



UNIVERSITÄT
BAYREUTH

Retsch
Group

Thermal Conduction in Anisotropic Granular Mixtures

Comsol Conference 2023, Munich

Flora Lebeda

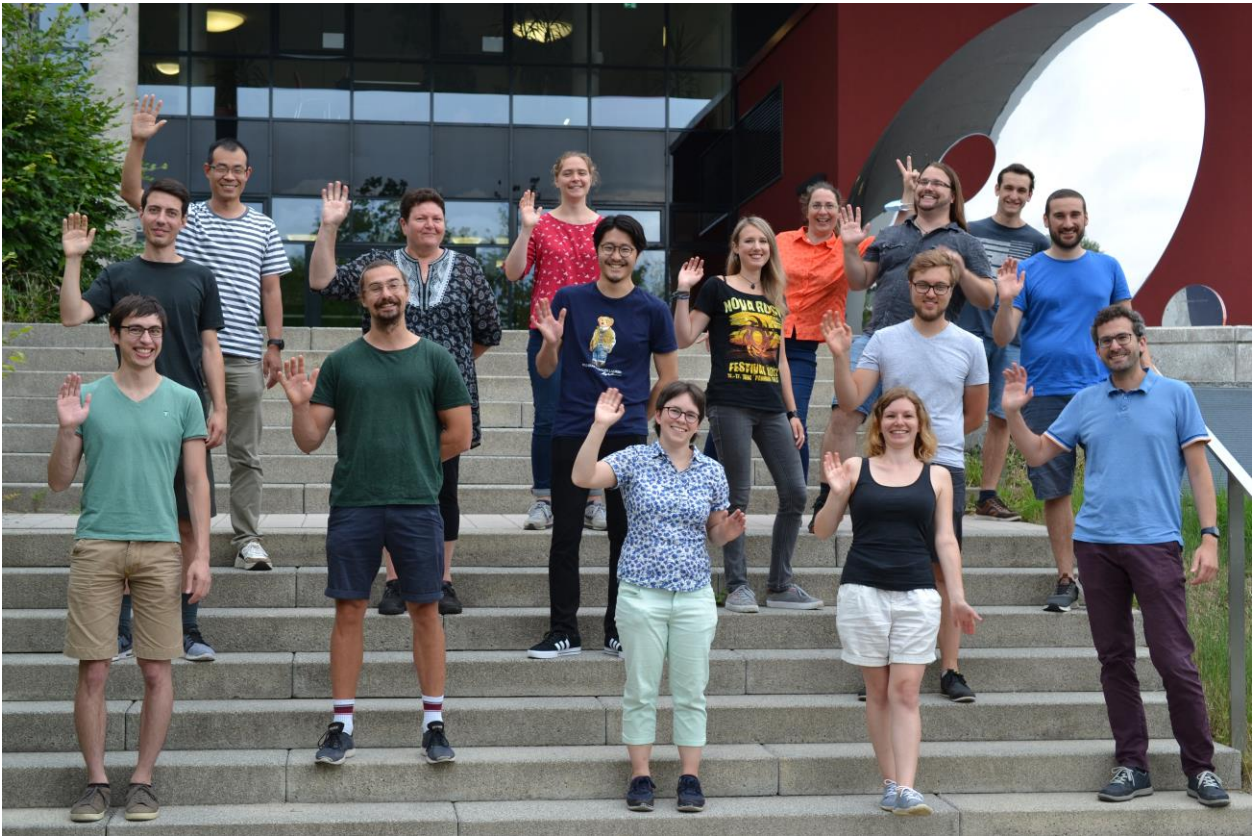
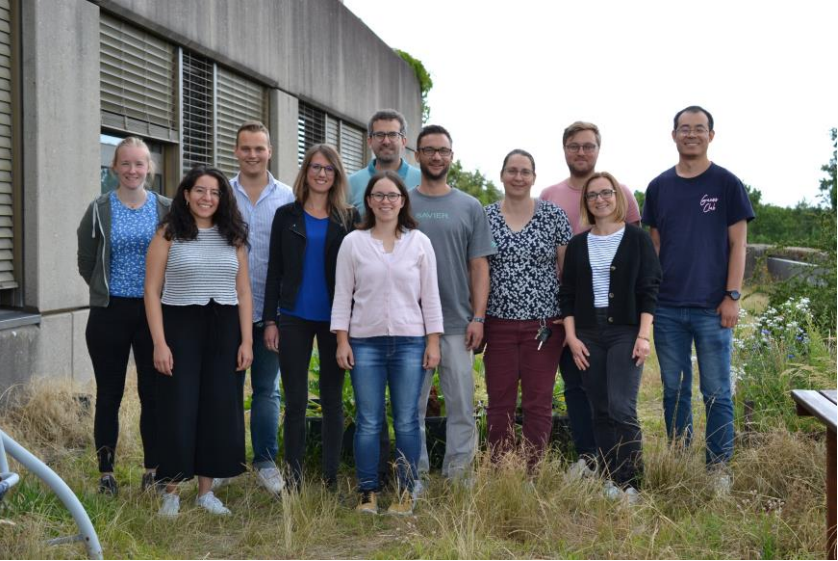
University of
Bayreuth

Thanks to my colleagues!



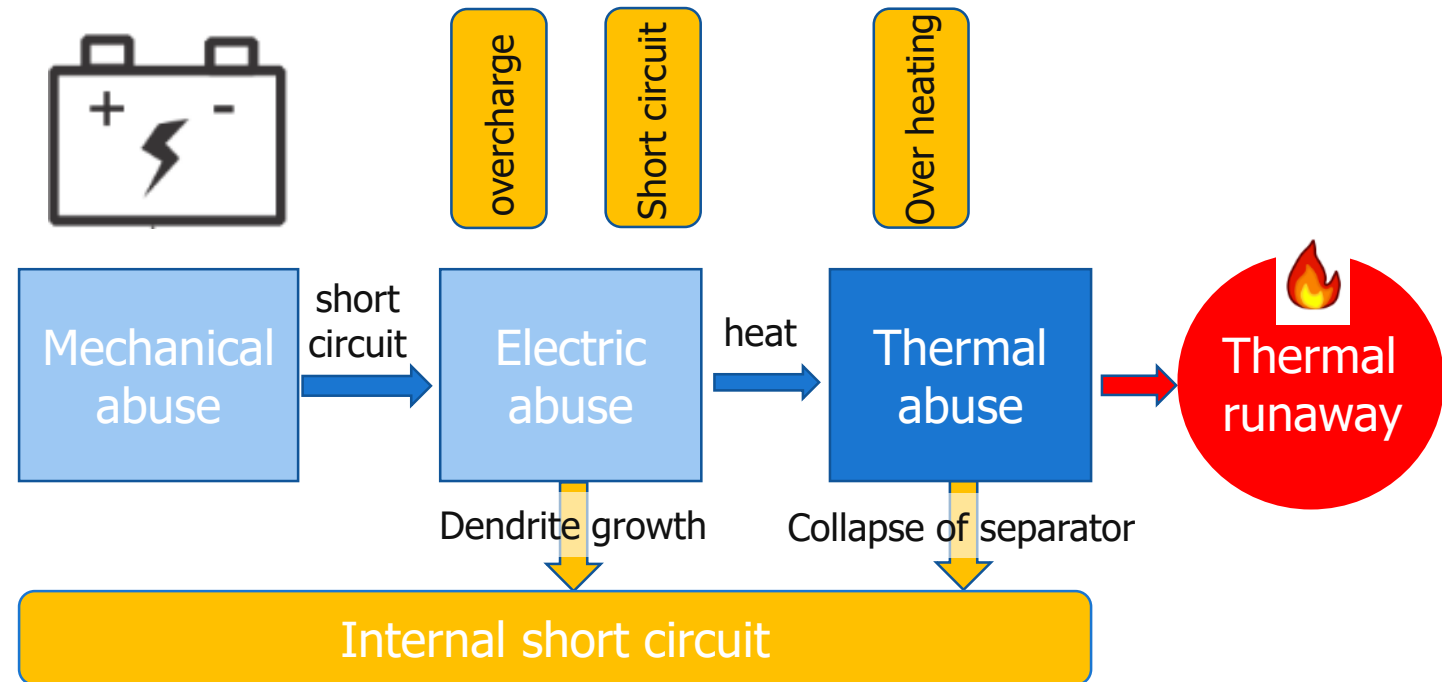
Bayerisches Zentrum für Batterietechnik

CHRISTIANE NÜSSEIN-VOLHARD-STIFTUNG



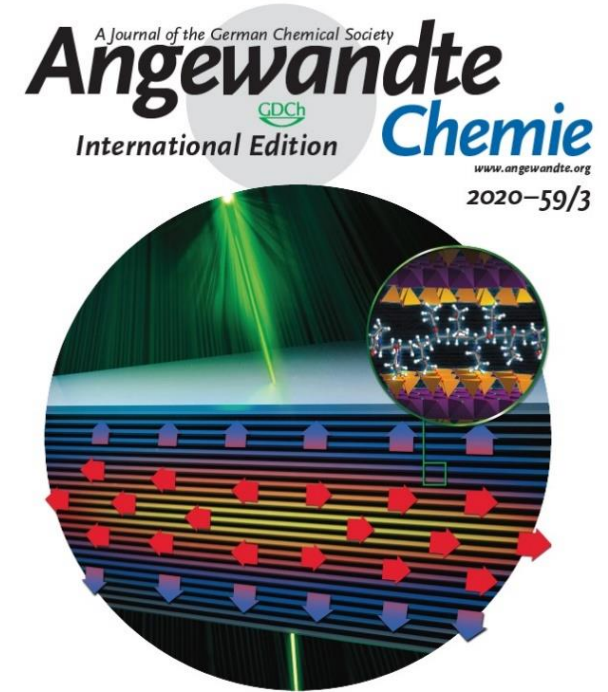
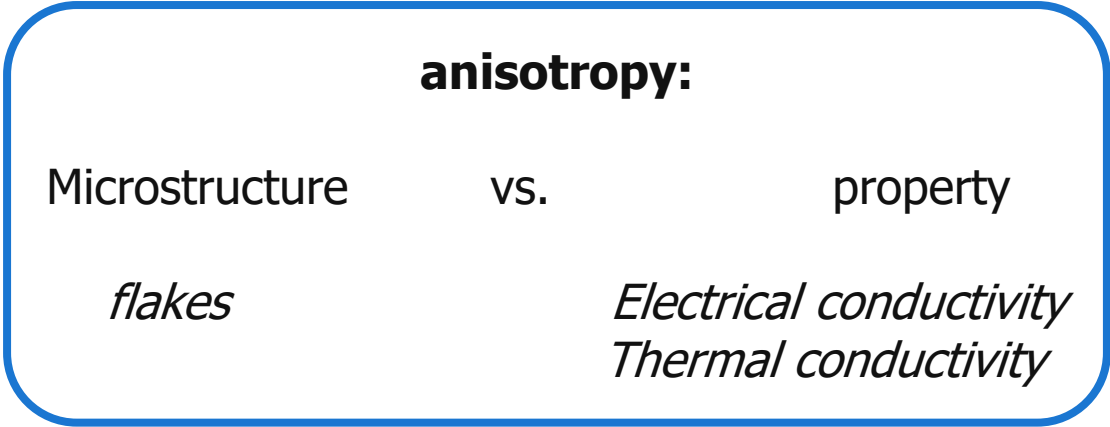
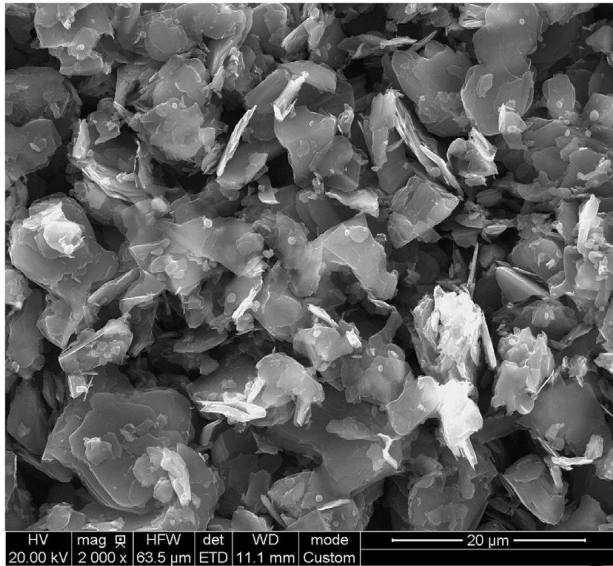
Prevention of heat release begins in the microscale!

About half of all products recalled for fire hazards are lithium-ion batteries.



Microstructure of battery electrodes?

Typical graphite powder



Cover Picture
 M. Retsch, J. Breu, G. Fytas et al.
 Tunable Thermoelastic Anisotropy in Hybrid Bragg Stacks with Extreme Polymer Confinement
 ACEFS 59 (3) 961–1356 (2020) | ISSN 1433-7851 | Vol. 59, No. 3

WILEY-VCH

Quantification of preferred orientation in graphite electrodes for Li-ion batteries with a novel X-ray-diffraction-based method

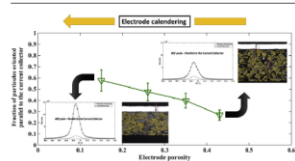
Simon Malifarge ^{a, b}, Bruno Delobel ^b, Charles Delacourt ^{a, *}

^a Laboratoire de Réactivité et Chimie des Solides, CNRS UMR 7314, Université de Picardie Jules Verne, 80039, Amiens Cedex, France
^b Renault Technocentre, 78084, Guyancourt, France

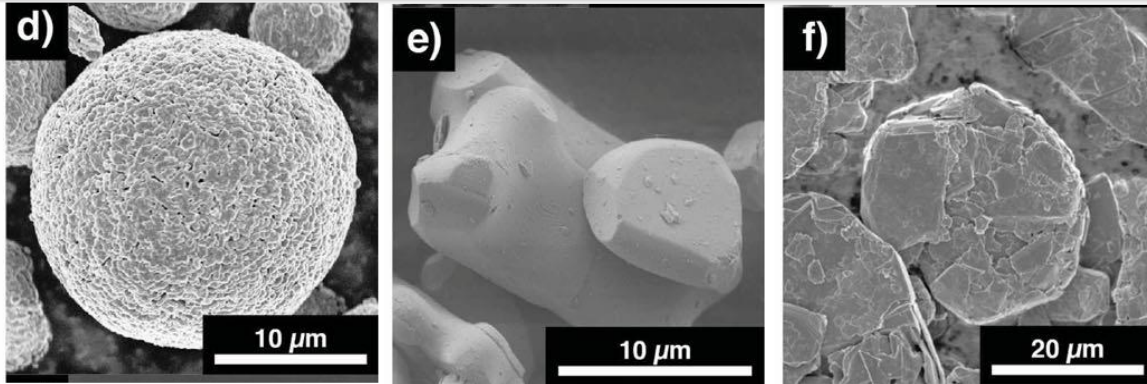
HIGHLIGHTS

- Particle orientation in an electrode is quantified by an X-ray diffraction method.
- A step function is used as the orientation distribution function.
- Anisotropic particle orientation increases with electrode calendaring.

GRAPHICAL ABSTRACT



Anisotropic materials in batteries? Random distribution!



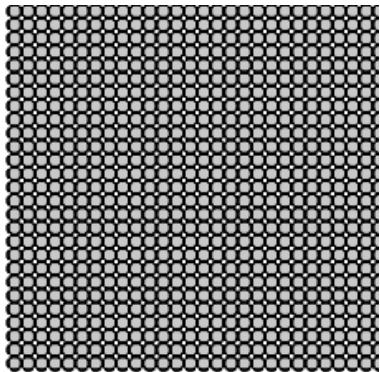
NMC

LCO

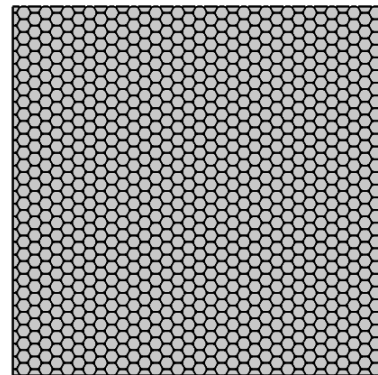
graphite

Assumptions: spherical particles
no additives, no electrolyte, narrow
size distribution

2D lattices

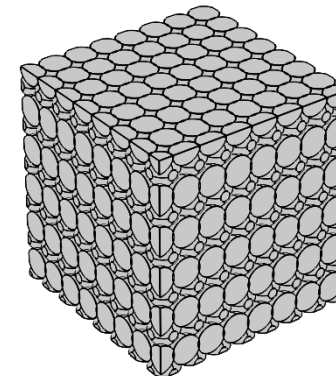


primitive cubic lattice
(cP)

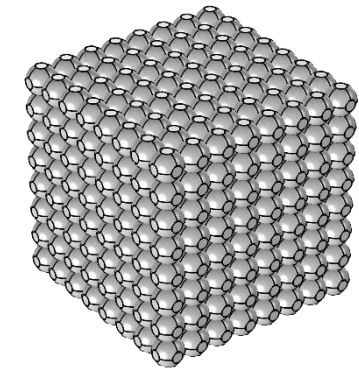


hexagonal lattice (fcc)

3D structure



hexagonal lattice (fcc)



primitive cubic lattice

simplification

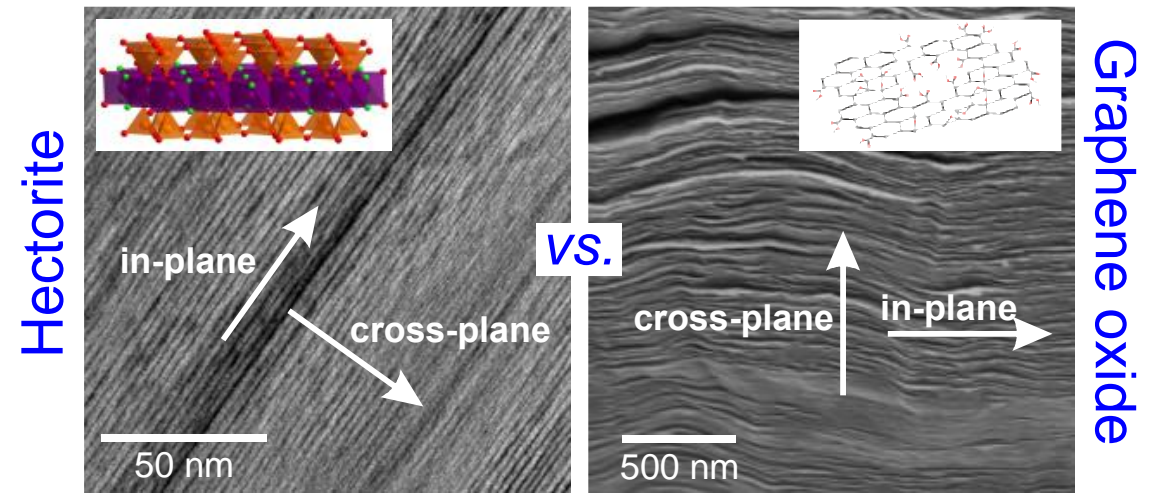
Rotation matrix for anisotropy in COMSOL

- Material property with anisotropy: tensor of 2D-rotation matrix

$$A = \begin{pmatrix} k_x (\cos \varphi)^2 + k_y (\sin \varphi)^2 & (k_x - k_y) \sin \varphi \cos \varphi & 0 \\ (k_x - k_y) \sin \varphi \cos \varphi & k_x (\sin \varphi)^2 + k_y (\cos \varphi)^2 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

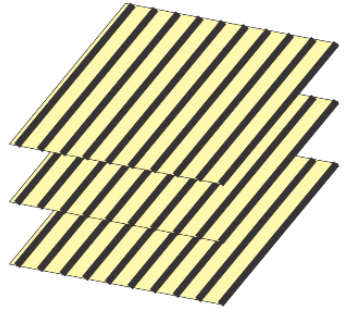
- isotropic material $\kappa = 100 \frac{W}{m K}$

- anisotropic material $\kappa = A \frac{W}{m K}$



proof: IR thermography of Laminates

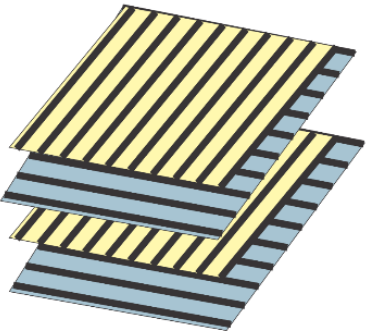
a) thermally anisotropic laminate



parallel alignment of prepregs
=> preferred conduction along carbon fibers



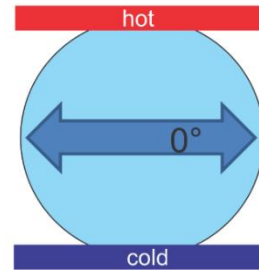
b) thermally isotropic laminate



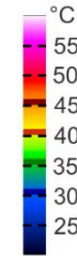
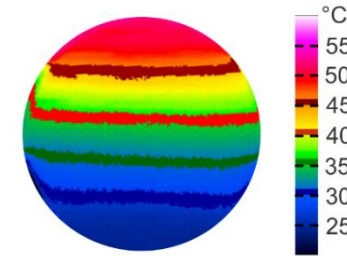
orthogonal alignment of prepregs
=> no direction-dependency of laminate



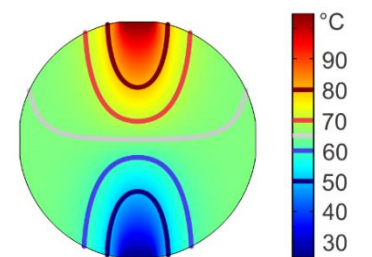
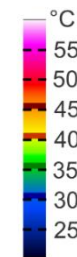
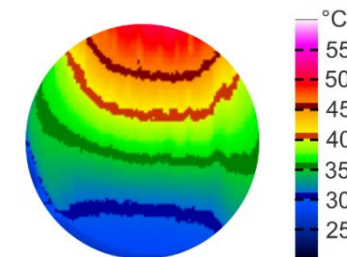
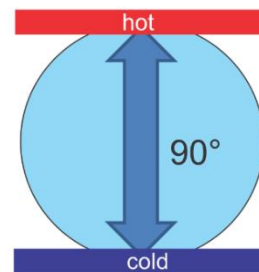
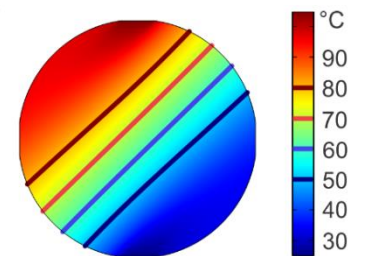
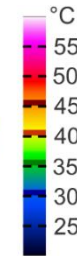
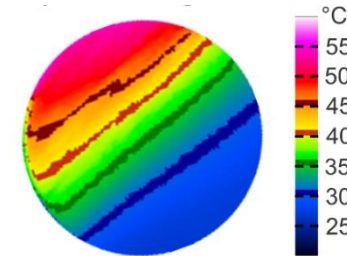
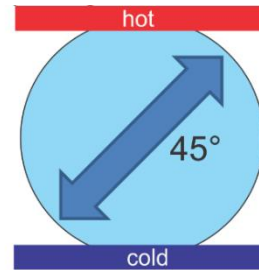
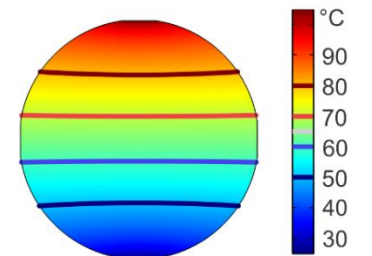
Rotation



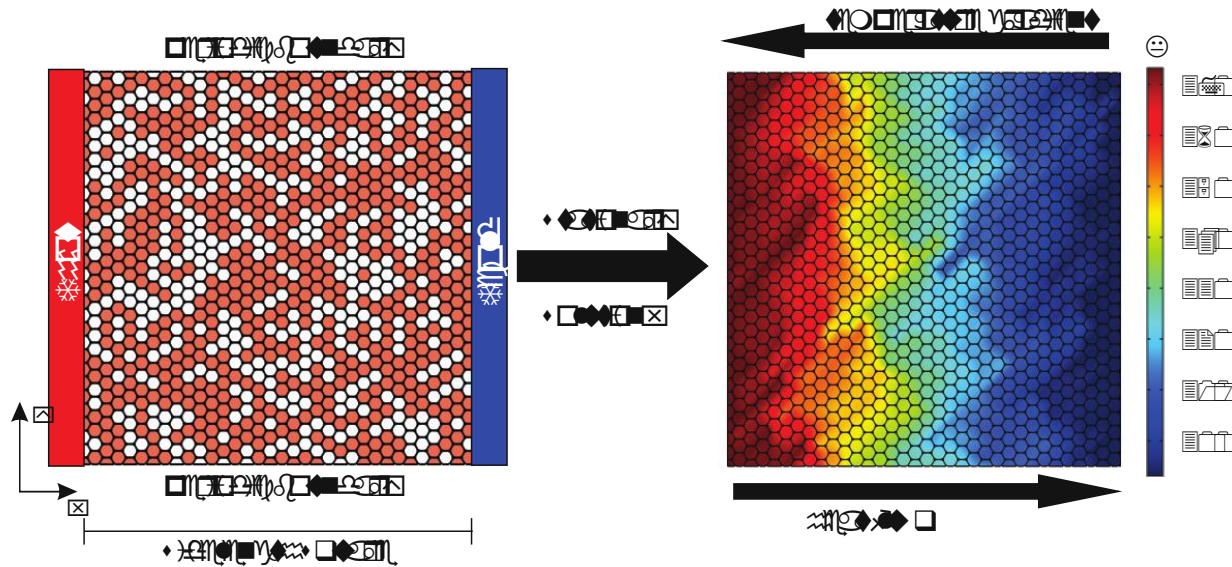
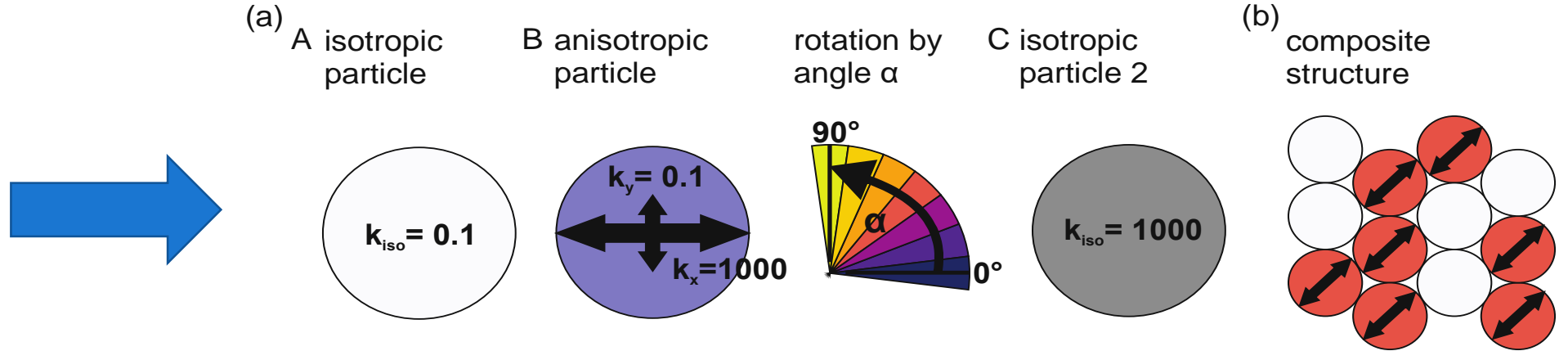
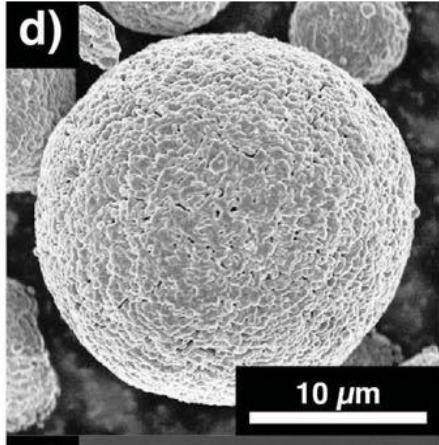
Thermogram



COMSOL



Modelling heat transfer of electrode

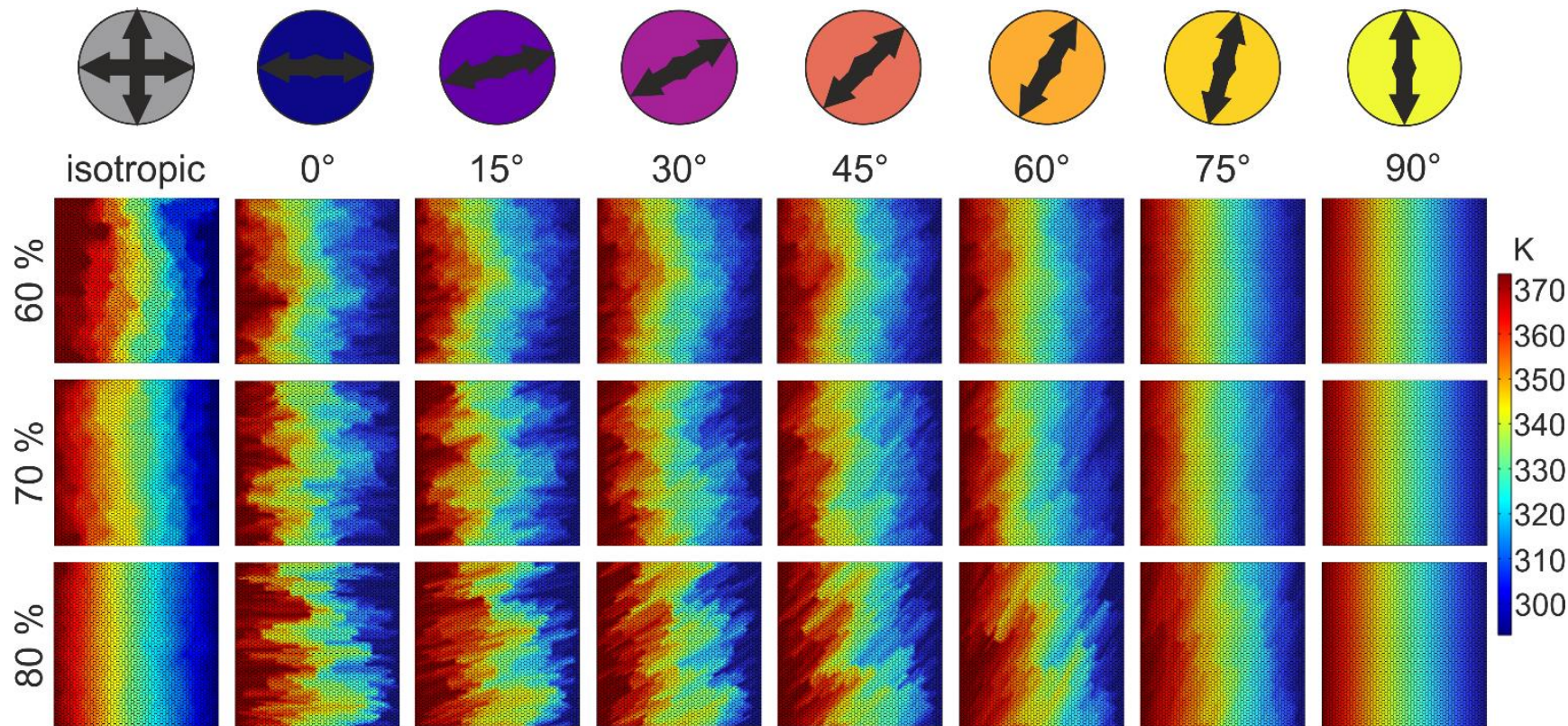


Automization:
Application Builder!

Influence of anisotropy?

Depends on:

- Amount of anisotropic particles
- Ratio of anisotropy in the single particles

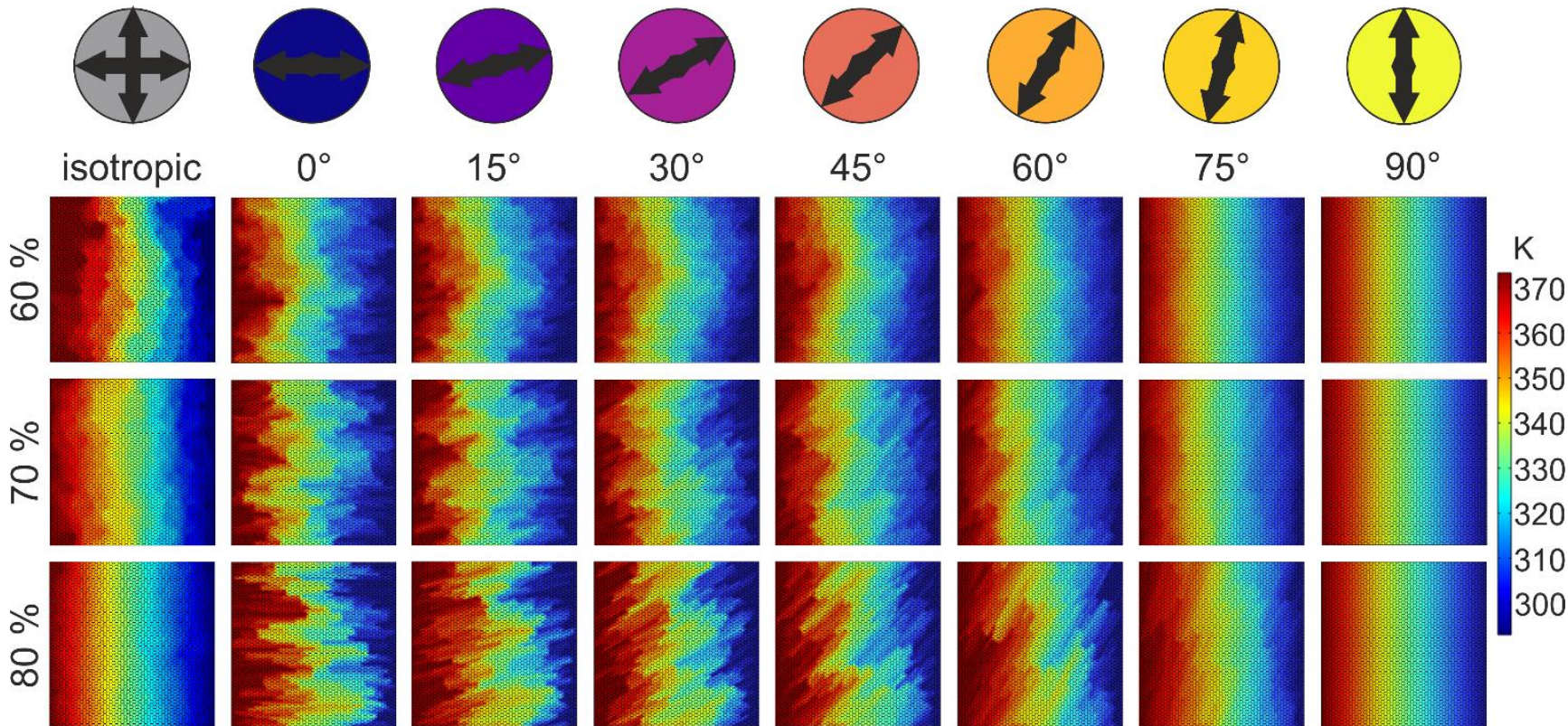


Internal temperature
distribution changes
drastically!

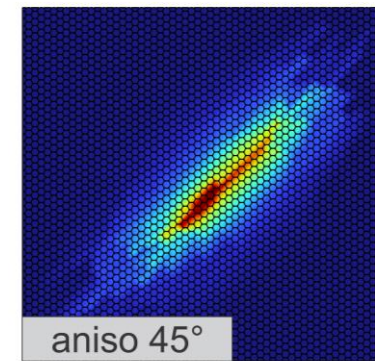
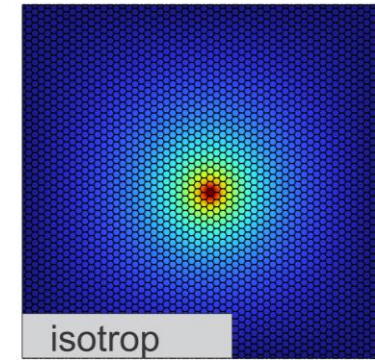
Influence of anisotropy?

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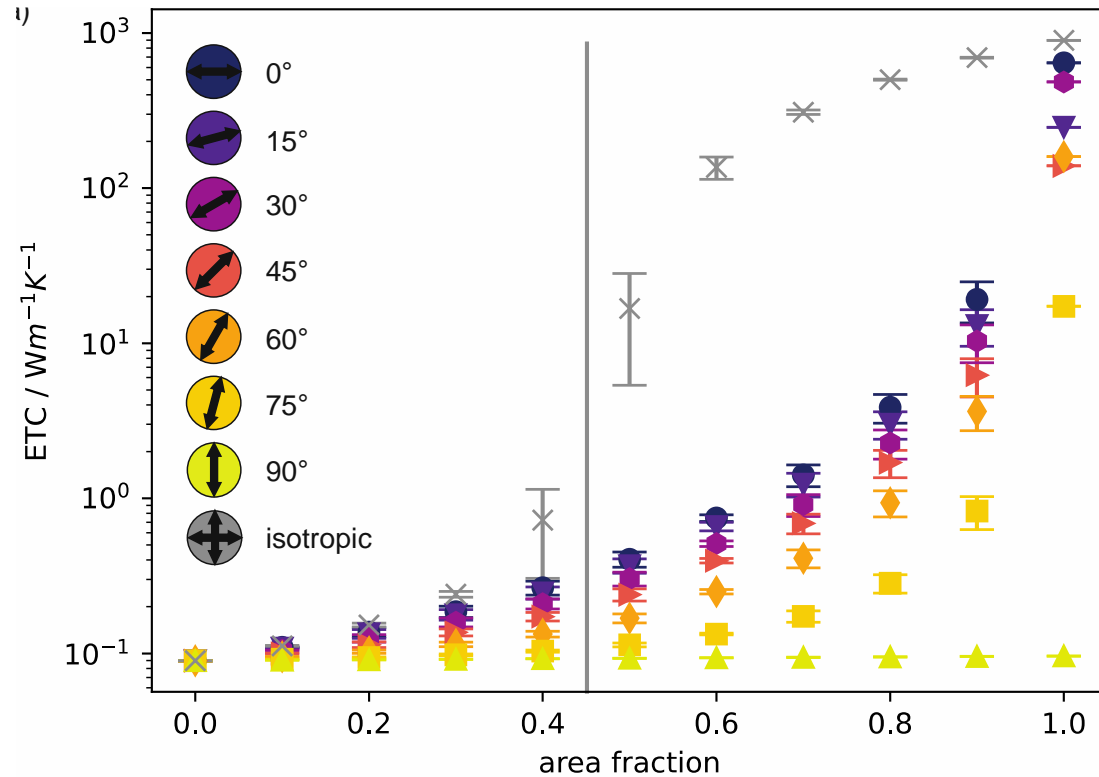
Heat source at center



Risk of hot spots!

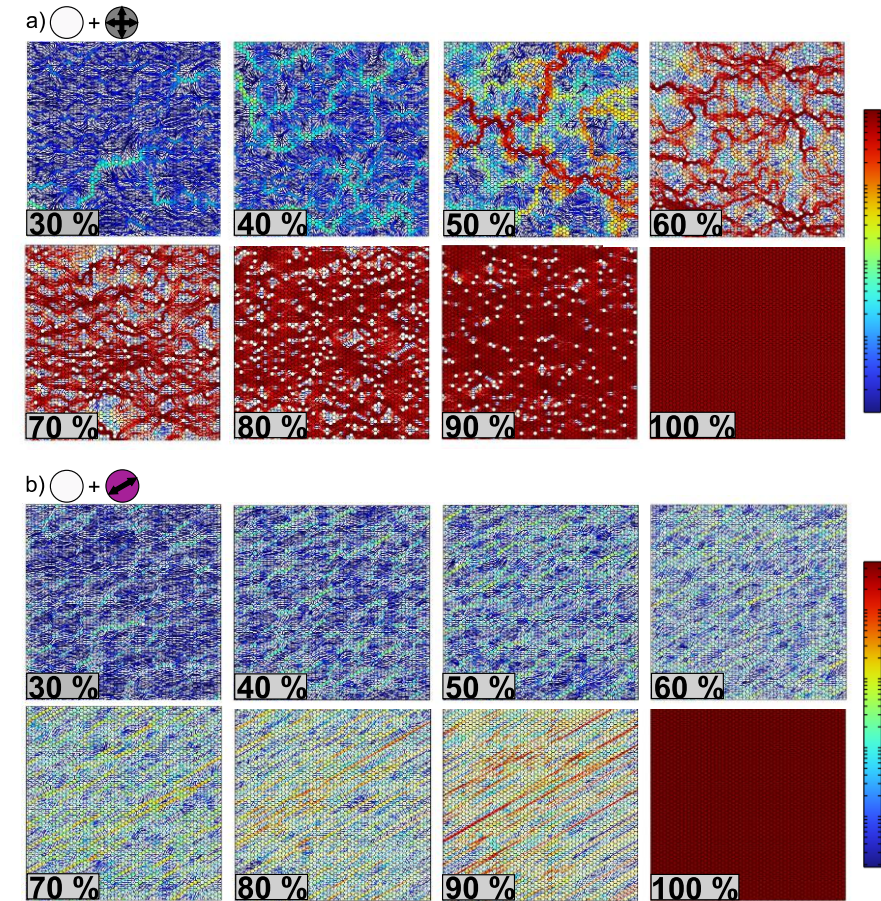
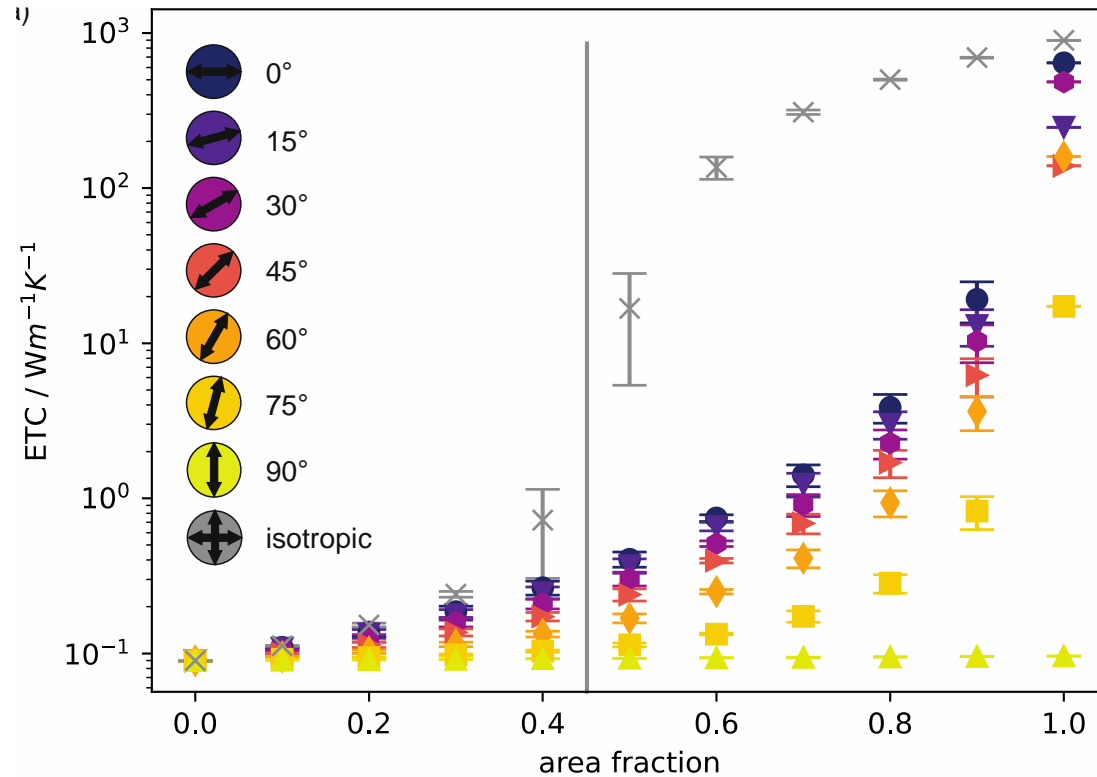
So, avoid anisotropic components?

- Effective thermal properties can be tailored specifically

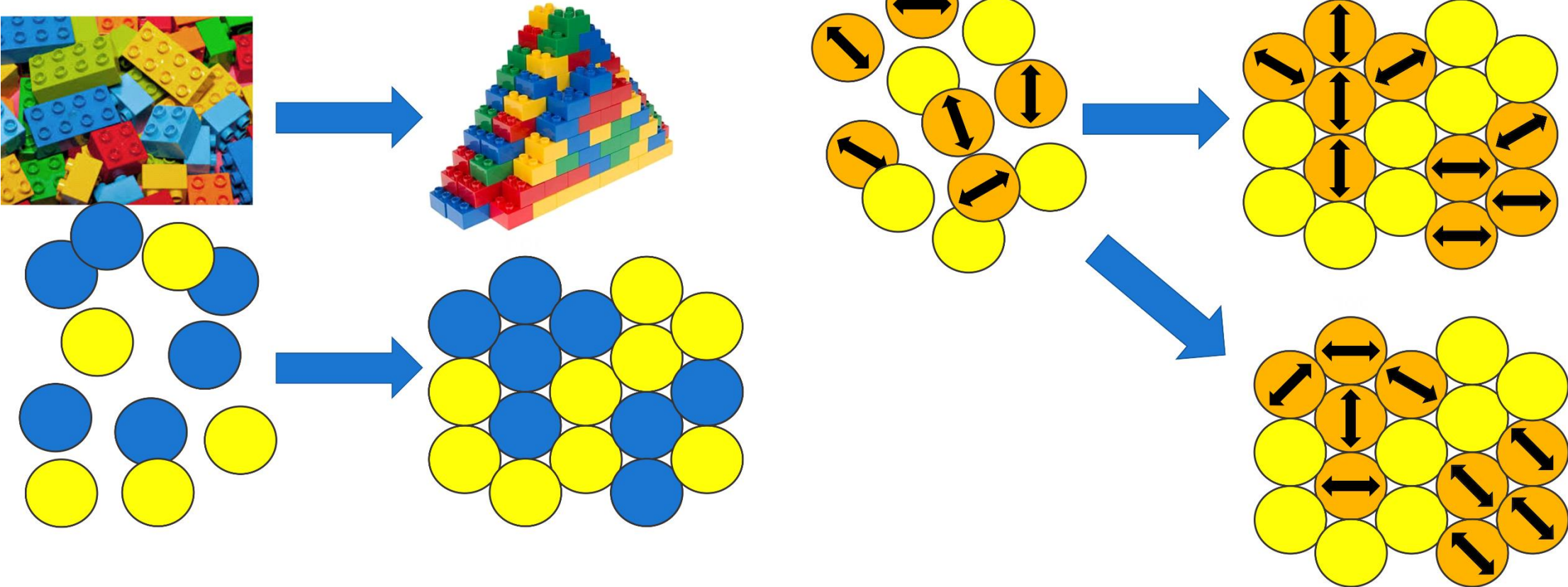


So, avoid anisotropic components?

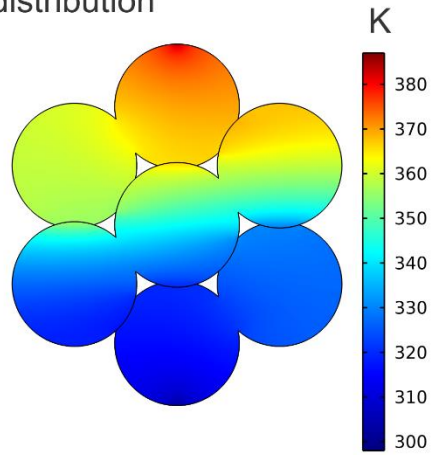
- Effective thermal properties can be tailored specifically



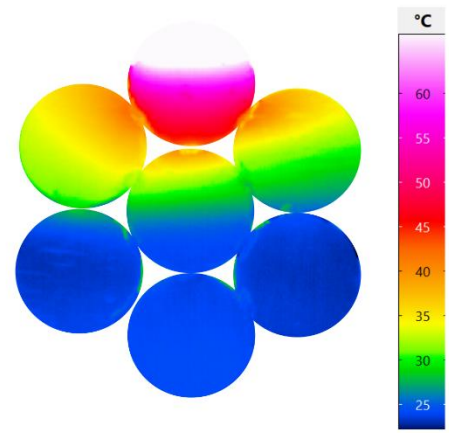
Application – Design of novel materials!



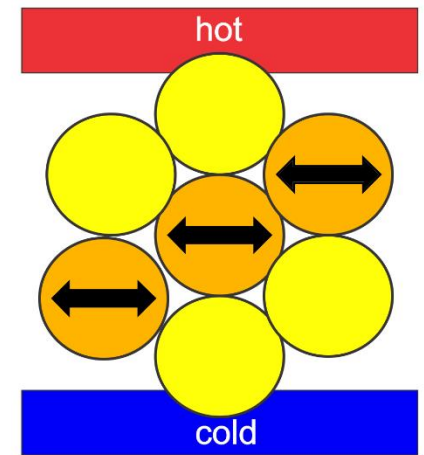
a) simulated temperature distribution



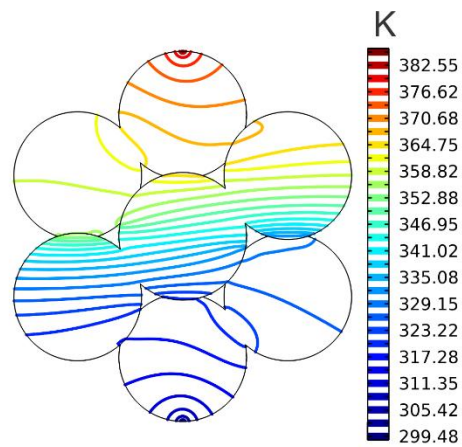
b) measured temperature



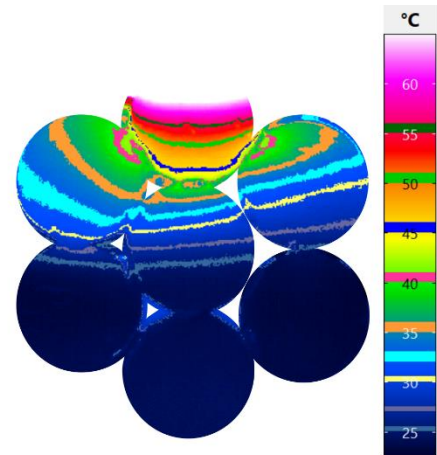
e) arrangement of the laminates

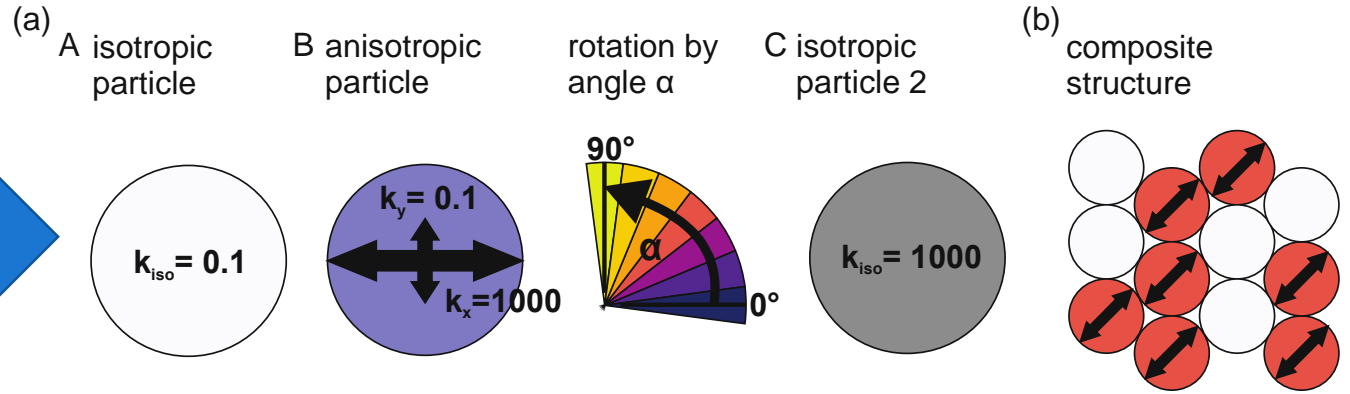
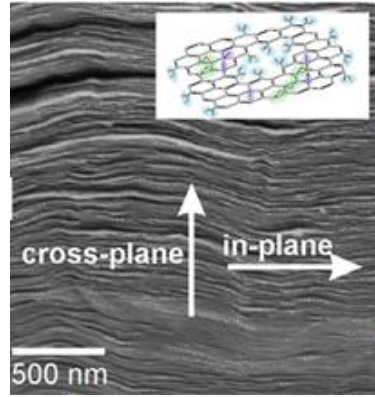
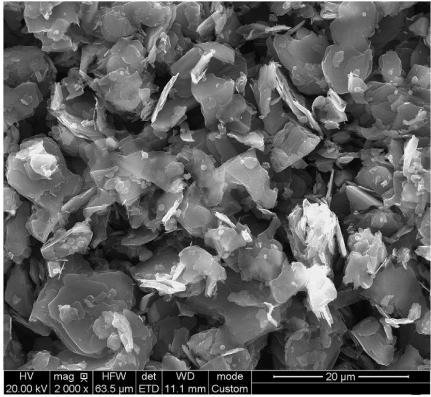


c) simulated isotherms



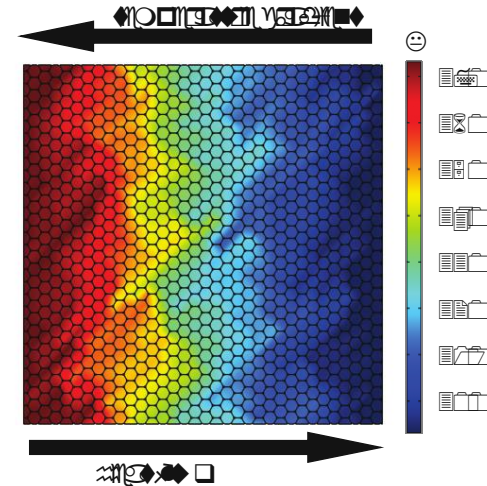
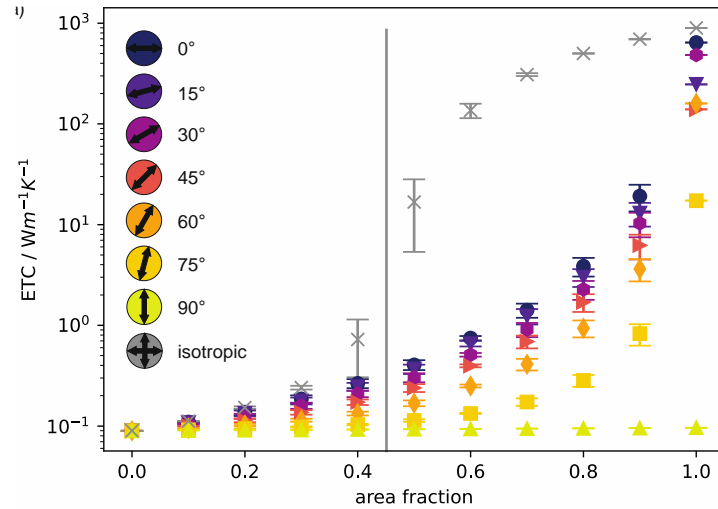
d) measured isotherms





Anisotropic graphite

Tailored thermal conductivity



Strong internal temperature gradients