



REPM 2025

NIMS

TSUKUBA

Thu. July 31
Theory & Simulations
[O14-4] 11:40 – 11:55

Phase-field simulation of liquid-phase sintering coupled with a CALPHAD database of Nd-Fe-B-Cu system

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¹ National Institute for Materials Science



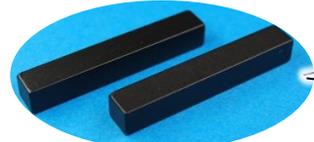
Background

*<https://www.webcg.net/articles/-/38278>

**<https://motor-fan.jp/tech/article/35211>



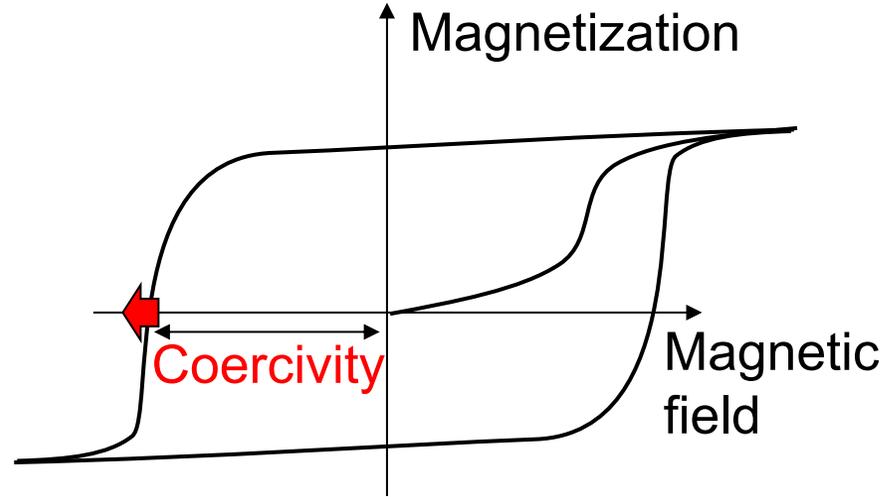
EV·HEV*



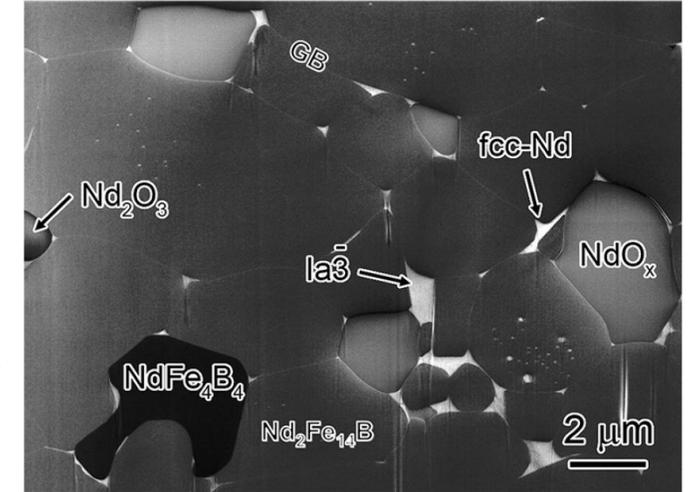
Nd-Fe-B magnets



Motor**



Magnetization Curve



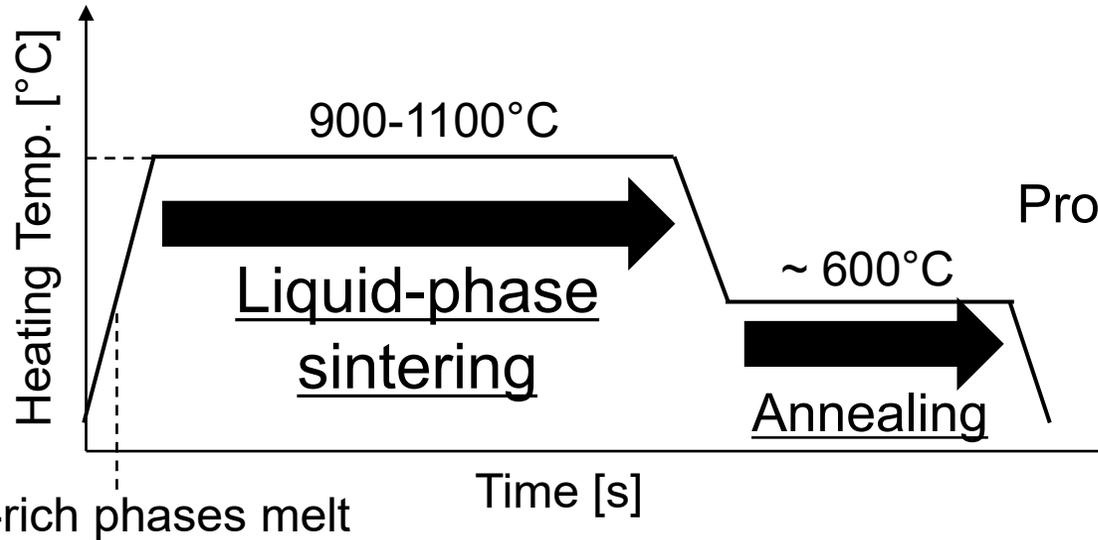
T.T. Sasaki et al., *Acta Mater.* **115** (2016) 269–277.

Microstructure



Nd-Fe-B-...

Packing



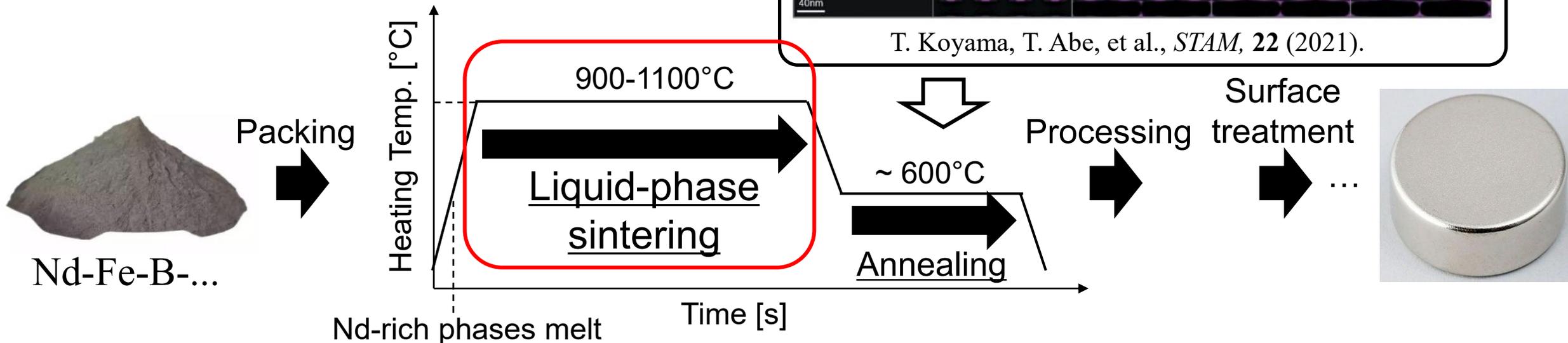
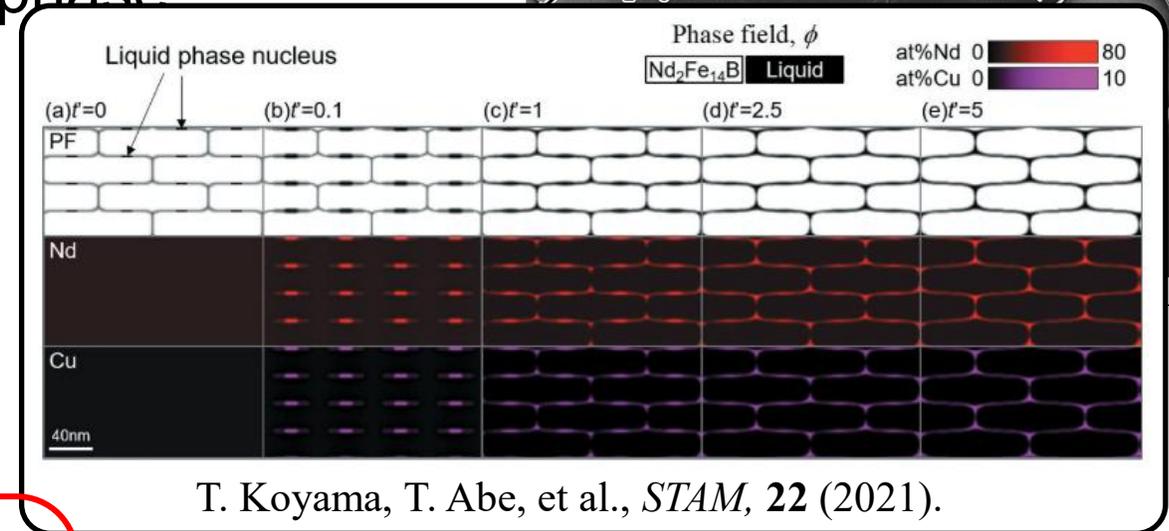
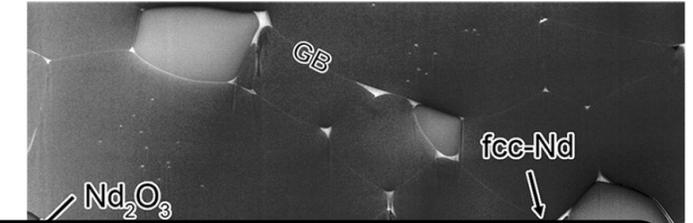
Processing

Surface treatment

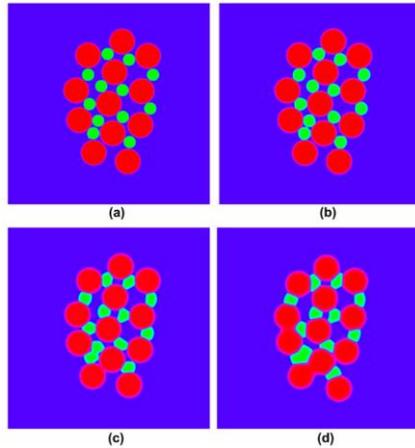


Key factors enhancing the coercivity:

- ✓ High density
- ✓ Small crystal grains of $\text{Nd}_2\text{Fe}_{14}\text{B}$ (T_1) phase
- ✓ High volume fraction of the T_1 phase
- ✓ Thin grain boundary phases uniformly cover the T_1 phases

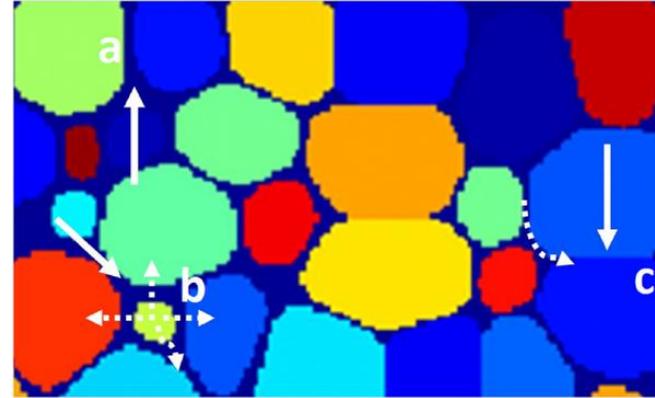


Phase-field Model of Liquid-phase Sintering



Villanueva model

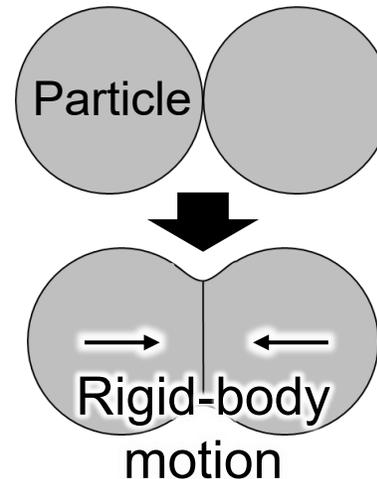
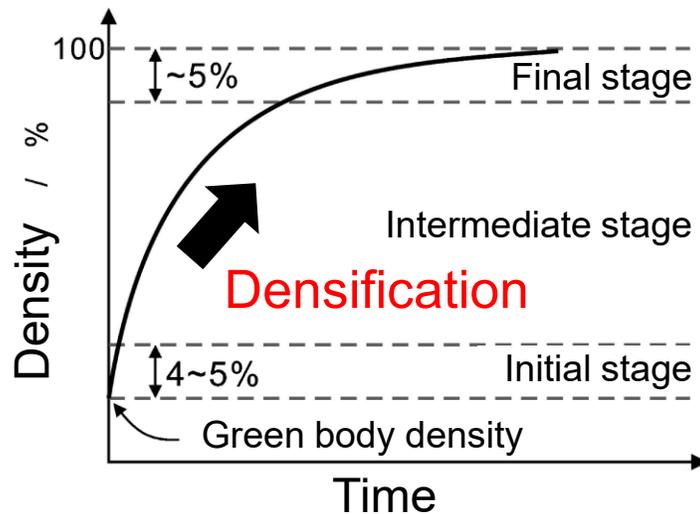
W. Villanueva et al., *Comput. Mater. Sci.* **47** (2009) 512–520.



Ravas model

H. Ravash et al., *J. Eur. Ceram. Soc.* **37** (2017) 2265–2275.

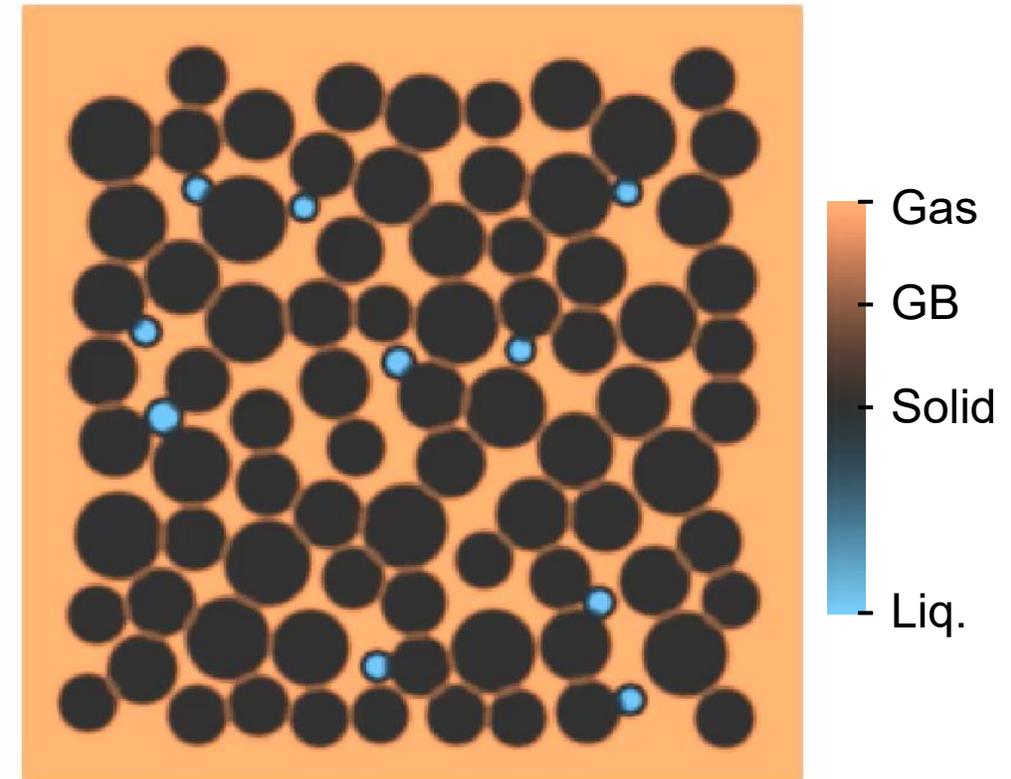
NOT considering rigid-body motion



New phase-field model of liquid-phase sintering

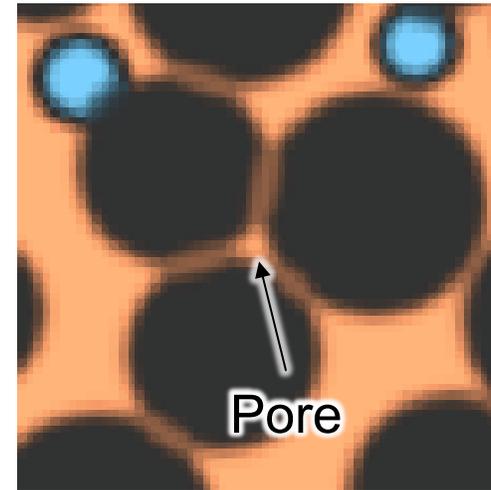
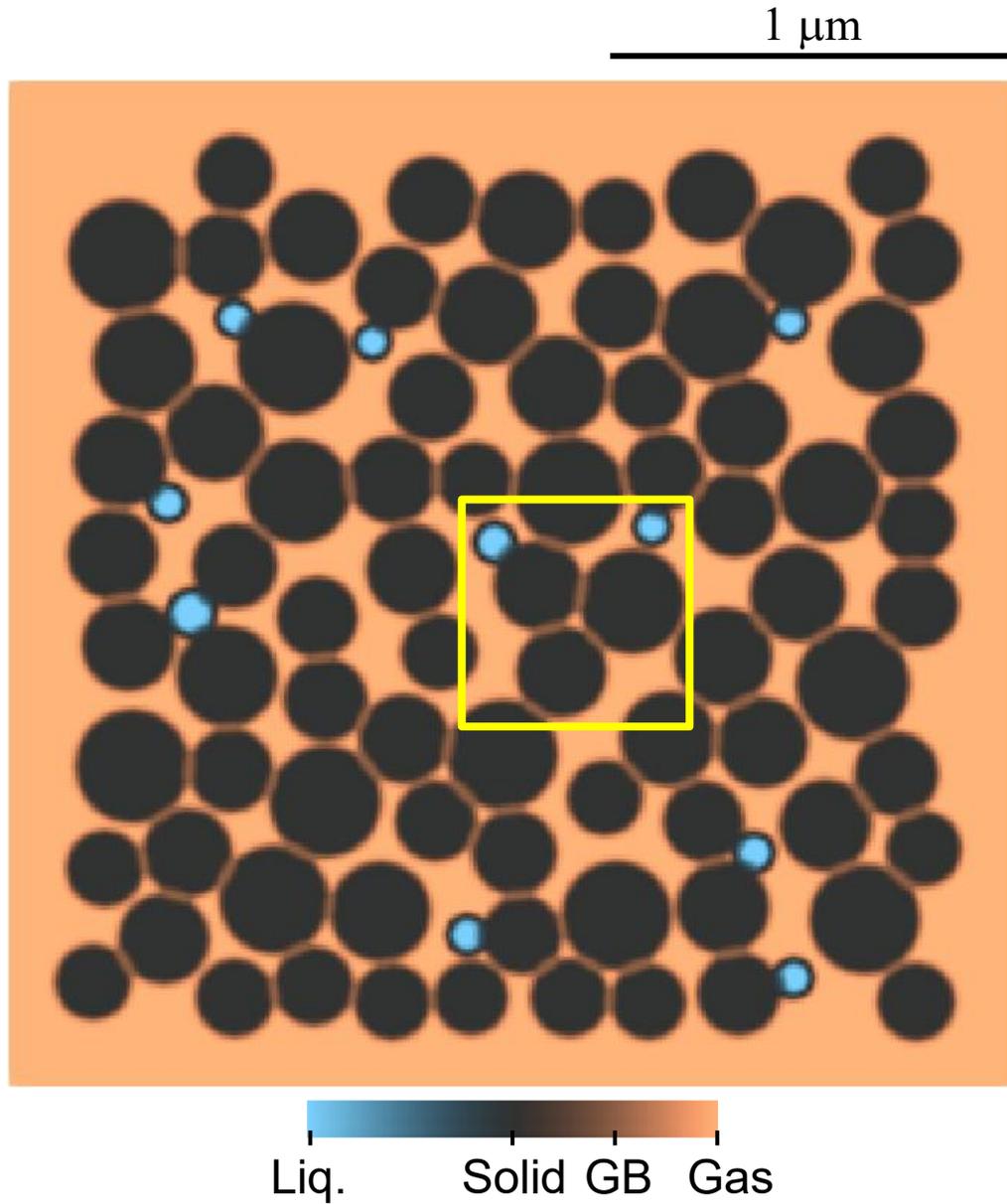
A. Ishii et al., Mater. Today Commun. **40** (2024) 110116.

Time: 0 [-] 1 μm

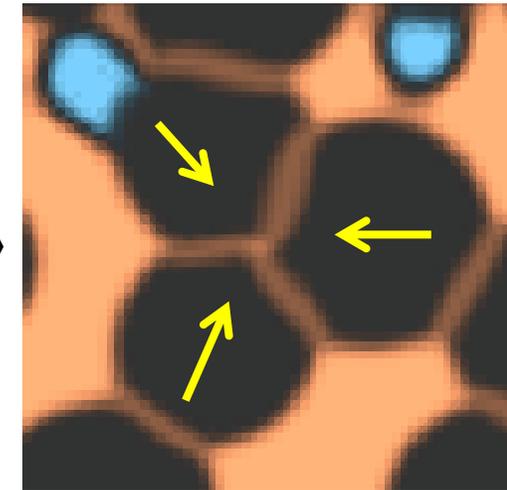


LPS simulation for model validation using hypothetical ternary system.

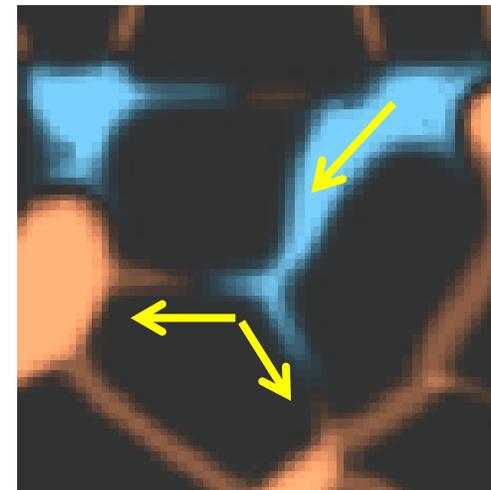
Microstructural Evolution (Hypothetical material)



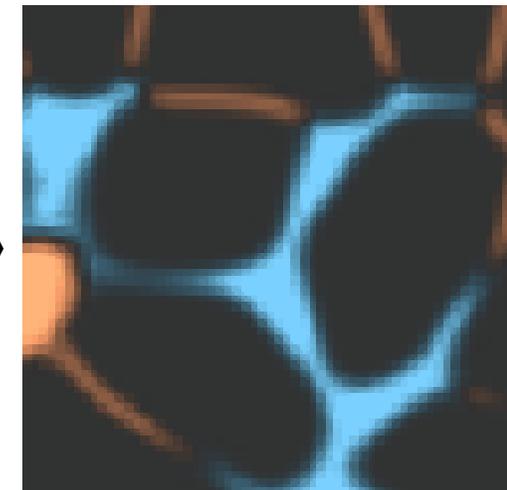
Initial state



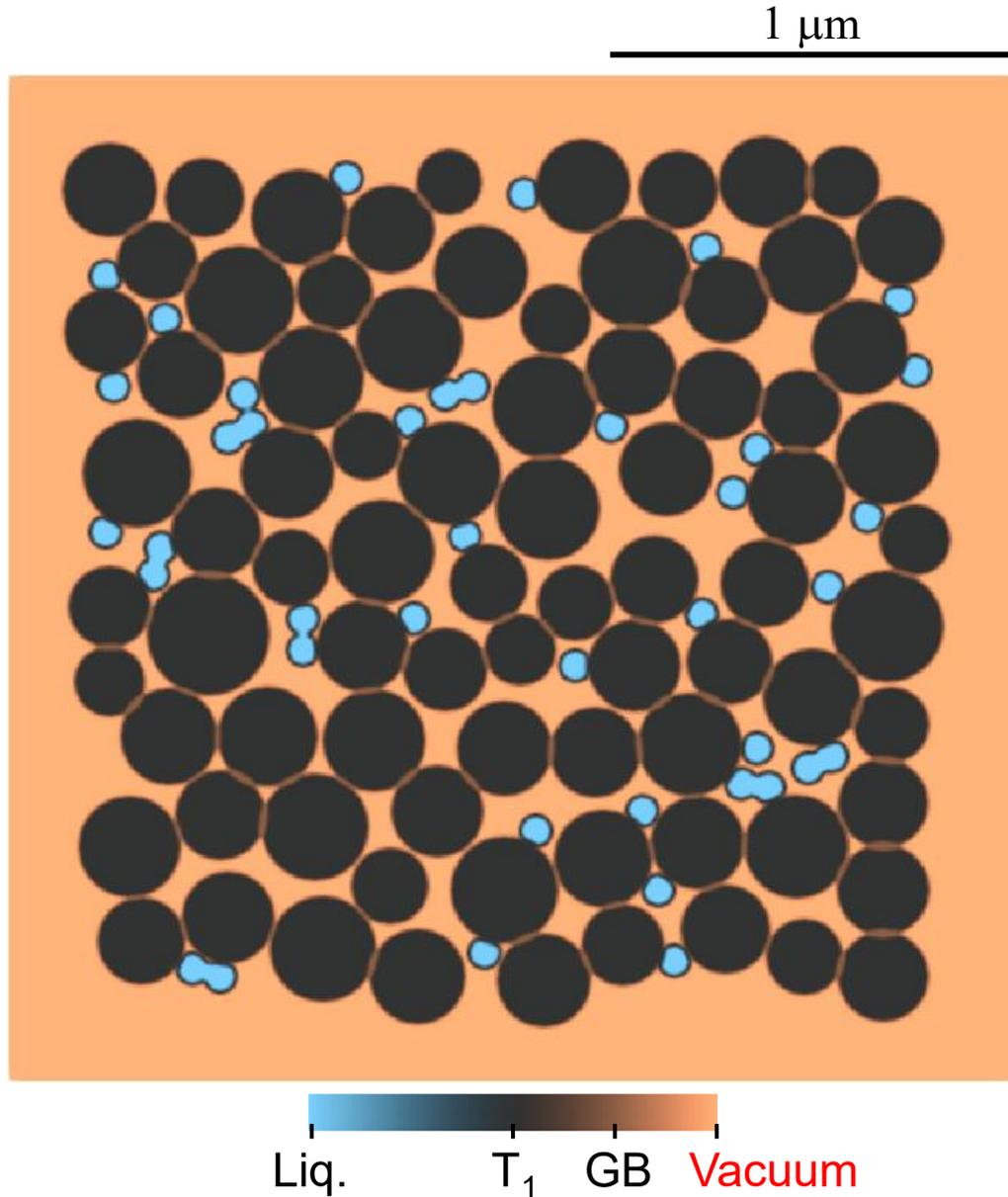
Densification



Penetration



Rearrangement



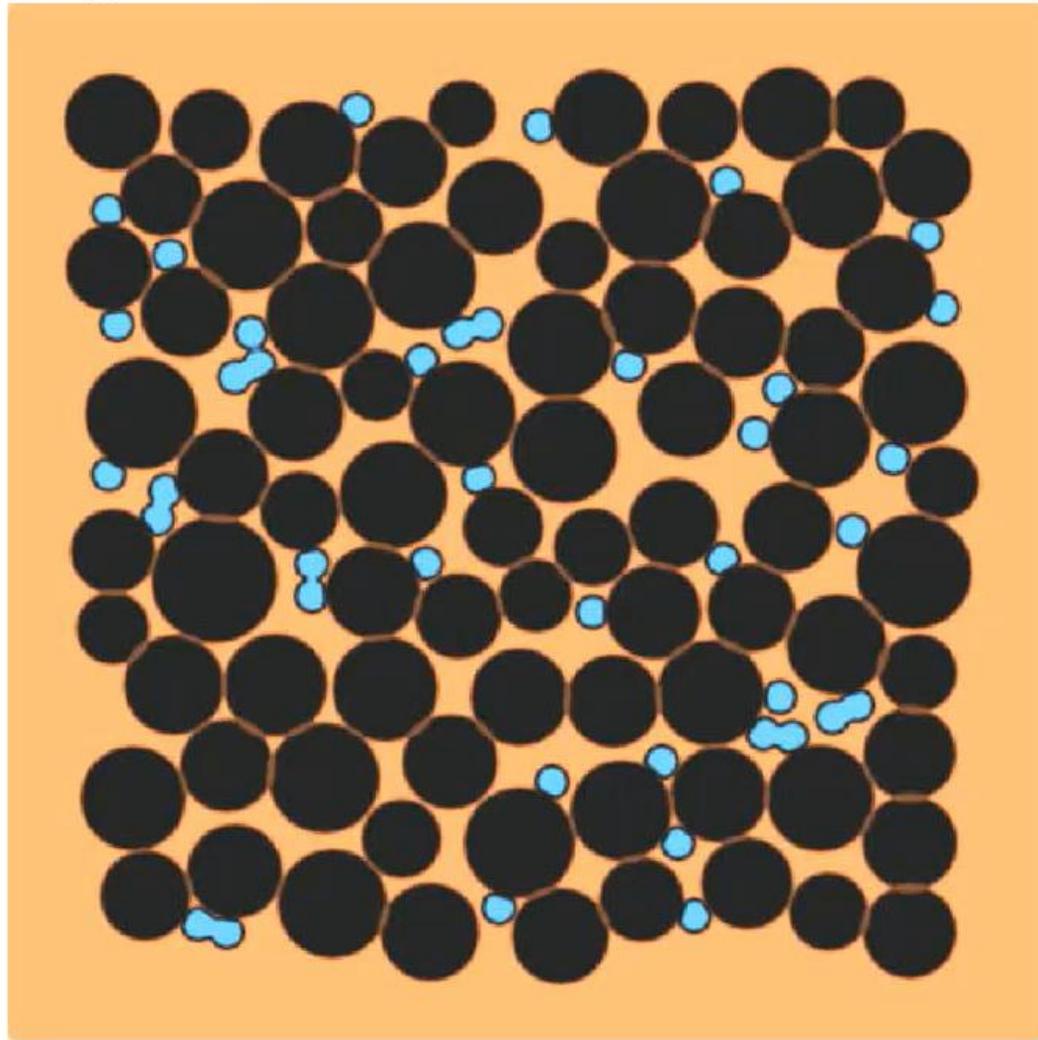
Simulation conditions

- Nd-Fe-B-Cu quaternary system
- Thermodynamic (CALPHAD) database
[T. Abe et al., *STAM* **22** (2021) 557–570.]
- Initial composition: Fe-6.0B-15.0Nd-0.1Cu (at%)
- Temperature: 1000°C
- Diffusivity ratios:
Solid : GB : Liquid = 1 : 10 : 100
- Interfacial energy ratios:
 $\sigma_{\text{solid-pore}} = 1.92 \text{ J/m}^2$
[Y. Ainaï et al., *Appl. Phys. Exp.* **13** (2020) 045502.]
 $\sigma_{\text{solid-solid}} = 0.77 \text{ J/m}^2$, $\sigma_{\text{solid-liquid}} = 0.47 \text{ J/m}^2$
 $\sigma_{\text{liquid-pore}} = 1.54 \text{ J/m}^2$

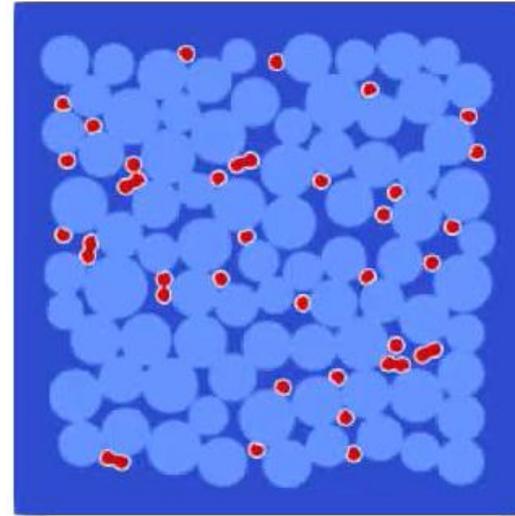
Results (Nd-Fe-B-Cu system)

Steps: 0

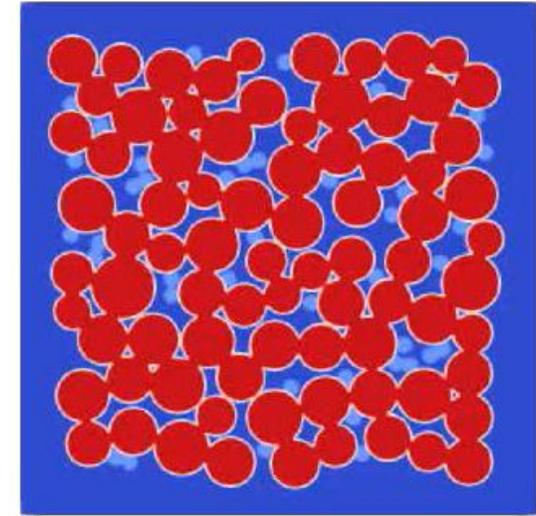
1 μm



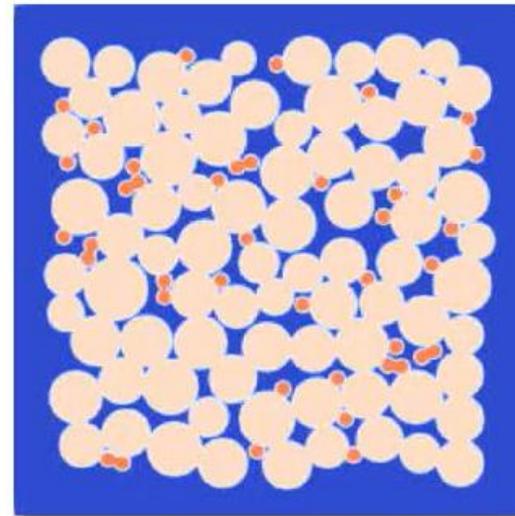
Liq. T₁ GB Vacuum



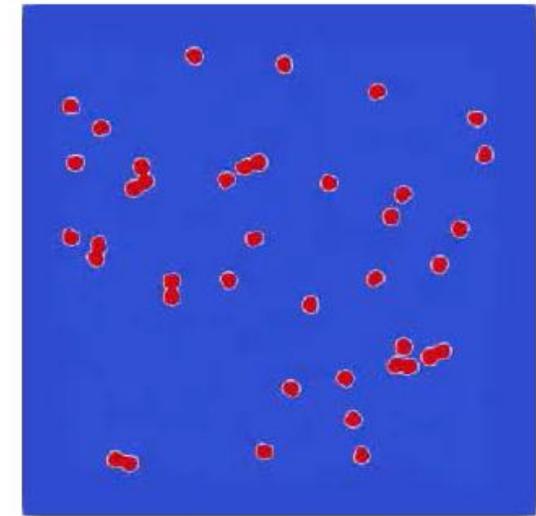
c^{Nd}
0.77
0.00



c^{Fe}
0.82
0.00

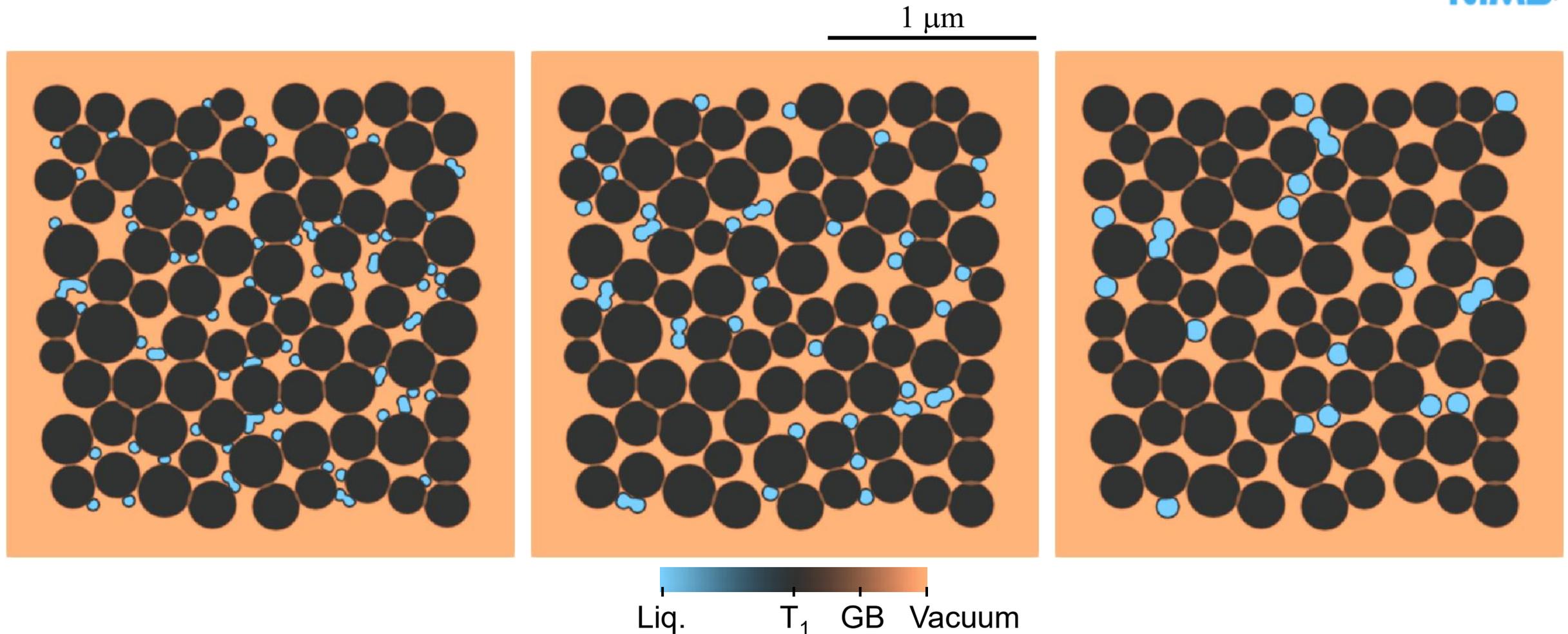


c^{B}
0.10
0.00



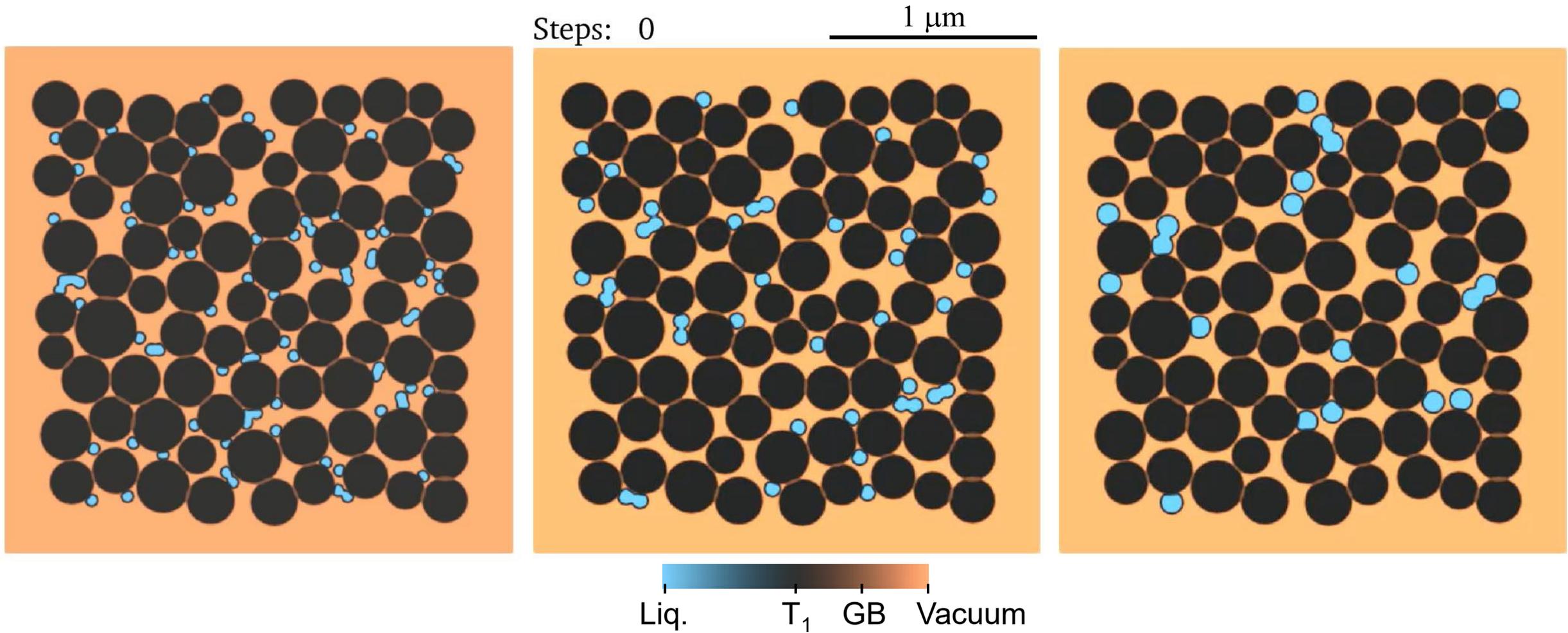
c^{Cu}
0.01
0.00

Initial liquid phase distributions (Nd-Fe-B-Cu system)



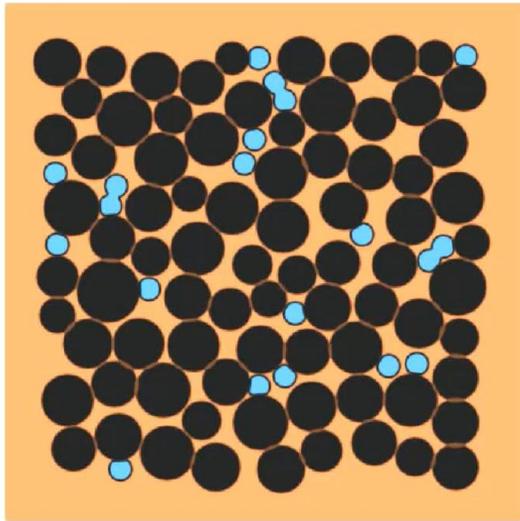
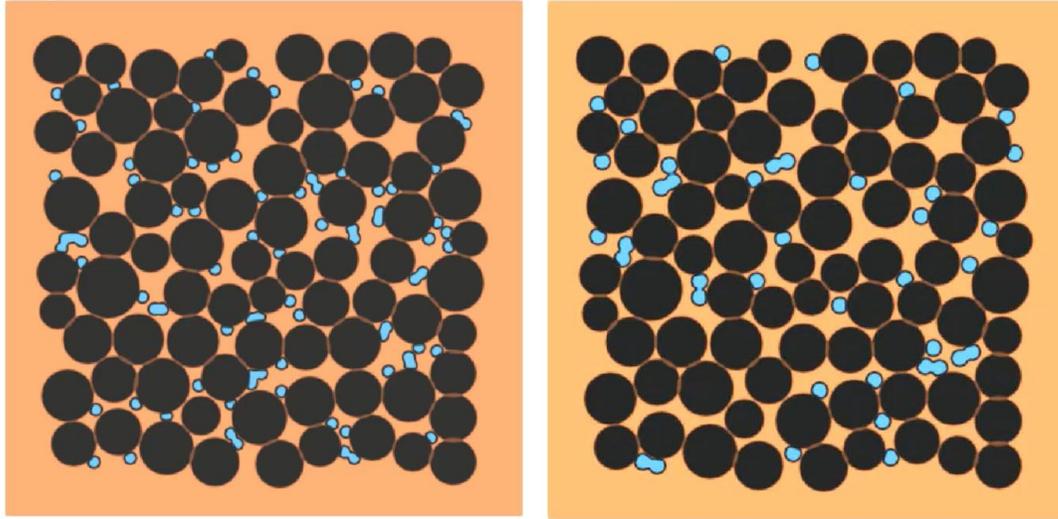
- Only the initial liquid phase distribution was changed.
- T_1 phase distribution, liquid phase volume, and compositions were not changed.

Simulation results (Nd-Fe-B-Cu system)



Comparison (Nd-Fe-B-Cu system)

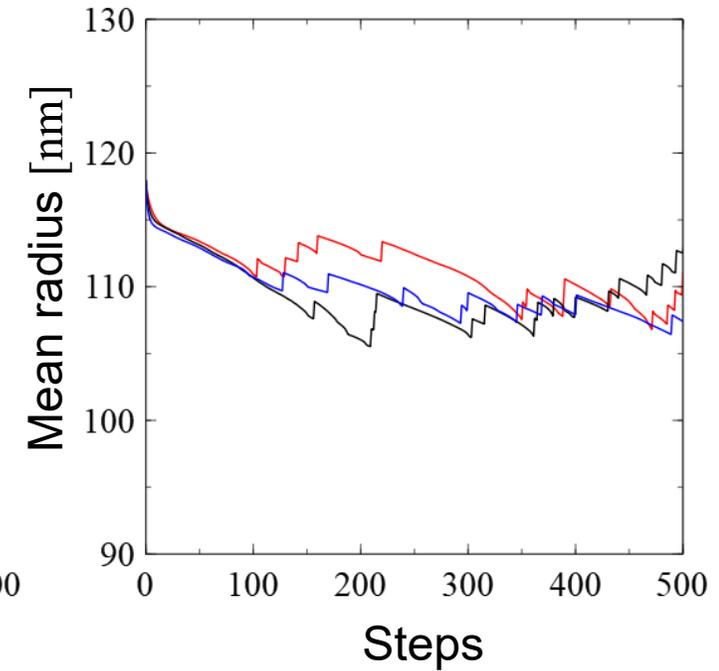
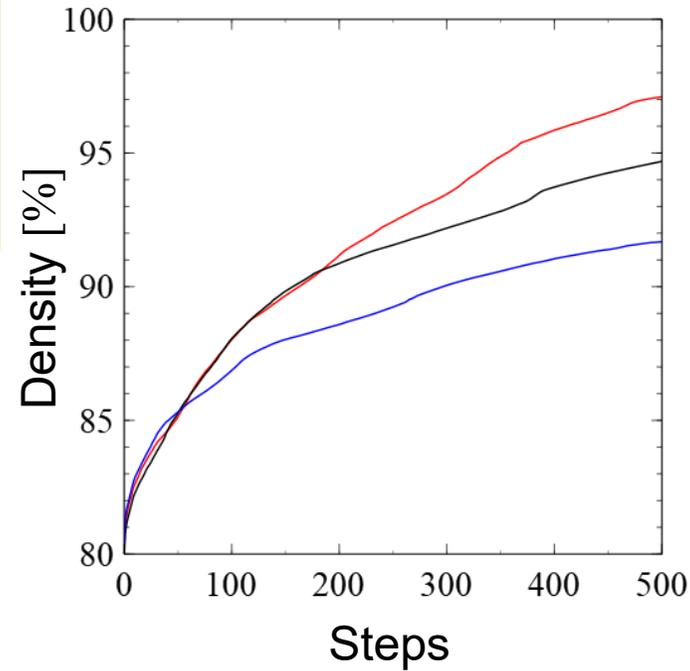
Steps: 0



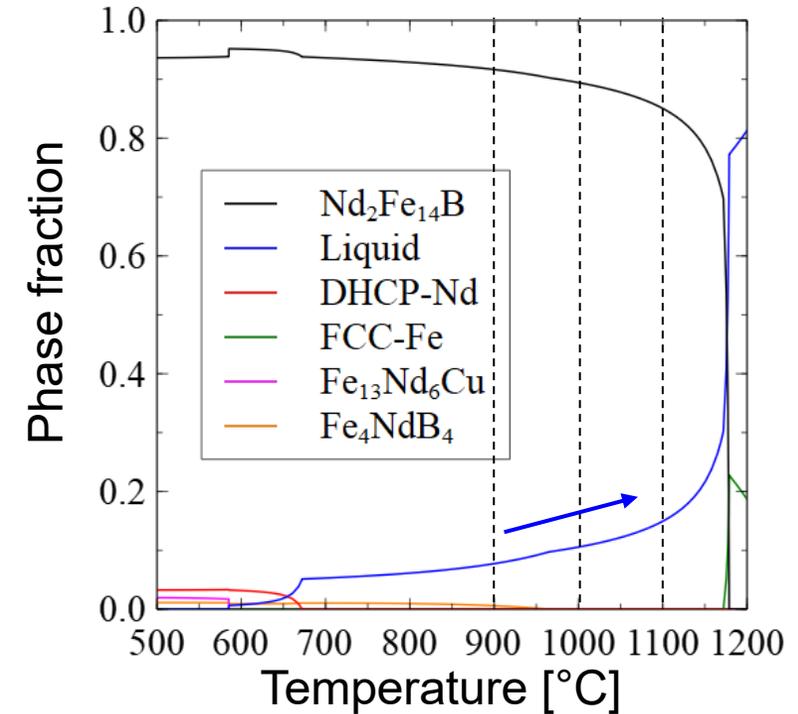
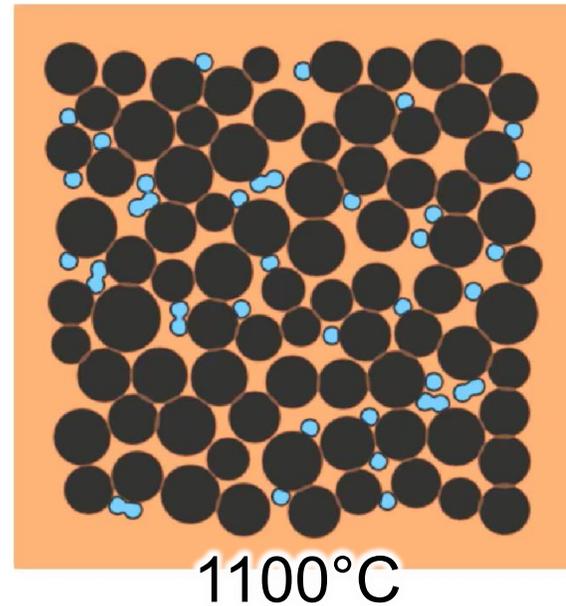
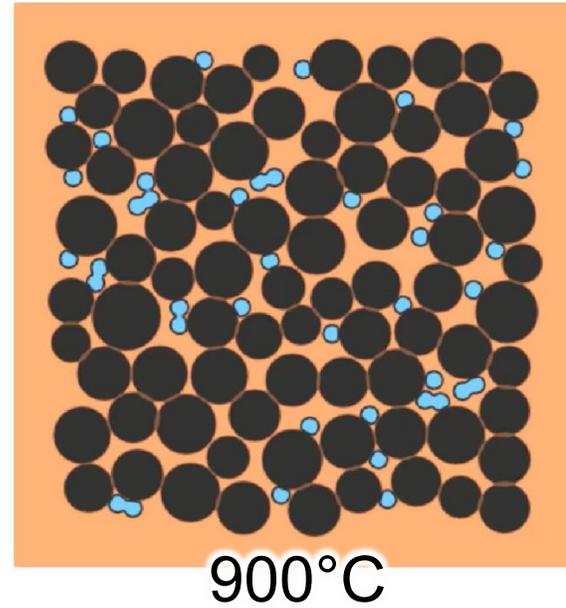
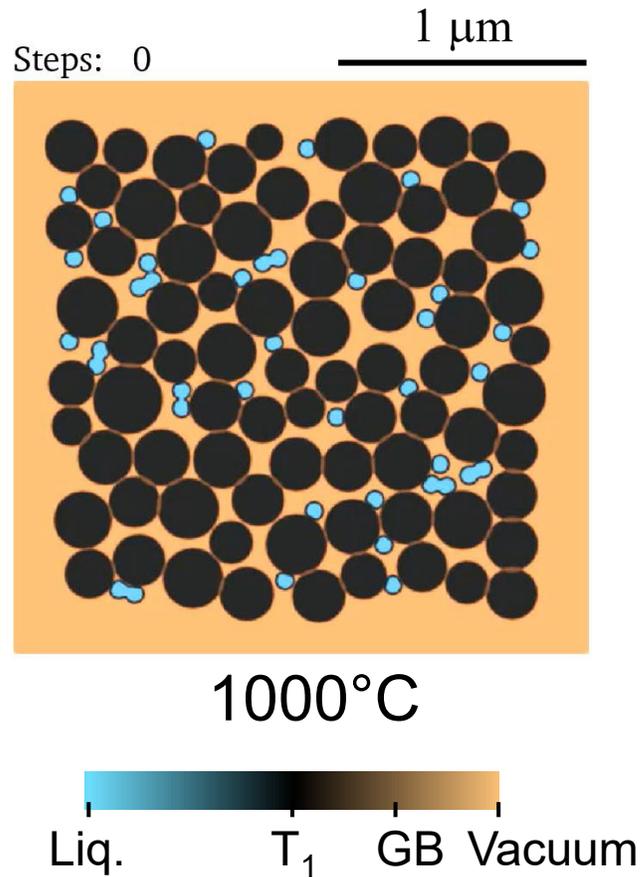
Liq. T_1 GB Vacuum

Radius of the initial liquid phases

— 29.8 nm — 40 nm — 56.1 nm

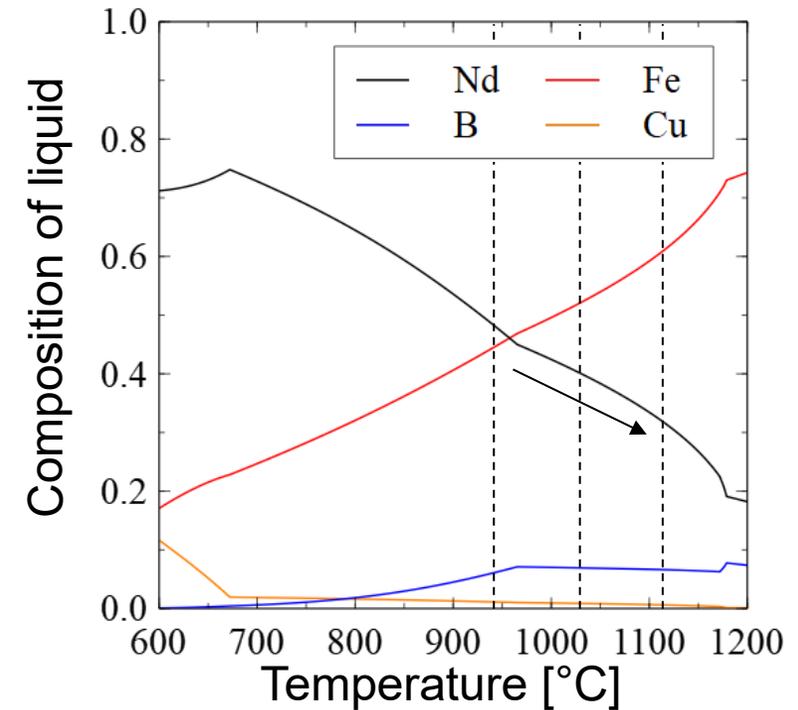
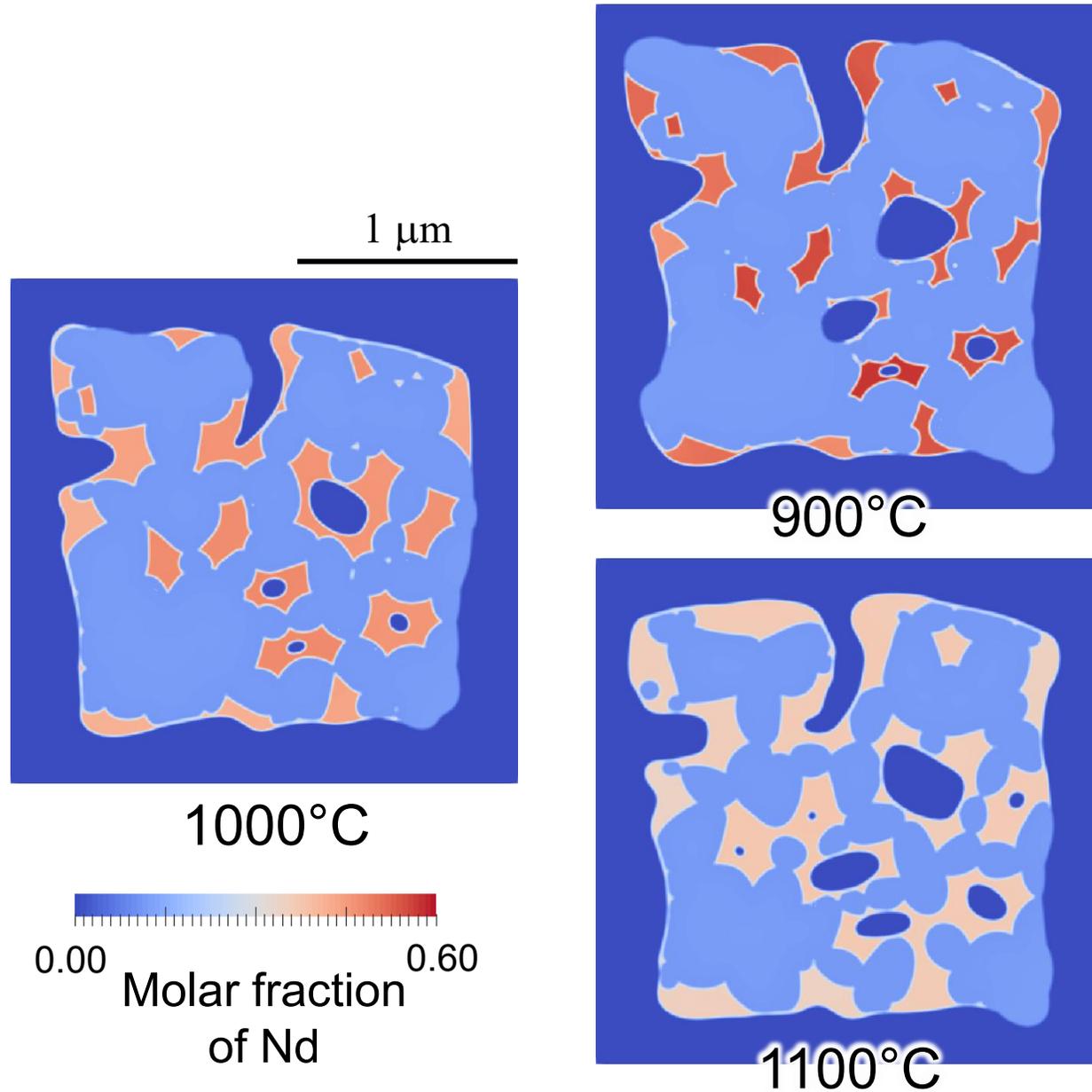


Effect of sintering temperature



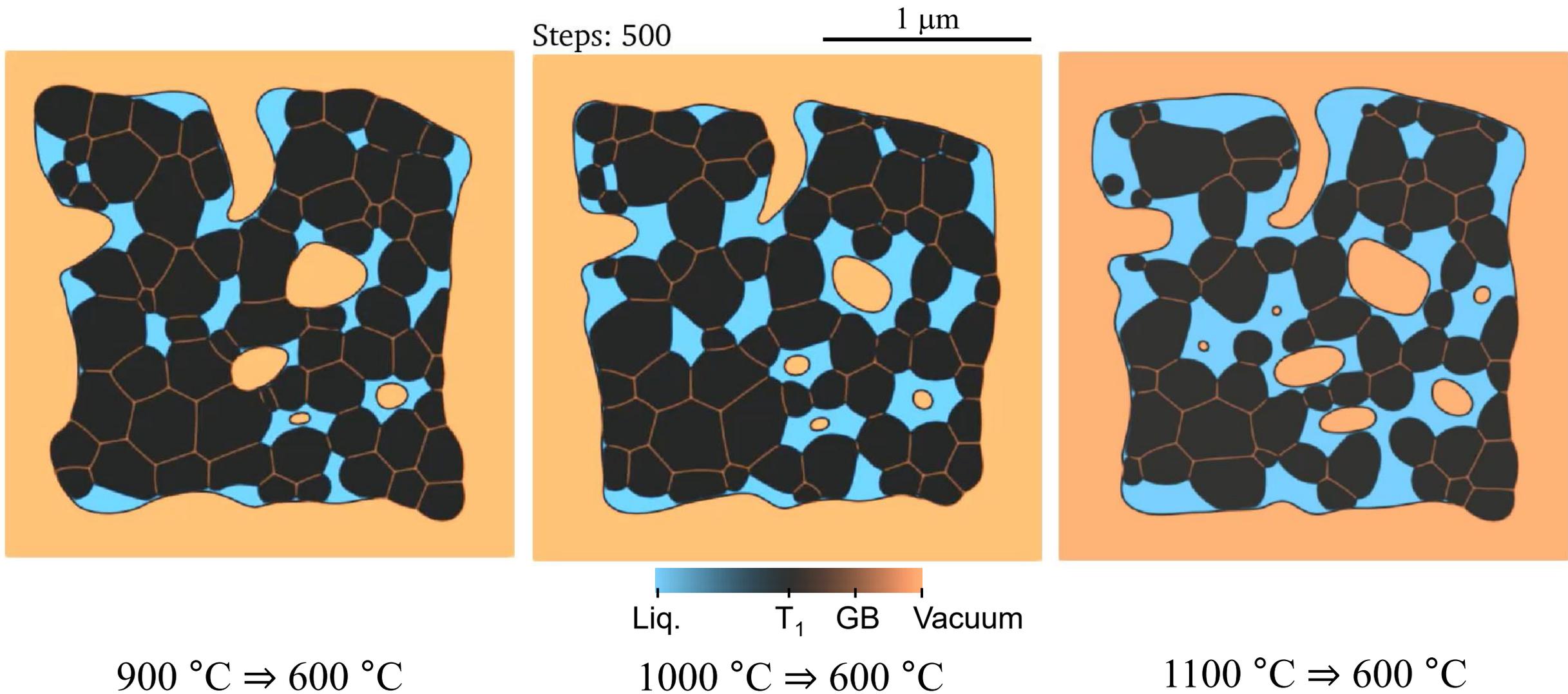
Temperature dependence of phase fractions obtained from CALPHAD calculation

Comparison of Nd concentration distribution



Temperature dependence of liquid composition obtained from CALPHAD calculation

Additional simulation of solidification



- We developed a new framework to simulate microstructural evolution of Nd-Fe-B sintered magnets during liquid-phase sintering.
- A new phase-field model of liquid-phase sintering was developed and coupled with an Nd-Fe-B-Cu thermodynamic database.
- The simulation results demonstrate that our framework has the potential to provide useful insights for the development of the Nd magnets.

Related papers • Model details \Rightarrow A. Ishii et al., *Mater. Today Commun.* **40** (2024), 110116.
• Further Discussions \Rightarrow A. Ishii et al., *J. Alloy. Compd.*, **1025** (2025) 180266.

Acknowledgement

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the Materials Open Platform for Permanent Magnet at NIMS