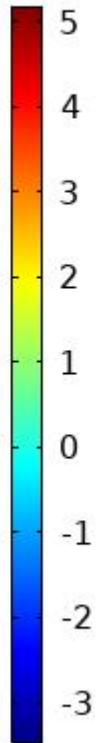
Heat source locally activated by strain

Time=0.5 s

Surface: Strain tensor, XX component (1)



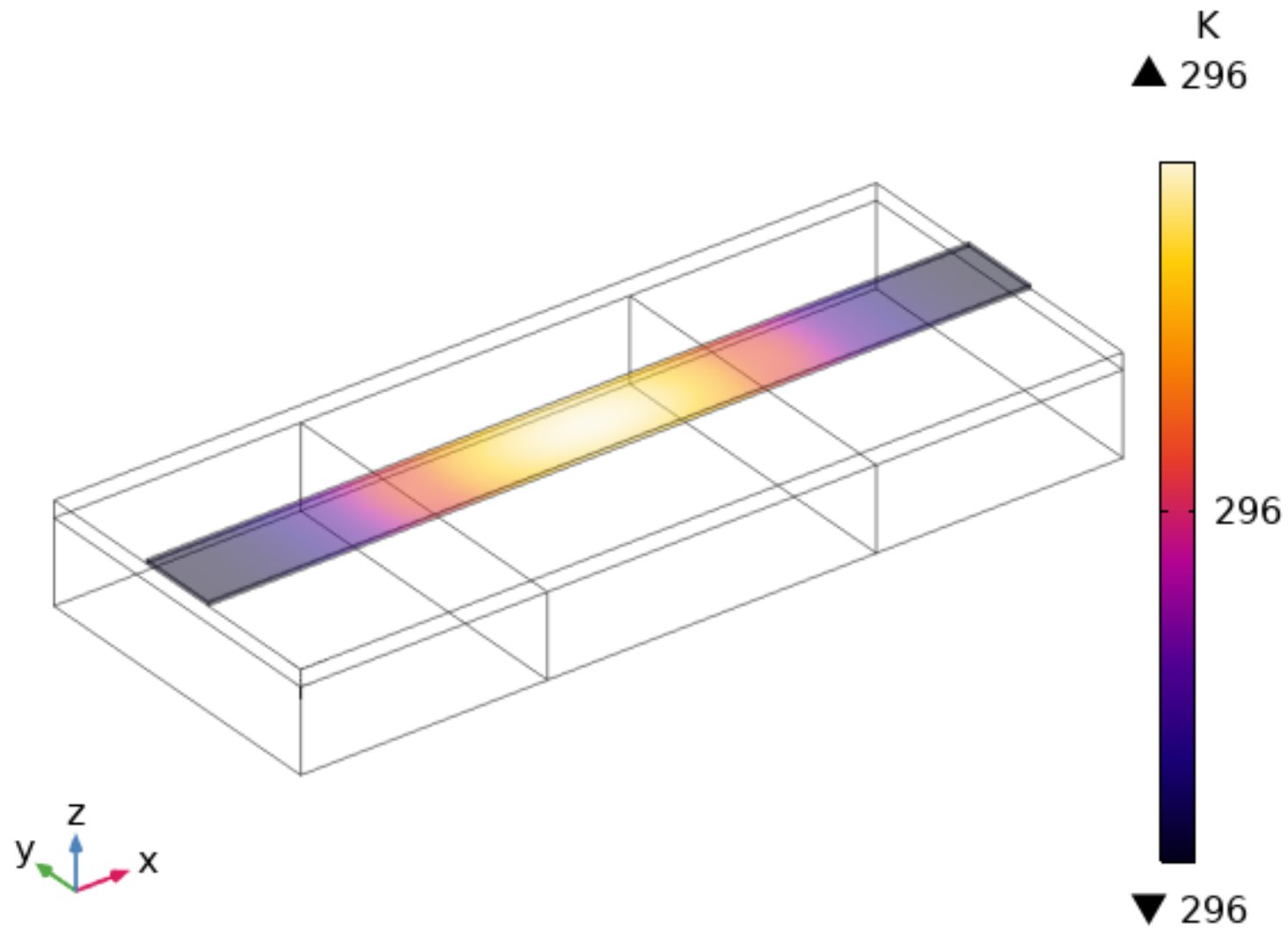
$\times 10^{-3}$





Time=0.5 s

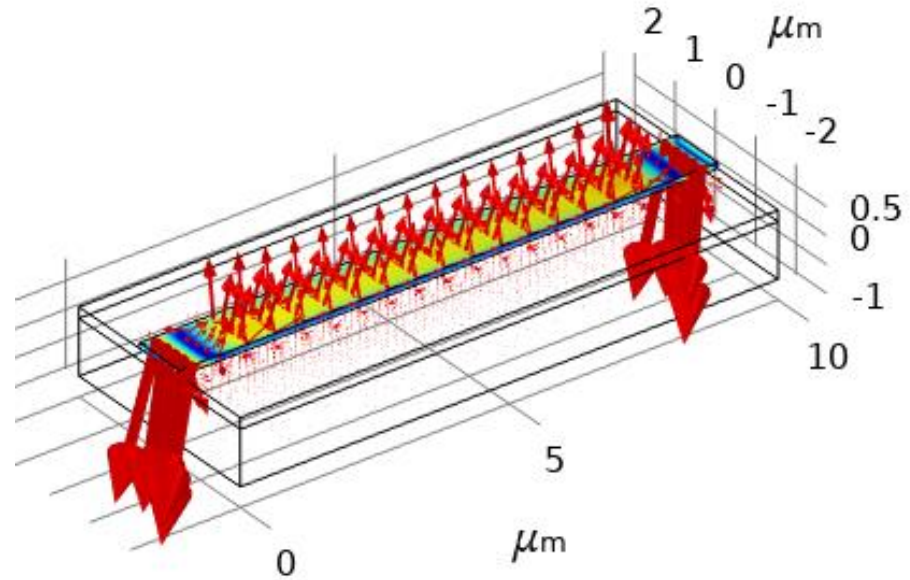
Slice: Temperature (K)



Summary

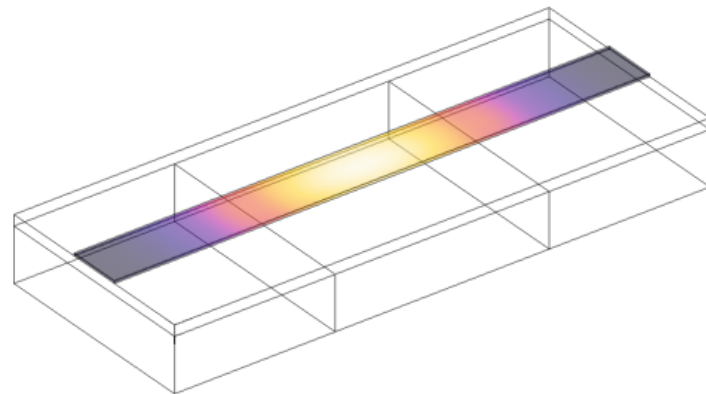
- Piezomagnetický jev

- Magnetization control
- MRAM



- Elastokalorický jev

- Phase transition control
- Solid state cooling



Díky za pozornost



EUROPEAN UNION
European Structural and Investment Funds
Operational Programme Research,
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MINISTRY OF EDUCATION,
YOUTH AND SPORTS