FEMS EUROMAT23

Multi-phase field evolution in Ni-YSZ Fuel Cells with Temperature-Dependent Elasticity

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Sep 07 | 2023

1. Fuel Cells : Introduction

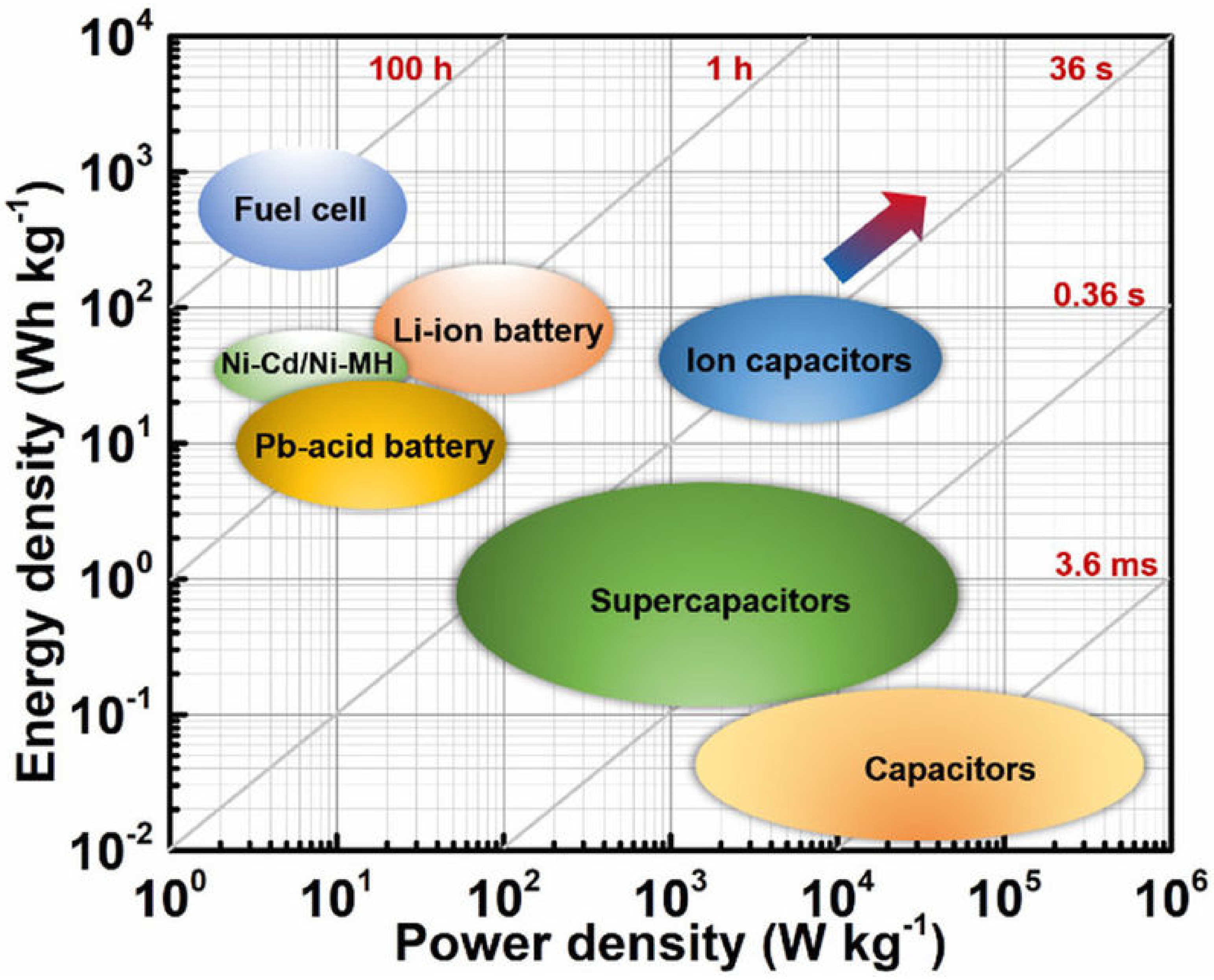
Fuel Cells: High Energy Density

- Store a lot of energy in a small space.

Capacitors: High Power Density

- Excel at releasing energy rapidly.

Other devices are in between Fuel cells and Capacitors including **batteries**.



Aravindan, Vanchiappan, et al. "Insertion-type electrodes for nonaqueous Li-ion capacitors." Chemical reviews 114.23 (2014): 11619-11635.

2. Nickel yttria-stabilized zirconia (Ni - YSZ)

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Y_2O_3

Stabilization

ZrO_2

Ni

YSZ

Ni - YSZ

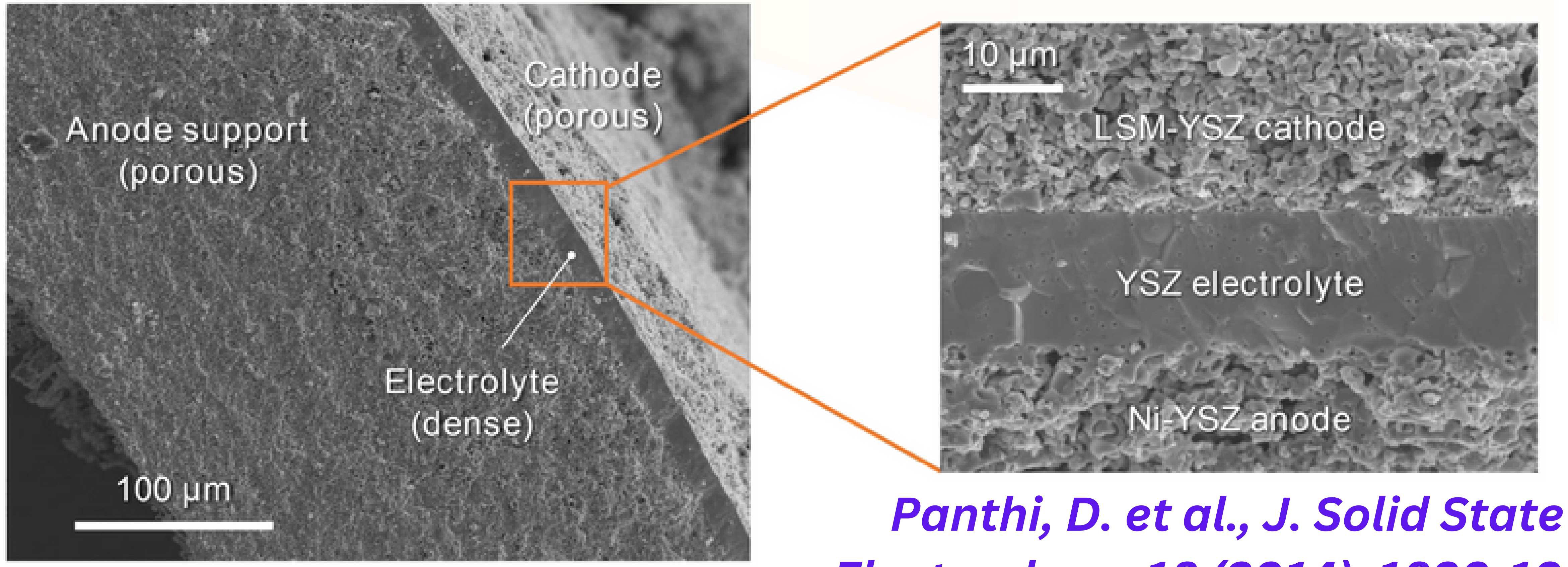
Applications in Solid fuel cells

Electrochemical reaction at three-phase boundary (TPB) regions

Electronic Conduction — Ni rich phase

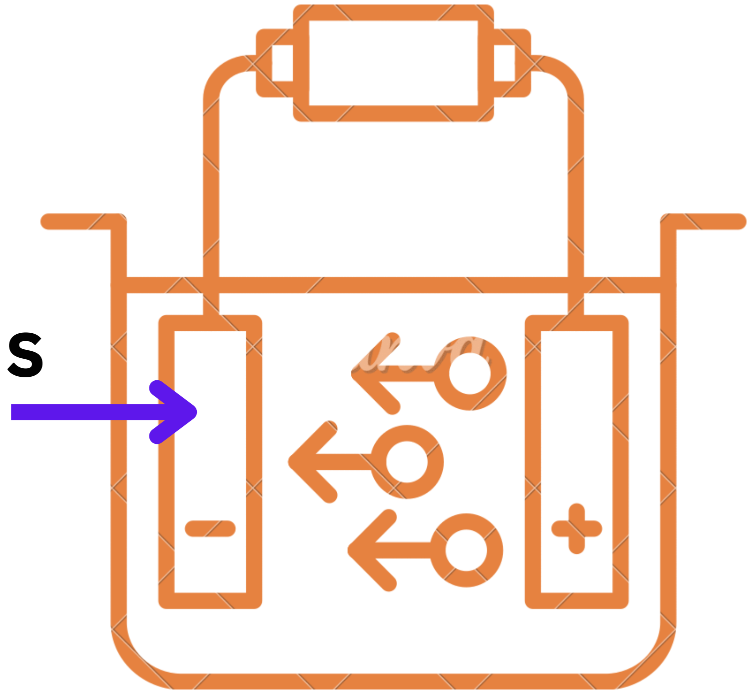
Ionic Conduction — YSZ rich phase

Anode as support



Panthi, D. et al., J. Solid State Electrochem. 18 (2014): 1899-1905

Ni-YSZ (Non-porous anode)



3. Nickel Coarsening

Nickel Coarsening
• Nickel particles can merge together • Decrease surface area for catalysis.

Ni coarsening parameters

- Processing parameters (powder particle size, sintering temperature, etc.)
- Operating parameters (temperature, fuel, H2O concentration)

4. Methodology Overview

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DFT

QUANTUM ESPRESSO

Temperature Dependent

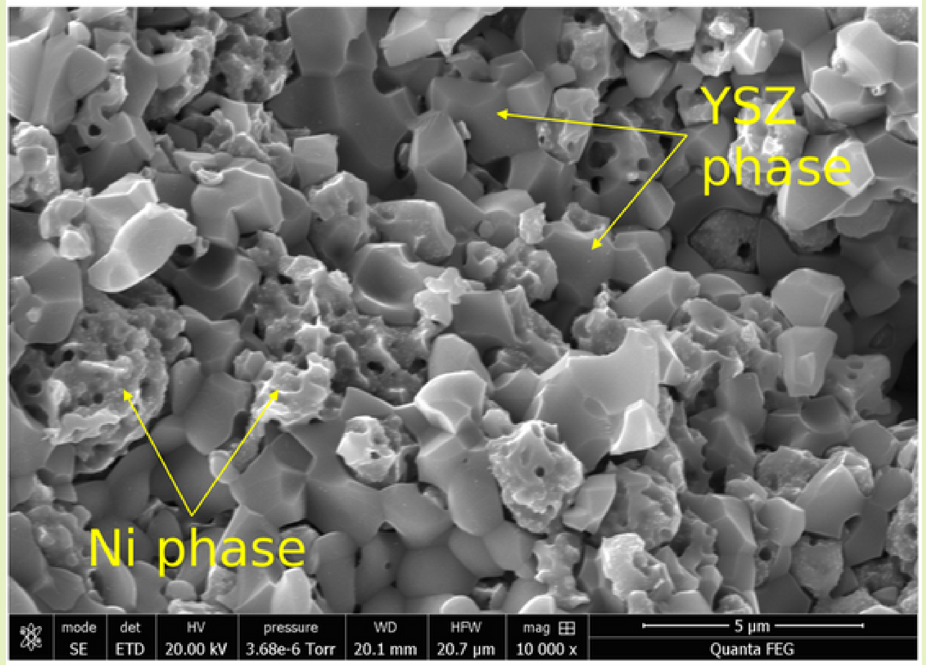
C *ijkl*

Phase Field

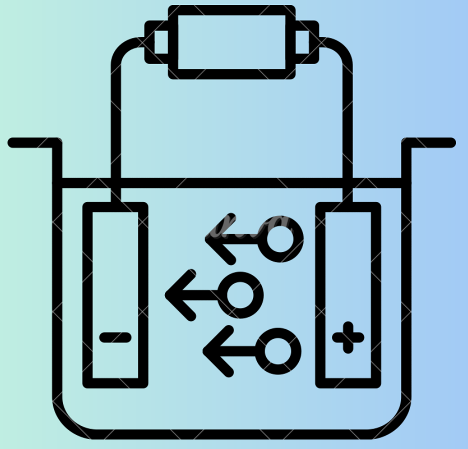
MOOSE

Microstructure Evolution

Experiments



Ni-YSZ



Scale-bridging Simulations for Microstructure study

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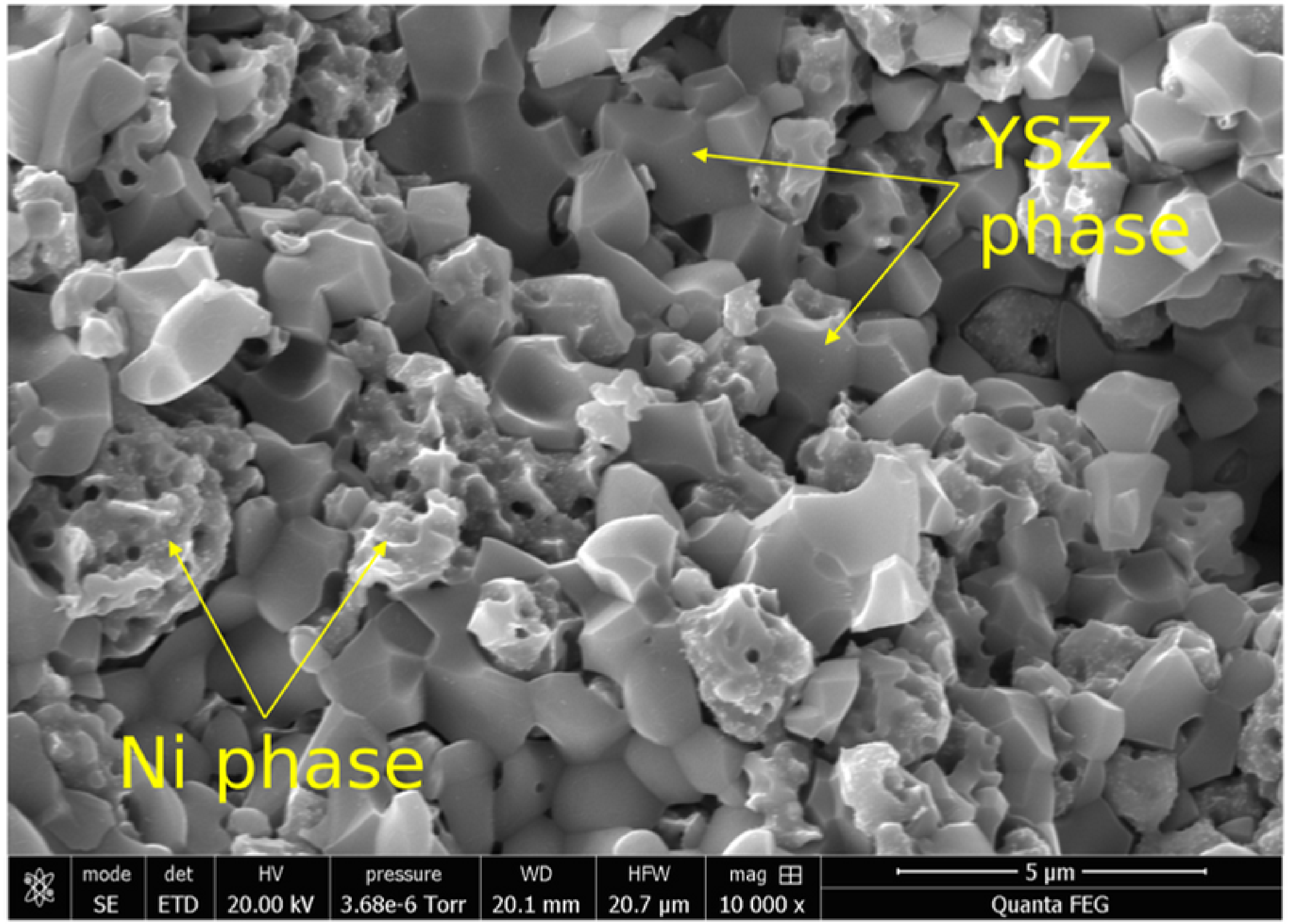
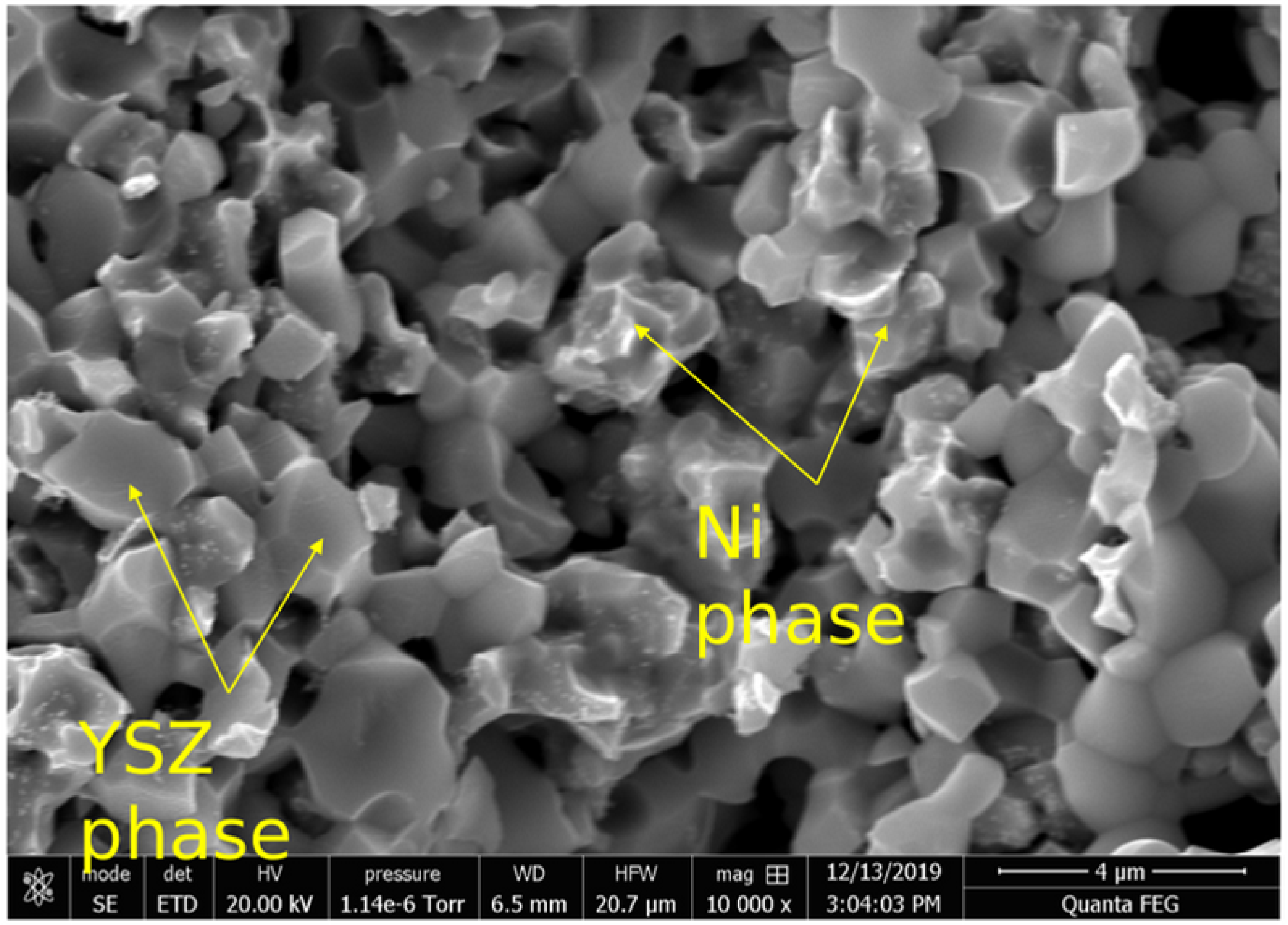
4.1 Insights for Digital Representation



11 h Operation



Max. Temperature: 973 K

Nature of Ni coarsening / agglomeration.

D.Panthi, Kent State University, USA.

4.2 Related Literature

- Anode microstructure evolution and resulting electrochemical performance degradation [1]
- Anode reduction process [2]
- Effective conductivity change during microstructure coarsening [3]
- Validation: Phase Field Model for Ni Coarsening in Solid Oxide Cells. [4]
- Quantitative 3D simulation of Ni coarsening (supported by ex-situ ptychographic nano-tomography) [5]

[1] Shikazono, N. et al., **J. Electrochem. Soc.** 160 (2013): F709

[2] Shikazono, N. et al., **J. Power Sources** 305 (2016): 10-16

[3] Lei, Y. et al., **J. Power Sources** 345 (2017): 275-289.

[4] M. Trini et. al, **Acta Mater.** (2021) 212(9):116887

[5] Yang, S. et al., **Acta Mater.** 246 (2023): 118708

Presented concept

$$\left.\begin{array}{c}\text{Ni}\\ \text{Zr}\\ \text{Y}\\ \text{O}\end{array}\right\}\ \text{4 component}$$

2 Phase

6 order parameter

Phase field simulations

YSZ is considered single component

Temperature-dependence of mechanical properties has not been undertaken

4.3 Physics behind phase field model

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Phase field equations

Conserved composition evolution equations

$i = 1, 2$

$$\frac{\partial c}{\partial t} = \nabla \cdot \left(\sum_i h_i M_i \nabla \left(\frac{\partial f_{\text{bulk}}}{\partial c_i} + \frac{\partial f_{\text{el}}}{\partial c_i} \right) \right)$$

Non-conserved order parameter

$N = 1 \text{ to } 6$

$$\frac{\partial \eta_i}{\partial t} = -L(\eta_1, \ldots, \eta_N) \left(\frac{\partial f_{\text{bulk}}}{\partial \eta_i} + \frac{\partial f_{\text{el}}}{\partial \eta_i} + \frac{\partial f_o}{\partial \eta_i} - \nabla \cdot \frac{\partial f_{\text{grad}}}{\partial (\nabla \eta_i)} \right)$$

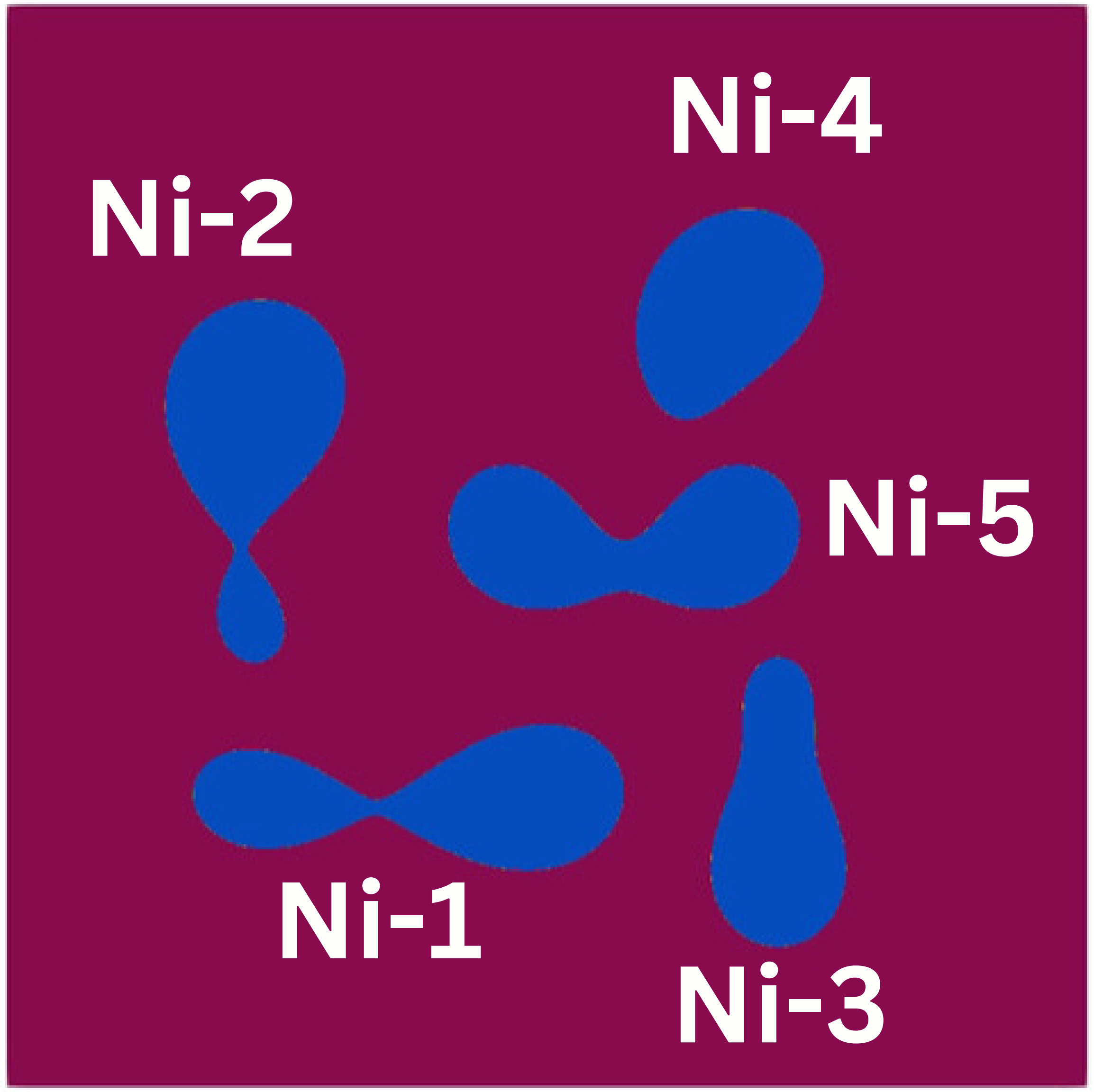
pycalphad

Curve fitting

Gibbs free energy

f_{bulk}

Ansara, I., A. T. Dinsdale, and M. H. Rand. "Al-Mg COST 507 Thermochemical database for light metal alloys." (1998).



700 nm x 700 nm

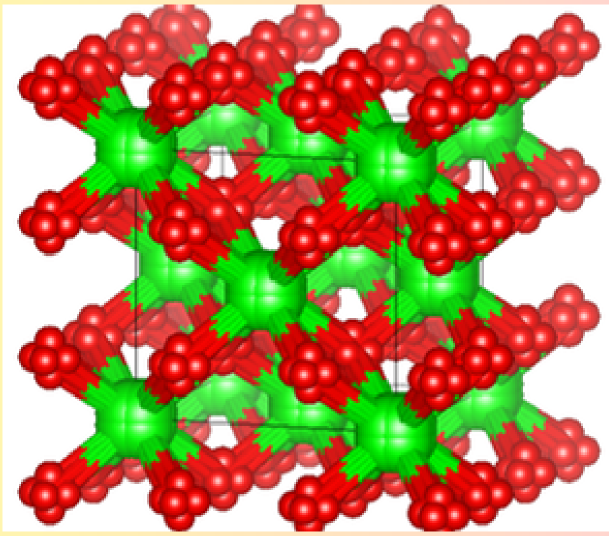
YSZ- matrix

4.4 Property Computation: DFT for Up-scaling

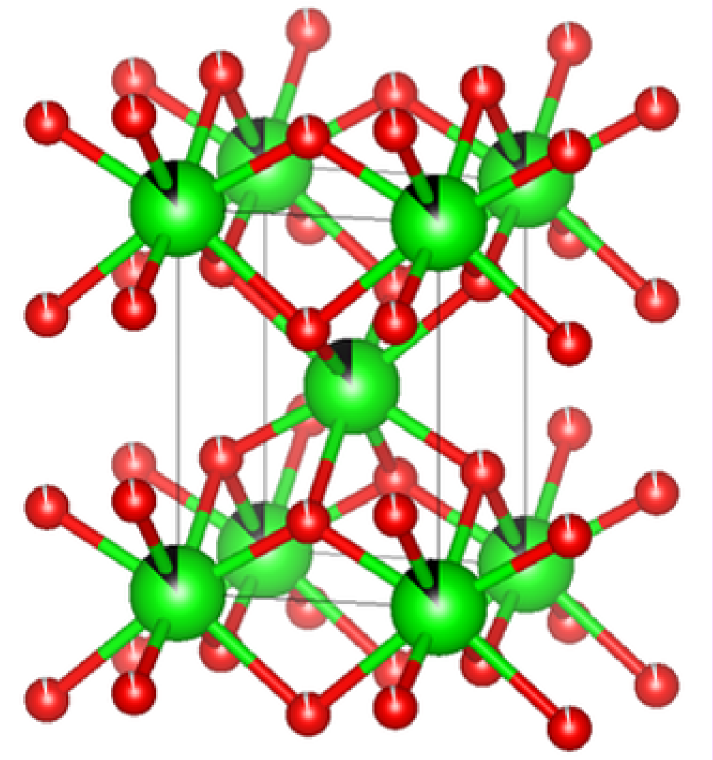
DFT: Temperature-dependent elastic Constants

Ysz

SG 225, F m -3 mc



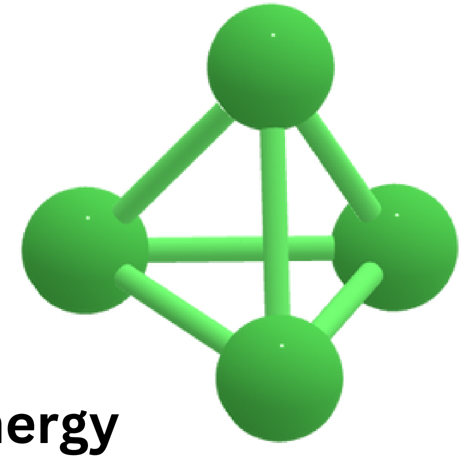
SG 137, P 42/n m c



Temperature-dependent property is yet to be computed

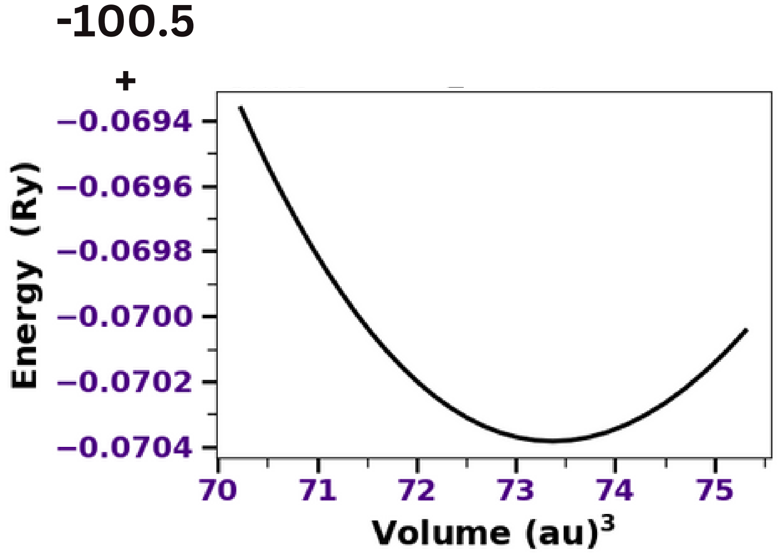
Convergence difficulties due to large atoms and complex crystal structure

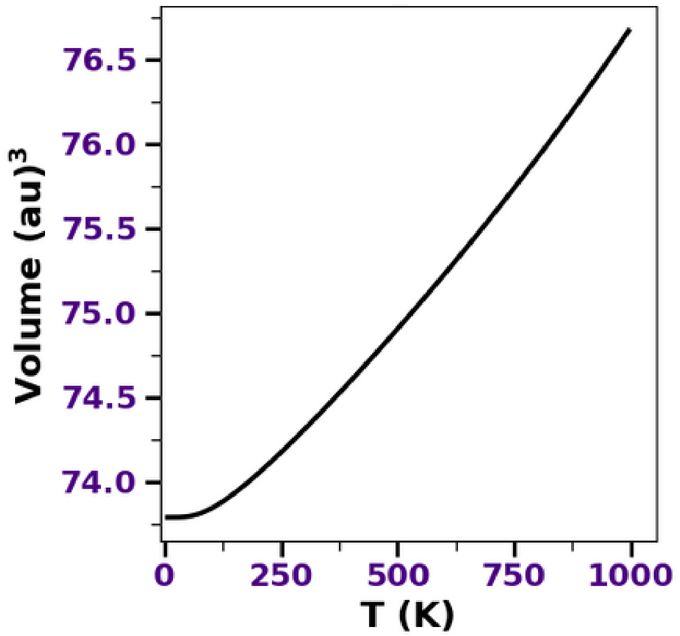
Ni

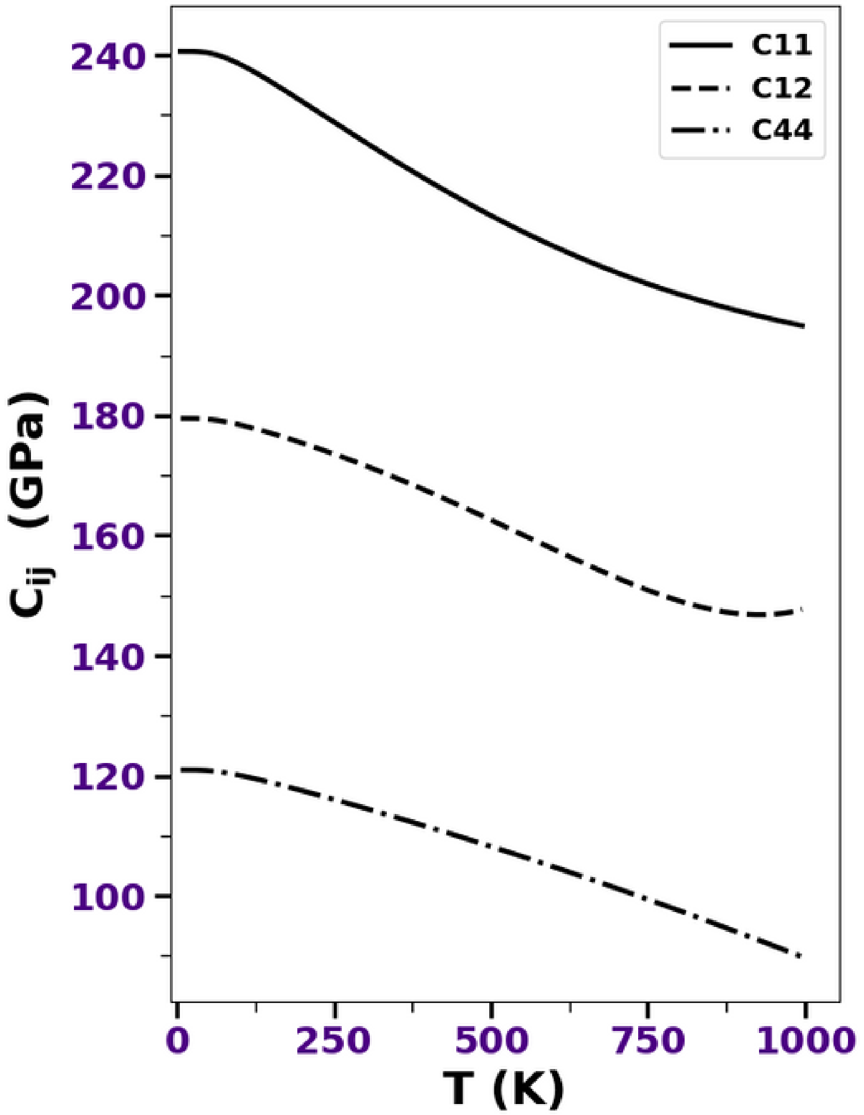


Helmholtz free energy

$$\tilde{C}^{T}_{ijkl} = \frac{1}{\Omega^{T}} \left(\frac{\partial^2 F_{hz}}{\partial \varepsilon_{ij} \partial \varepsilon_{kl}} \right)_{\varepsilon=0}$$







DFT Simulation Setup:

- Nickel lattice constant = 3.48 Å
- Cutoff Energies: ecutwfc=40.0 Ry,
- ecutrho=200.0 Ry.
- Space Group: 225.
- Pseudopotential: Ultrasoft
- K-points: 12x12x12.: 12x12x12.

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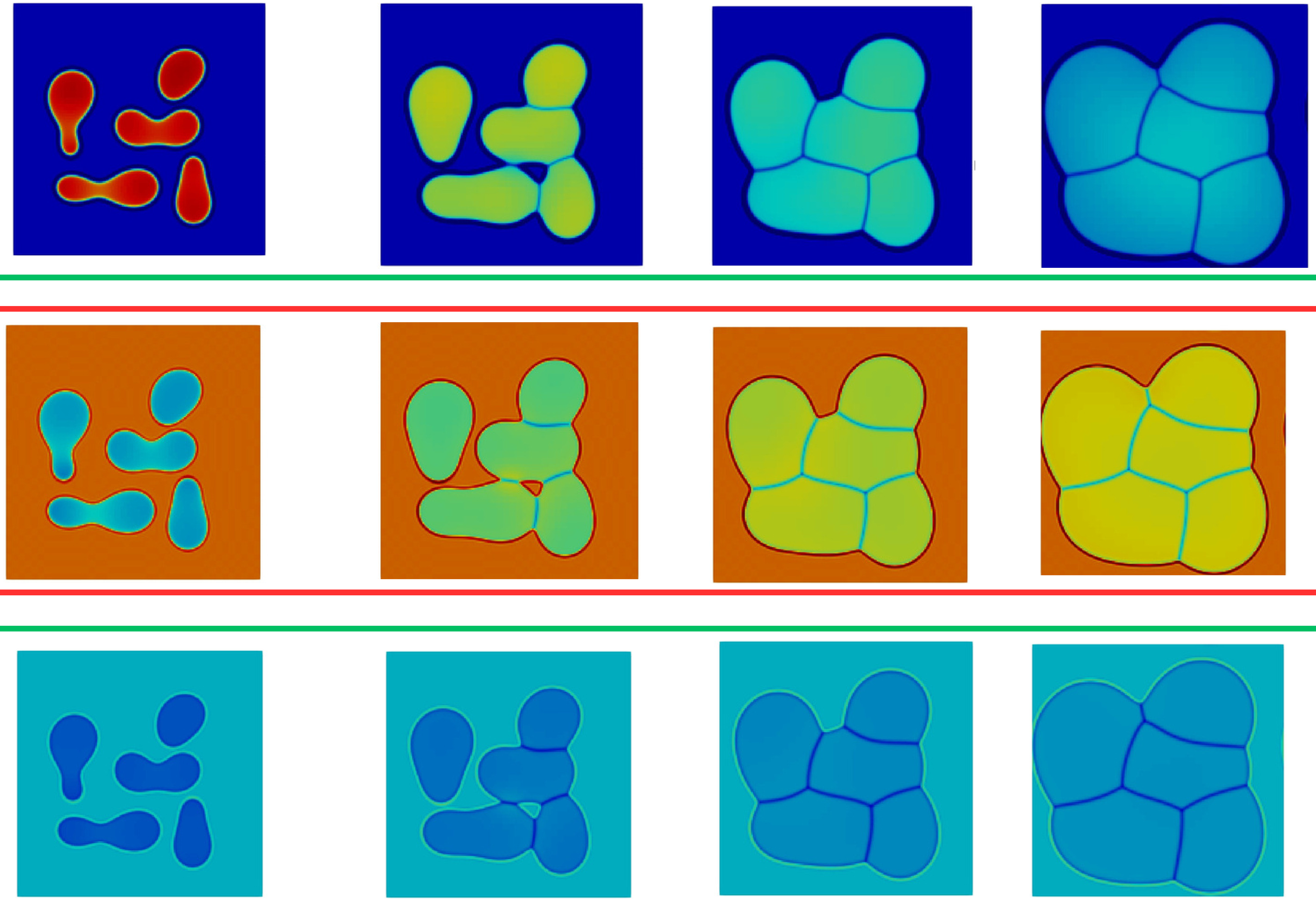
5.1 Phase Field Results: The Composition Plots

46 ms | 181 ms | 349 ms | 605 ms

cNi

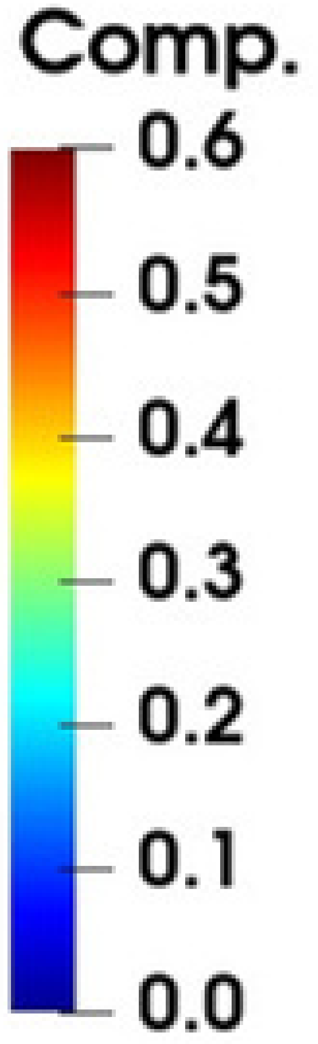
cZr

cY



scale

300 nm

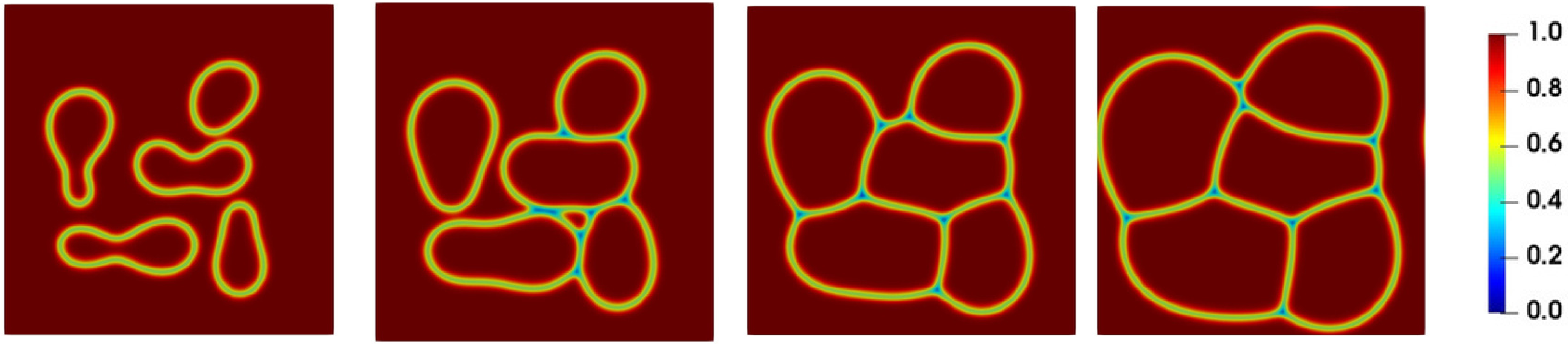


5.2 Phase-field Results: Order Parameters and Grain Growth

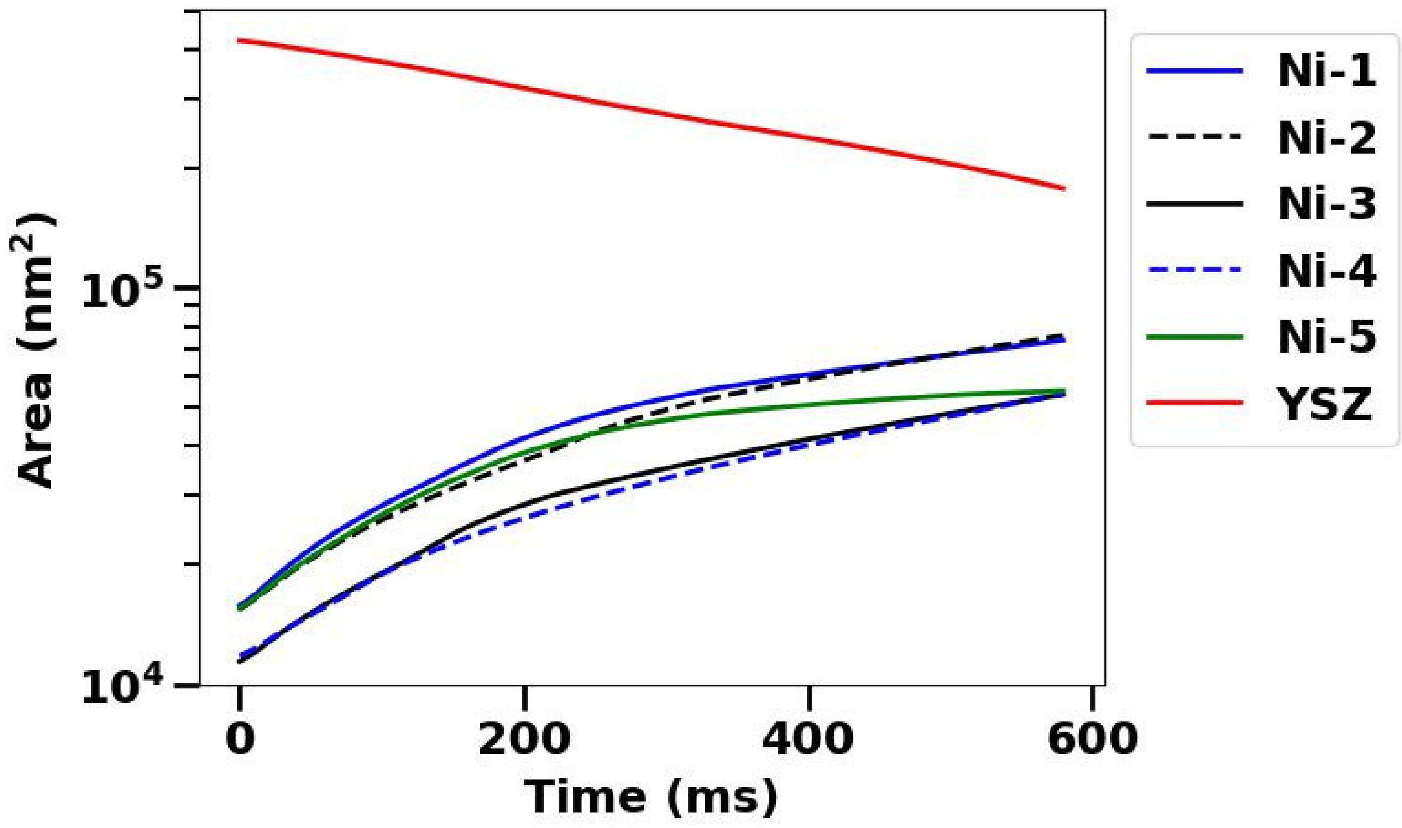
46 ms | 181 ms | 349 ms | 605 ms

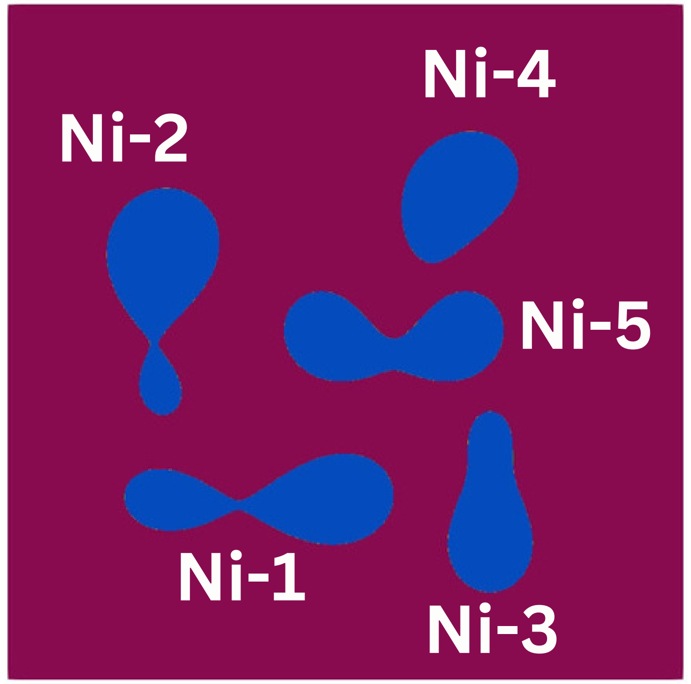
scale

300 nm



$$\sum_{i=1}^{3}(\eta_i)^2$$





6 Future Work

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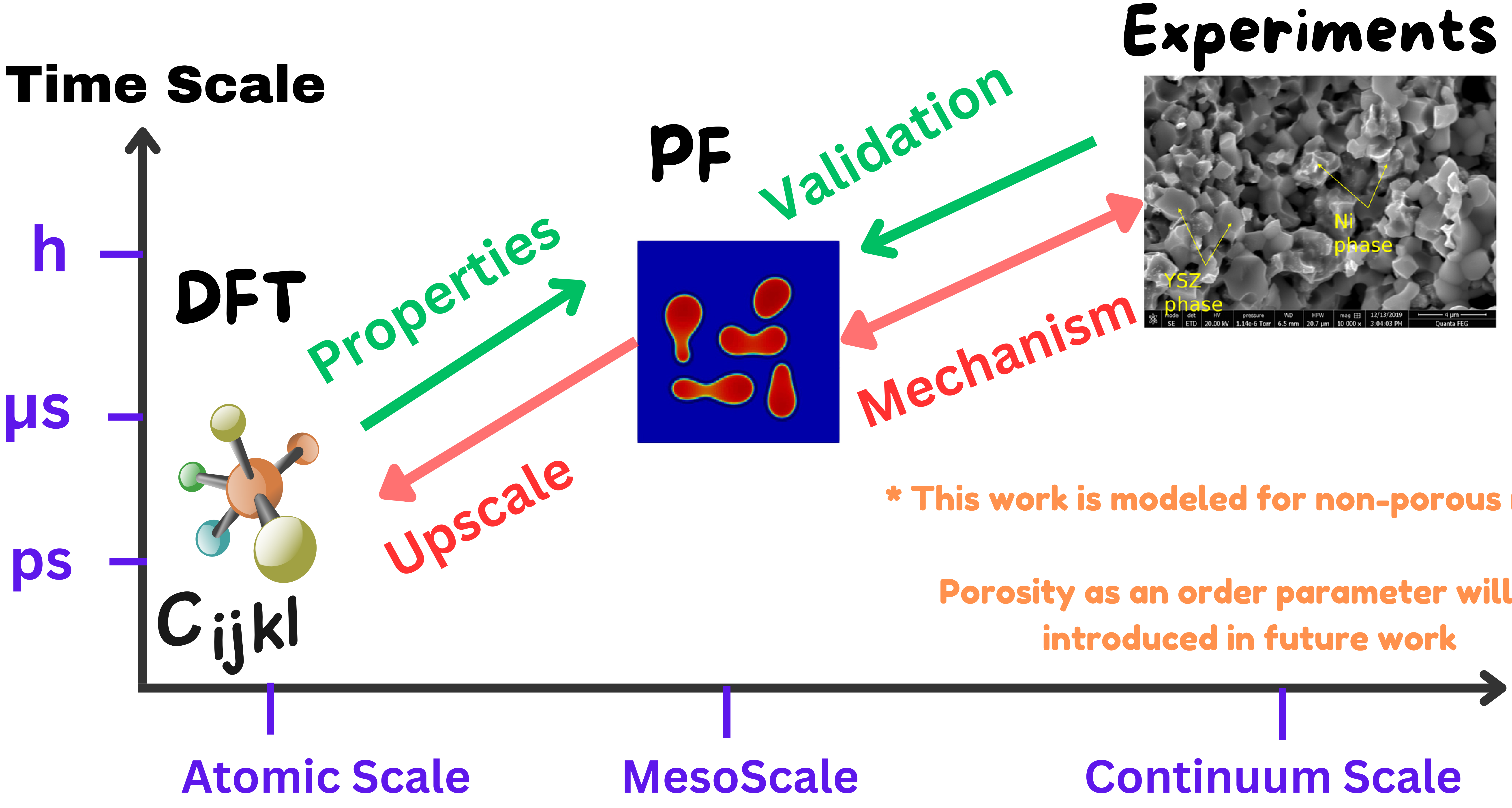

* This work is modeled for non-porous media.

Porosity as an order parameter will be introduced in future work

This work is supported by

National Science Centre Poland

Award Number: UMO-2021/42/E/ST5/00339

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