2024 May 21

NATIONAL SCIENCE CENTRE
POLAND
UMO-2021/42/E/ST5/00339

Temperature dependence of free energies in a phase field model for selective laser melting of tin powder on copper substrate.

Presenter: Upadesh Subedi

U. Subedi[1], N. Moelans[2], T. Tański[1], A. Kunwar[1]
[1]Silesian University of Technology
[2]KU Leuven

Politechnika Śląska

The 5th International Symposium on Phase-Field Modelling in Materials Science

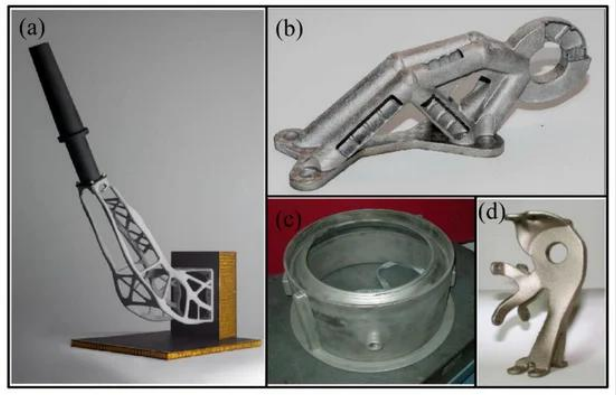
KU LEUVEN

Additive Manufacturing | Selective Laser Melting

Additive Manufacturing | Selective Laser Melting

SLM

Additive Manufacturing | Selective Laser Melting



Areospace parts fabricated via SLM [1]

Dental arc implant support produced via SLM [2]

SLM

Turbine components produced via SLM [3]

Active Heat Shield of an **automotive** produced by SLM [4]

[1] Fereiduni et. al., Aerospace, MPDI (2020), https://doi.org/10.3390/aerospace7060077
[2] Leon, et. al., European Journal of Prosthodentics and restorative dentistry (2017), https://doi.org/10.1922/EJPRD_RevillaLeon05
[3] Guo, et. al., Frontiers of Mechanical Engineering, (2013), https://doi.org/10.1007/s11465-013-0248-8
[4] Nikon SLM Solutions, SLM 280 Twin, AlSi10Mg, https://www.slm-solutions.com/industries/automotive

Existing Strategies for SLM modeling with PFM

SLM: Selective Laser Melting
PFM: Phase Field Modeling

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Entropy Functional (Yang et. al., 2019)

- Entropy functional
- Legendre transformation

$$S(e,\rho,\{\eta_i\}) = \int_{\Omega}\left[s(e,\rho,\{\eta_i\}) - \frac{1}{2}k_\rho|\nabla\rho|^2 - \frac{1}{2}k_\eta\sum_i|\nabla\eta_i|^2\right]d\Omega \quad [1]$$

$$F(T,\rho,\{\eta_i\}) = \inf_{\epsilon}\left[\epsilon(T,\rho,\{\eta_i\}) - TS(e,\rho,\{\eta_i\})\right] \quad [1]$$

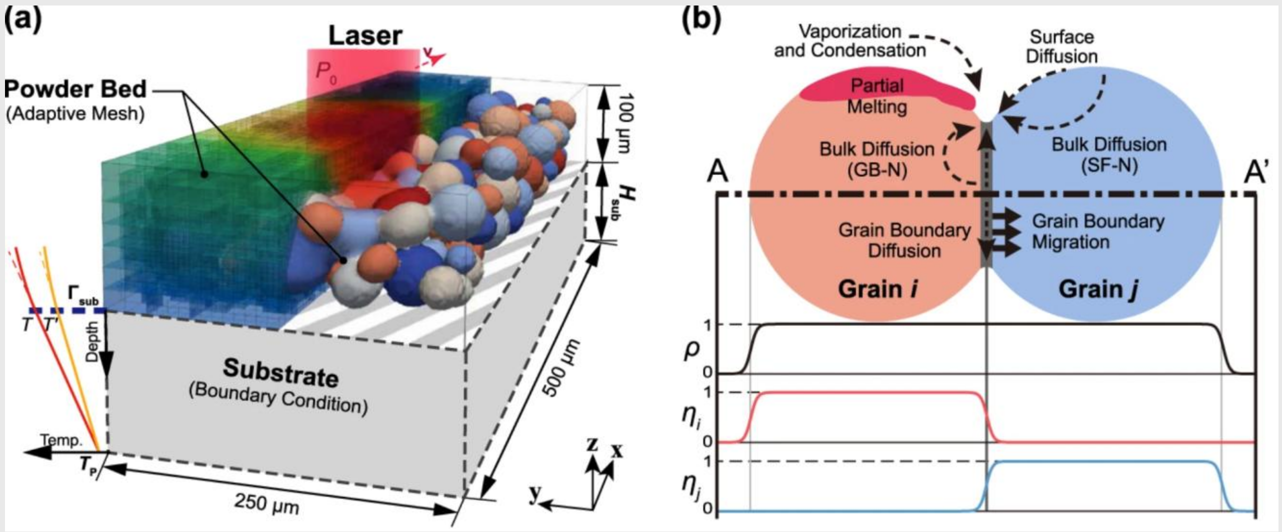

Fig. **(a)** Schematics of simulation domain.
(b) Order Parameter profile across A-A' section [1]

[1] Yang et. al., npj Computational Materials, (2019)5:81, https://doi.org/10.1038/s41524-019-0219-7

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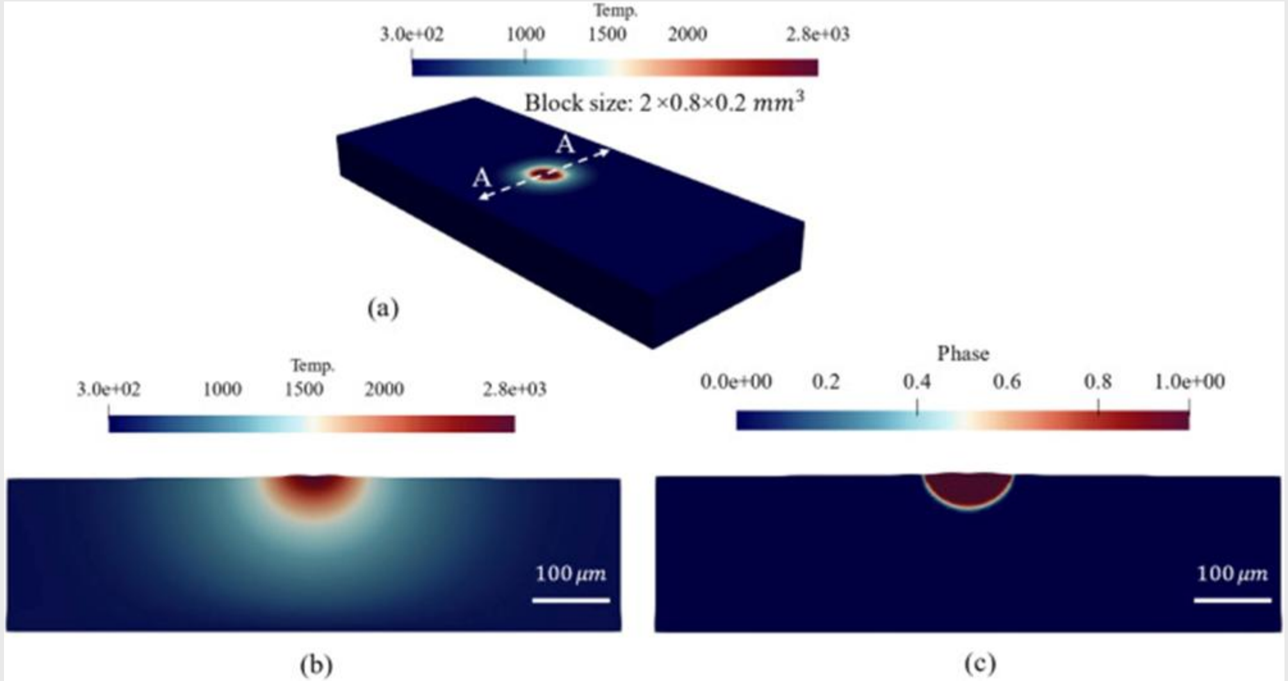

Fig. **(a)** Temperature evolution at center of trace.
(b,c) Temperature and Phase field variable along A-A [2]

Gibbs Energy Functional

- Minimization of Free energy functional
- Free energies extracted from CALPHAD database
- Free energies → Free energy densities

$$F(\phi) = \phi^2(1-\phi)^2 \quad \text{(Darabi et. al., 2023)}$$
$$p(\phi) = \phi^3(6\phi^2 - 15\phi + 10) \quad [2]$$

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[2] Darabi et. al., Applied Mathematical Modelling 122, (2023), https://doi.org/10.1016/j.apm.2023.06.021

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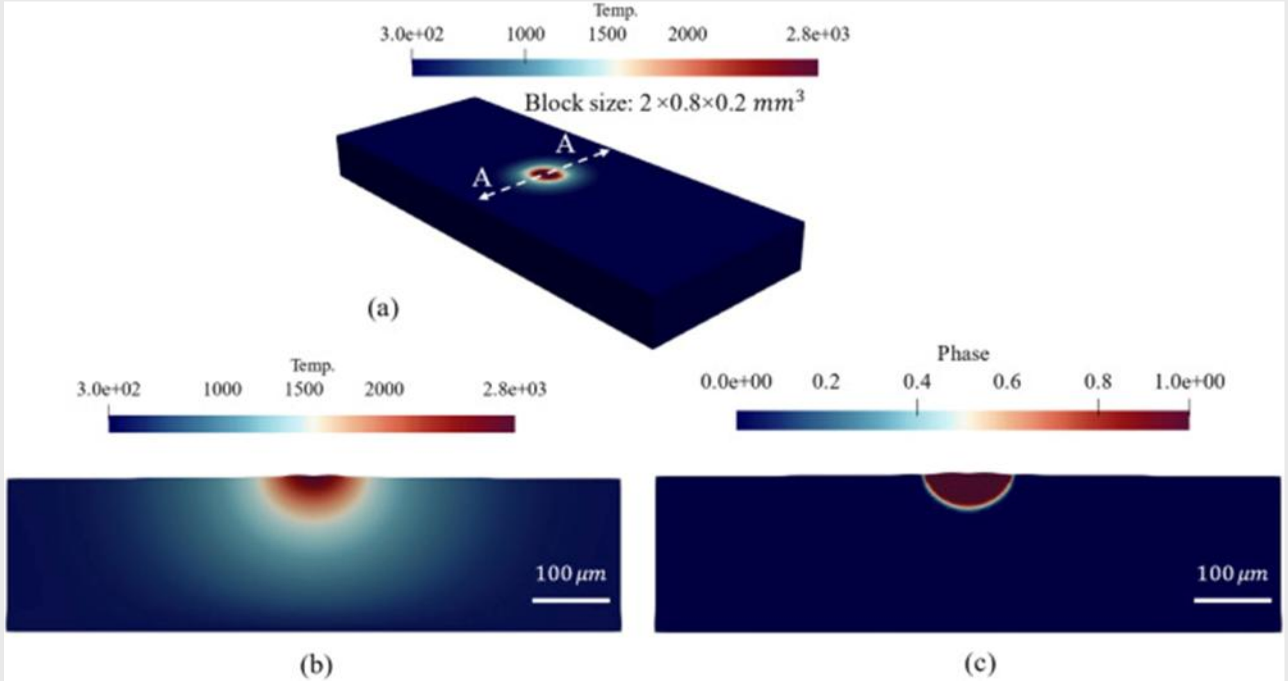

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- **Ease of Data Extraction**
- **Integrational ease with modular software**

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Multi-Physics Phase Field Formulation

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i → ith Phase
$\langle T \rangle$ → Temperature Dependence

Phase Field

Conserved; Bulk Free Energy density; Phase Mobility; Flow Velocity

$$\frac{\partial c_i}{\partial t} = \nabla . M_i\langle T\rangle \; \nabla\left(\frac{\partial f_b\langle T\rangle}{\partial c^i}\right) - \vec{u}.\nabla c_i$$

Non-Conserved; Interfacial Mobility

$$\frac{\partial \eta_i}{\partial t} = -L_i \left(\frac{\partial f_b\langle T\rangle}{\partial \eta_i} + \frac{\partial f_0}{\partial \eta_i} - \nabla . \frac{\partial f_{grad}}{\partial \nabla \eta_i}\right)$$

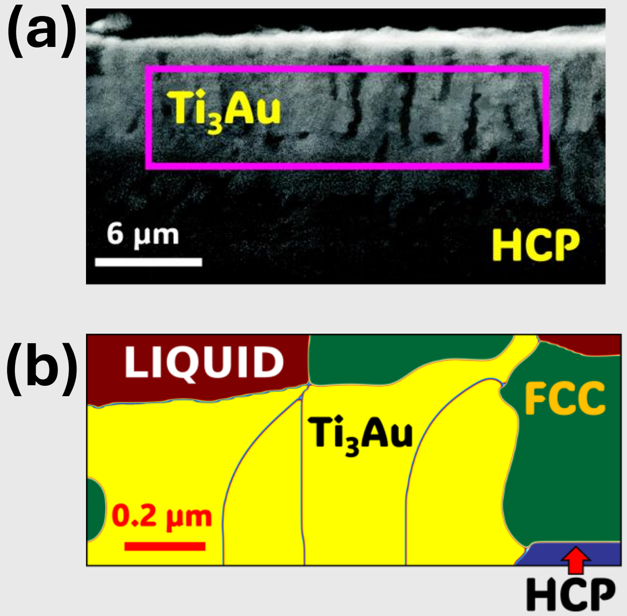

Fig. Microstructure Evolution of laser treated Au-Ti system in **(a)** Experiment [1] **(b)** Simulation

[1] Bialas et. al., JESTECH, 42, (2023), https://doi.org/10.1016/j.jestch.2023.101413

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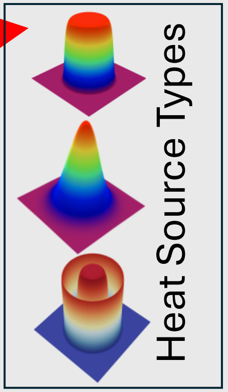
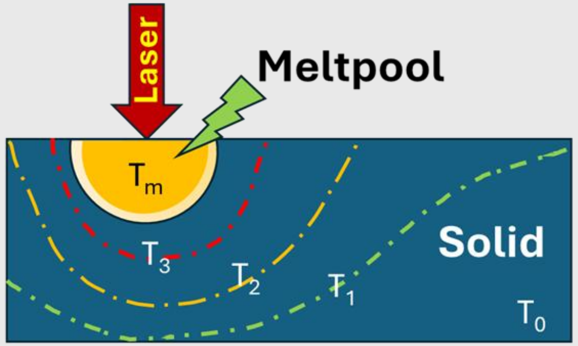
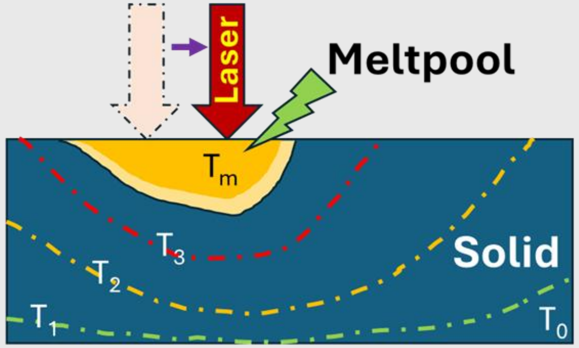
Energy

Density; Specific Heat; Thermal Conductivity; External Heat

$$\rho^i\langle T\rangle \, C_p^i\langle T\rangle \left(\frac{\partial T}{\partial t} + \vec{u} \, . \nabla T\right) = k_{th}^i\langle T\rangle \nabla^2 T + \boldsymbol{Q_{laser}}$$







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Conserved; Phase Mobility ($M_i\langle T\rangle$); Bulk Free Energy density ($f_b\langle T\rangle$); Flow Velocity ($\vec{u}$)

$$\frac{\partial \eta_i}{\partial t} = -L_i \left(\frac{\partial f_b\langle T\rangle}{\partial \eta_i} + \frac{\partial f_0}{\partial \eta_i} - \nabla . \frac{\partial f_{grad}}{\partial \nabla \eta_i}\right)$$

Non-Conserved; Interfacial Mobility (L_i)

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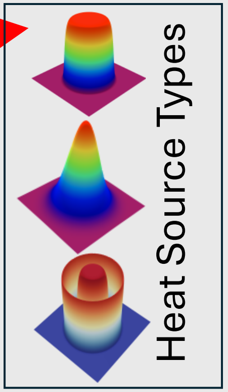

Fluid Flow

$$\nabla . \vec{u} = 0$$

Continuity Eqⁿ

$$\rho^{LIQ}\langle T\rangle \frac{\partial u}{\partial t} + \rho^{LIQ}\langle T\rangle(\vec{u}.\nabla)\vec{u} = -\nabla p + \mu^{LIQ}\langle T\rangle \nabla^2\vec{u} + F_{bou}$$

Pressure (p); Viscosity ($\mu^{LIQ}\langle T\rangle$); Boussinesq Approx. ($F_{bou}$)

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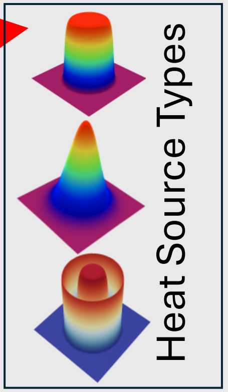

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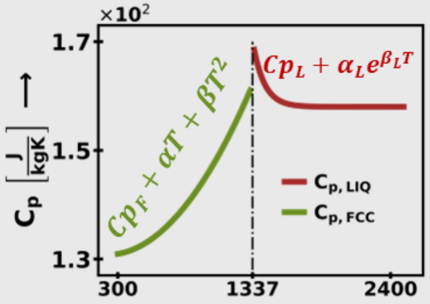
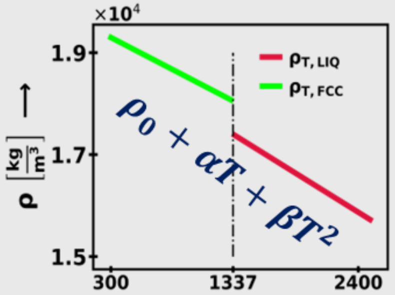
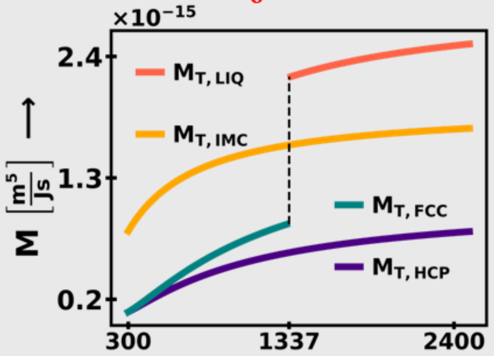




$$M = M_0 + e^{-Q_0/RT}$$



T-Dependent Mat. Prop. of Phases in Au-Ti System [1]

[1] Bialas et. al., JESTECH, 42, (2023), https://doi.org/10.1016/j.jestech.2023.101413

Simulation Setup

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MOOSE

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Multi-Physics Modules:

Simulation Setup

Multi-Physics Modules:

- **Phase Field**
- **Navier Stokes**
- **Heat Transfer**

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Simulation Setup

MOOSE

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Multi-Core Parallel Computation

Use of PETSc

Adaptive time

Auto-Scaling of variables

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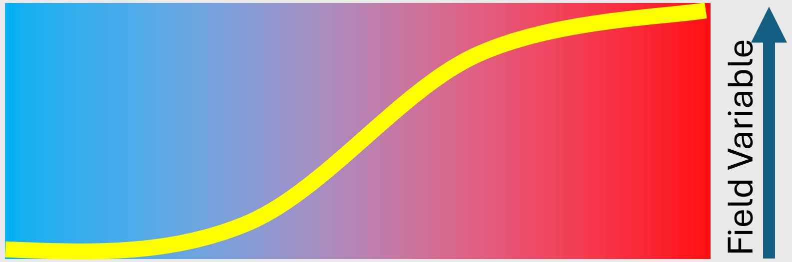

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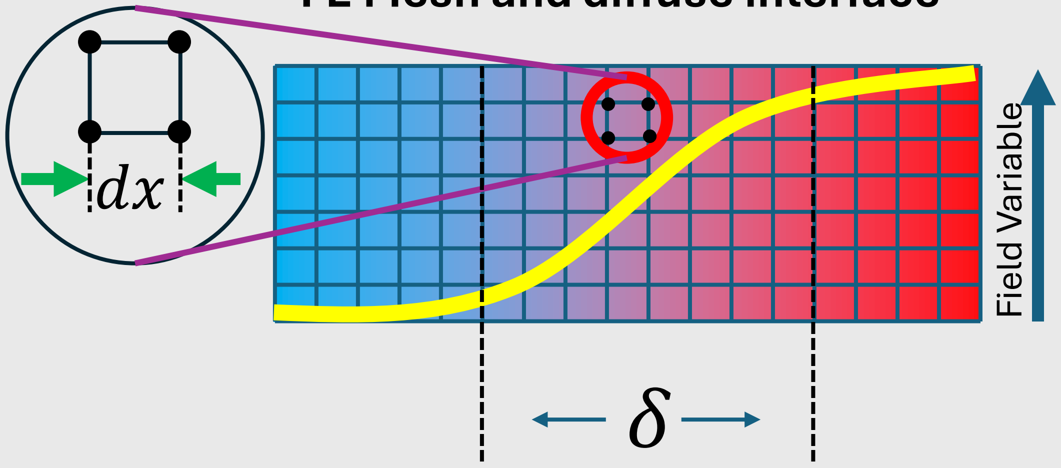

Diffuse Interface Width

Mesh Element Size & Interface width

$$\delta \geq 6.65\, dx \quad [1]$$

[1] Moelans, et. al., Physical Review B 78, 024113 (2008), https://doi.org/10.1103/PhysRevB.78.024113

T-Dependent Gibbs Free Energies & Simulation Results

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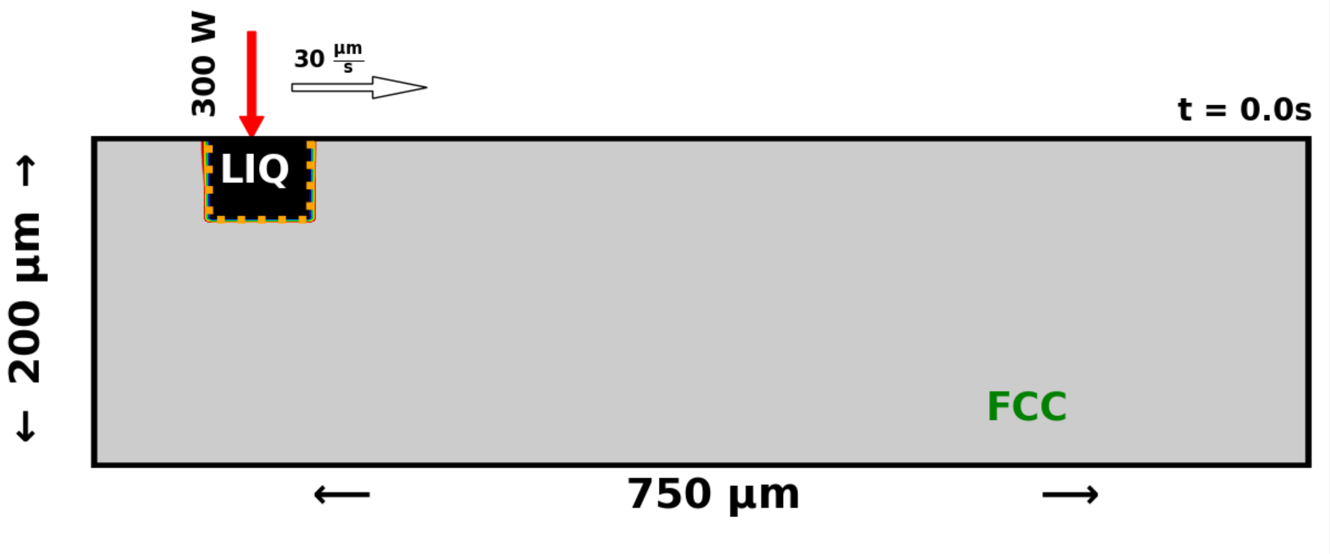
(A) 2 Phase Unary "Au" System



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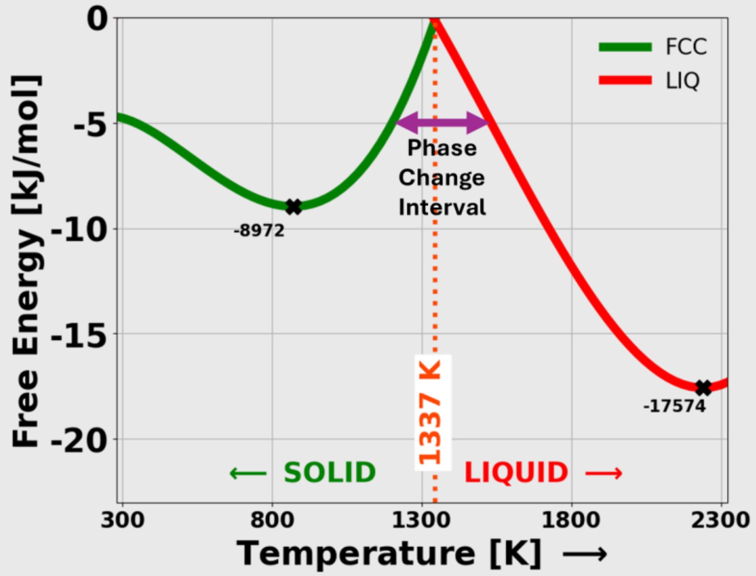

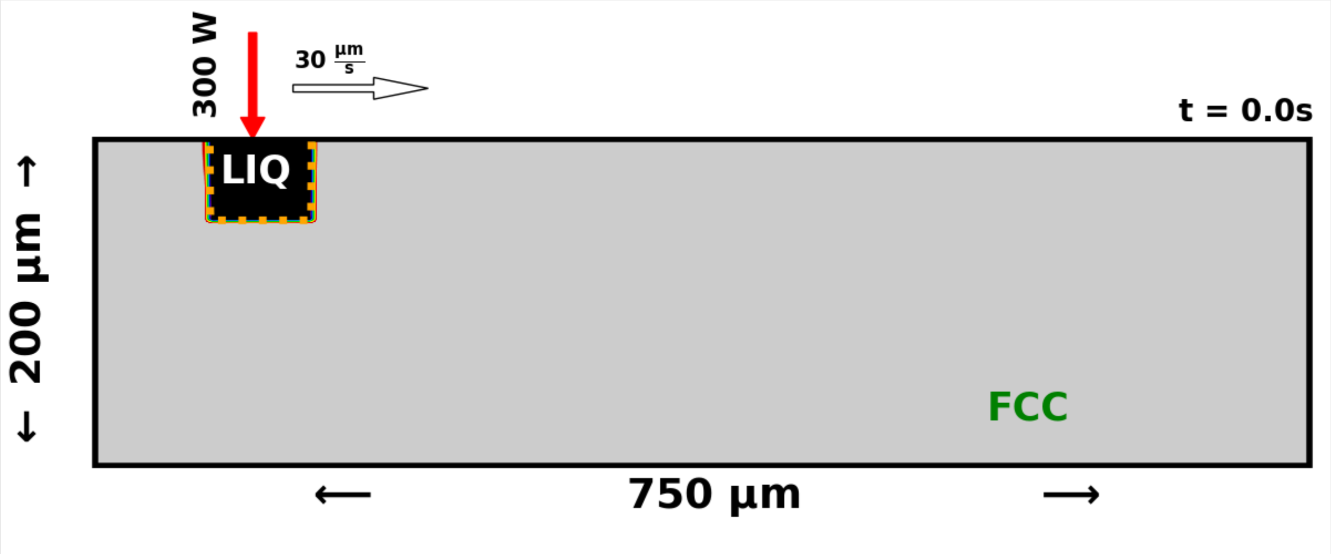

$$F^i(T) = a + b + c(T - T_0) + d(T - T_0)\ln(e\,T) + f(T - T_0)^2 + g(T - T_0)^3 + \frac{h}{T}$$

	a	b	c	d	e	f	g	h	T_0
LIQ	1337	18905	11.2	6.3	23e-4	34e-3	1.9e-5	-17.4	2227
FCC	300	4985	-49.6	-12	0.235	-1e-3	2e-5	-1e-3	235

.TDB file Source: Khvan et. al, Calphad 68 (2022), https://doi.org/10.1016/j.calphad.2019.101724

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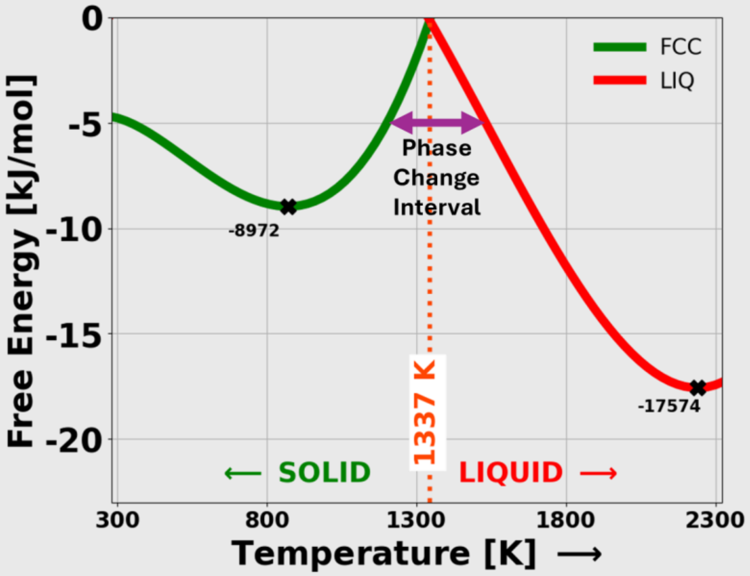

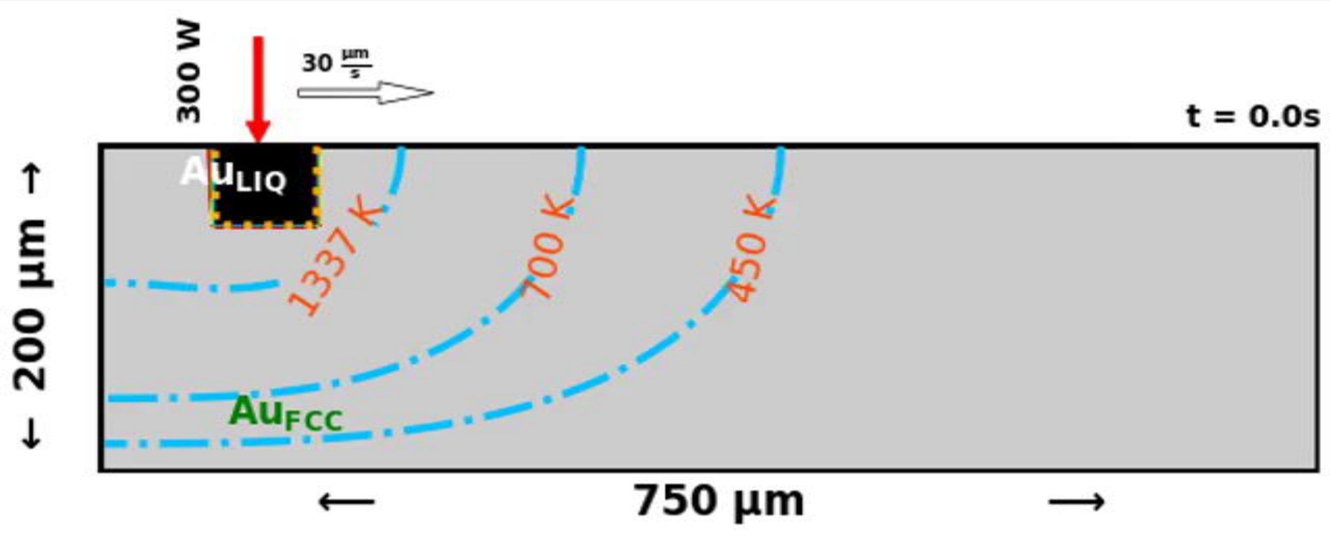

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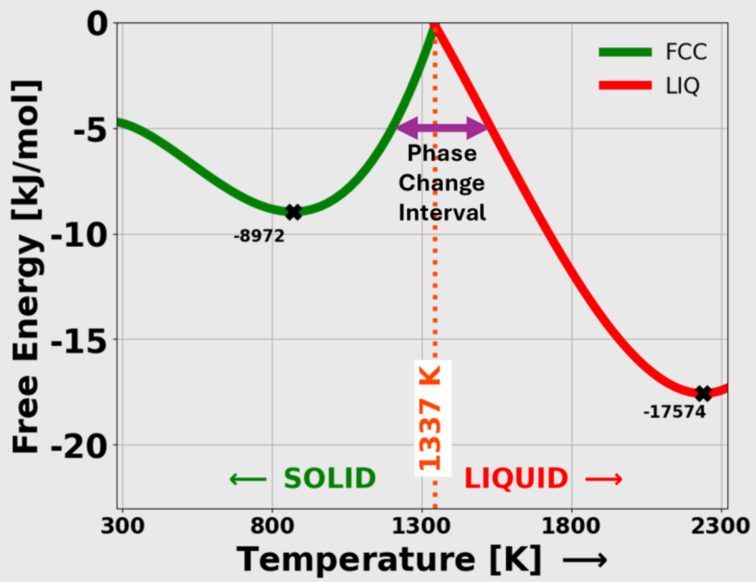

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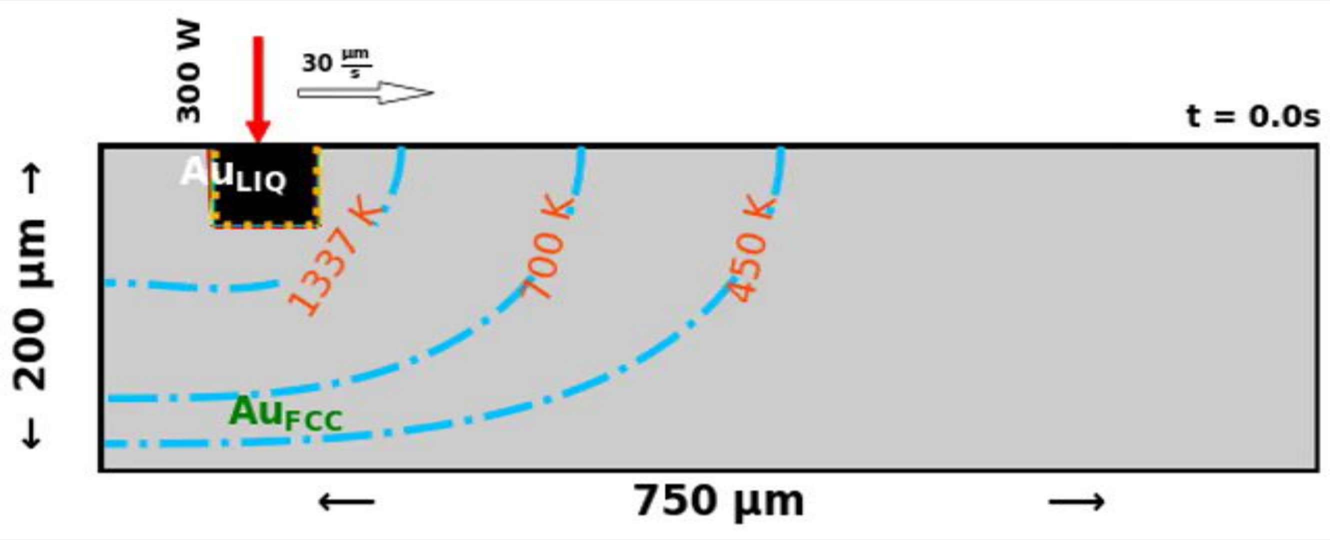

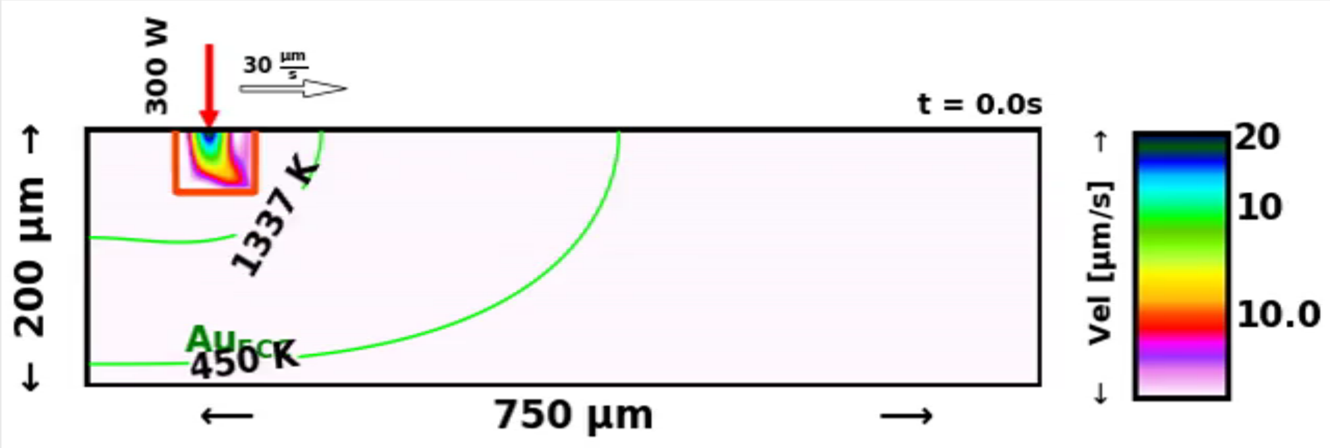

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(B) 4 Phase 7 η Binary "Au-Ti" System

Au rich FCC

Ti rich HCP

Ti3Au IMC

LIQUID

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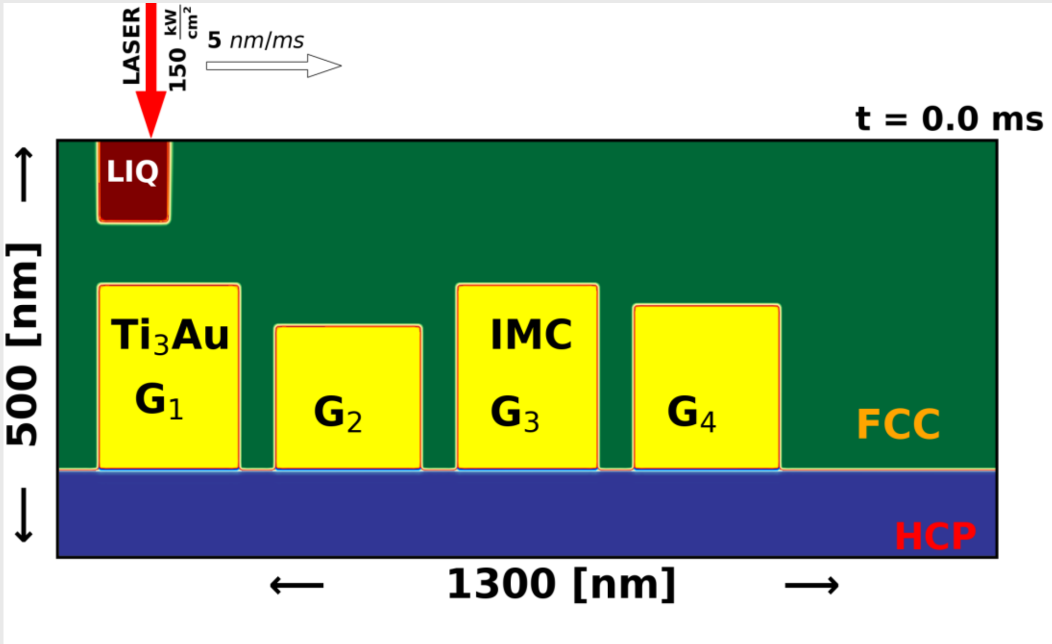

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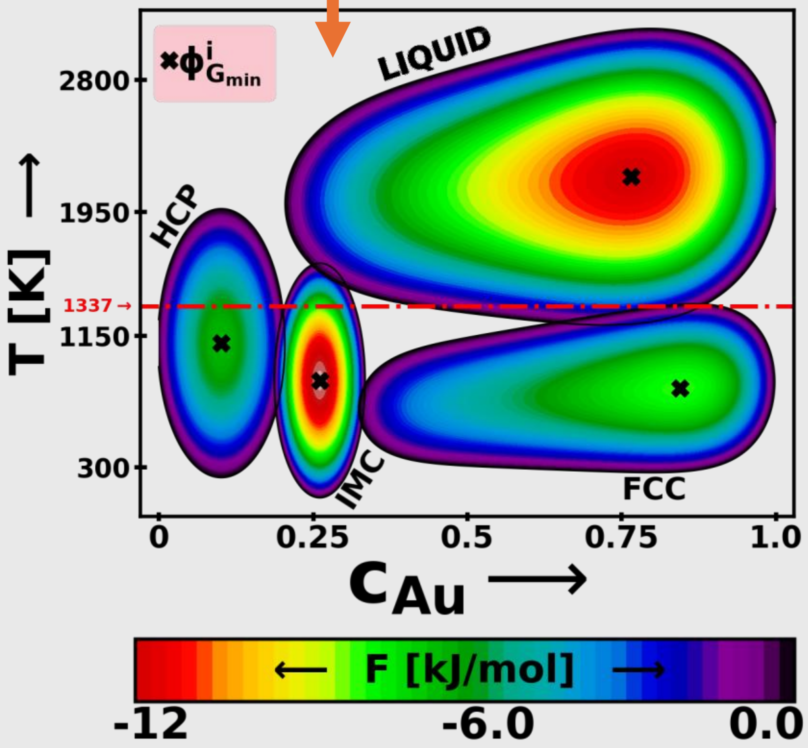
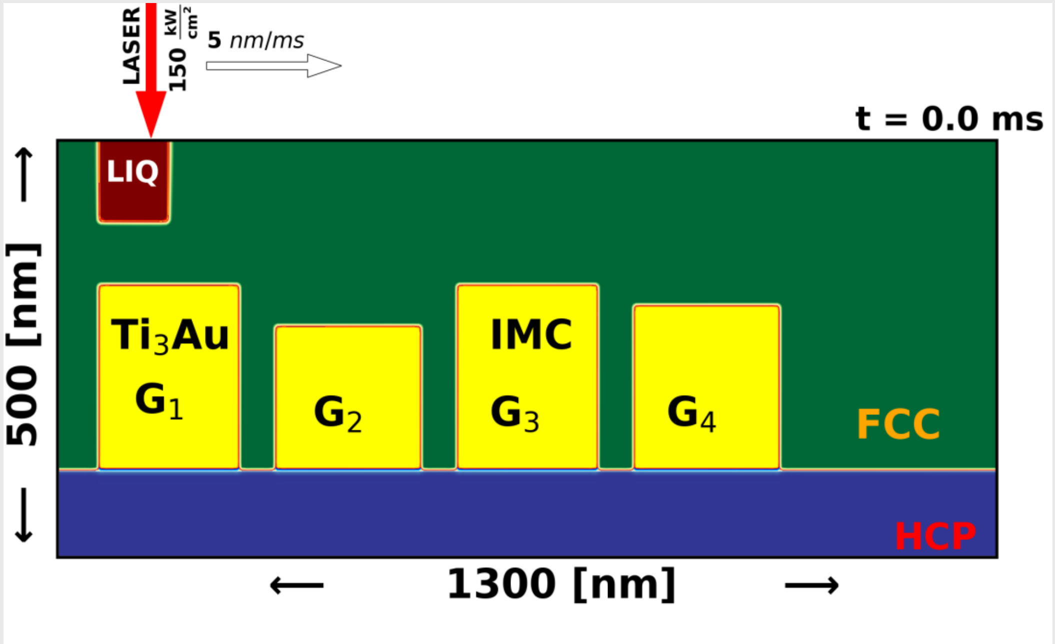


i → FCC, HCP, LIQ, IMC



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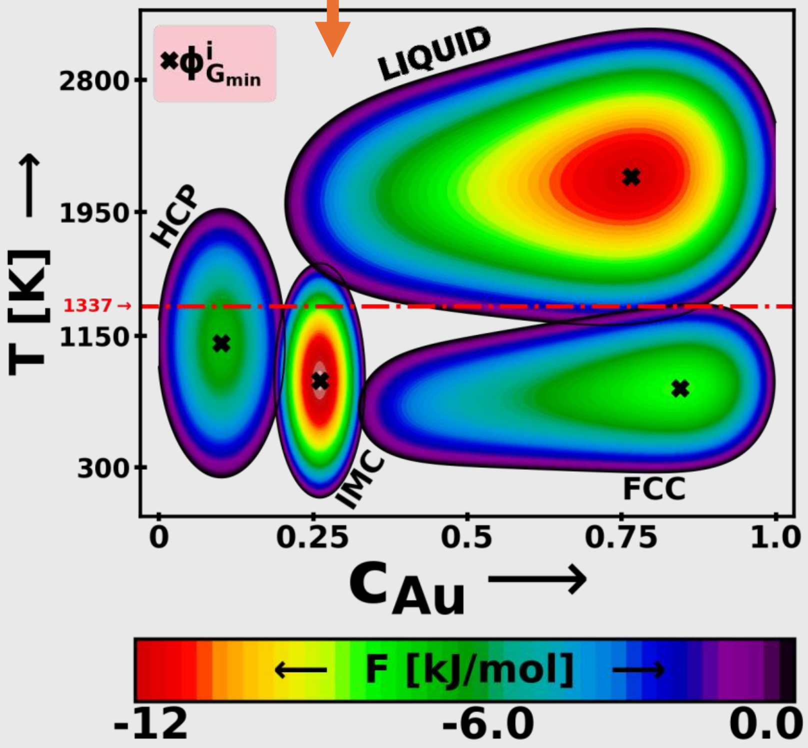

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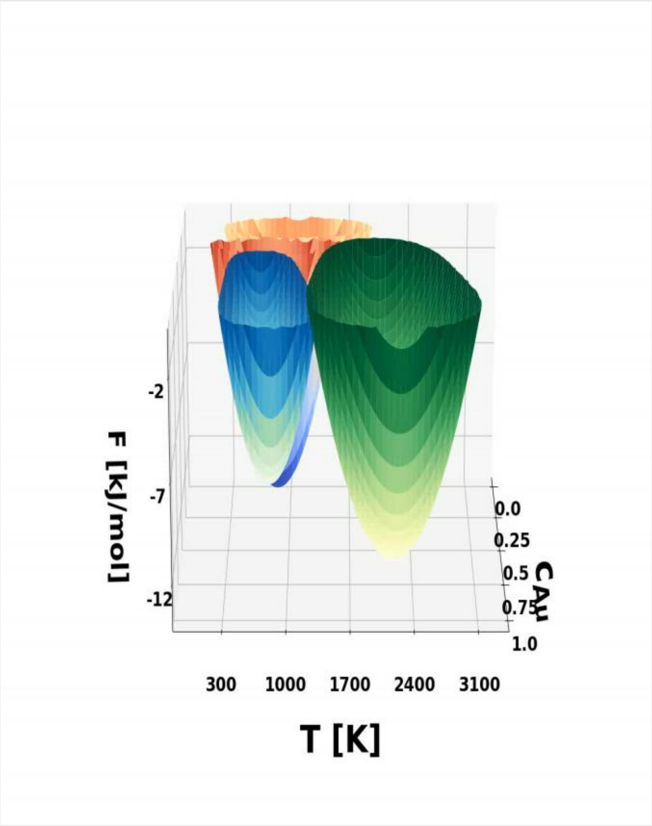

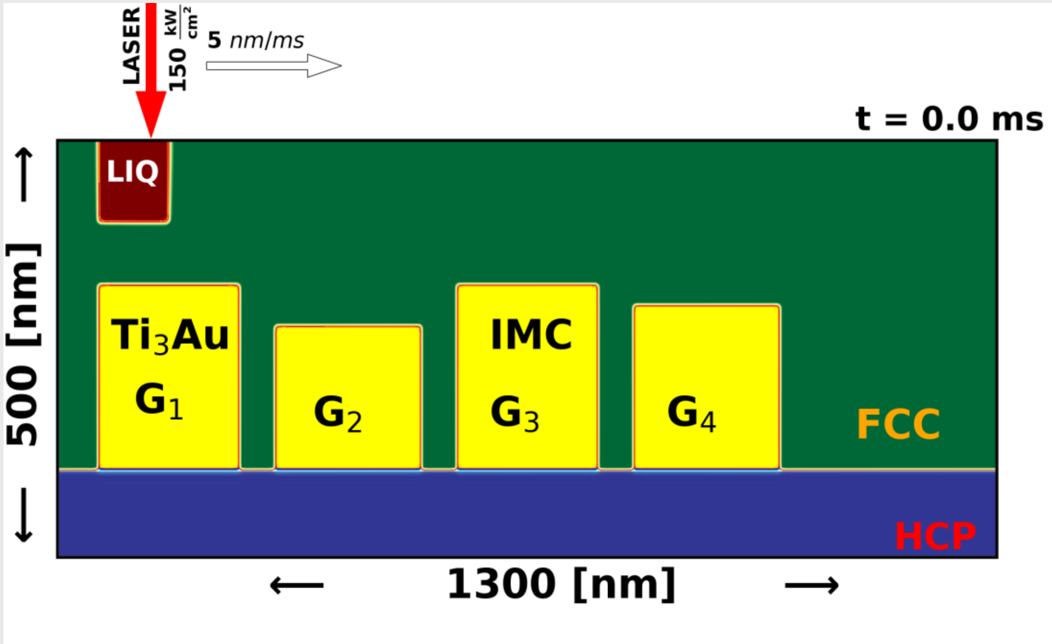

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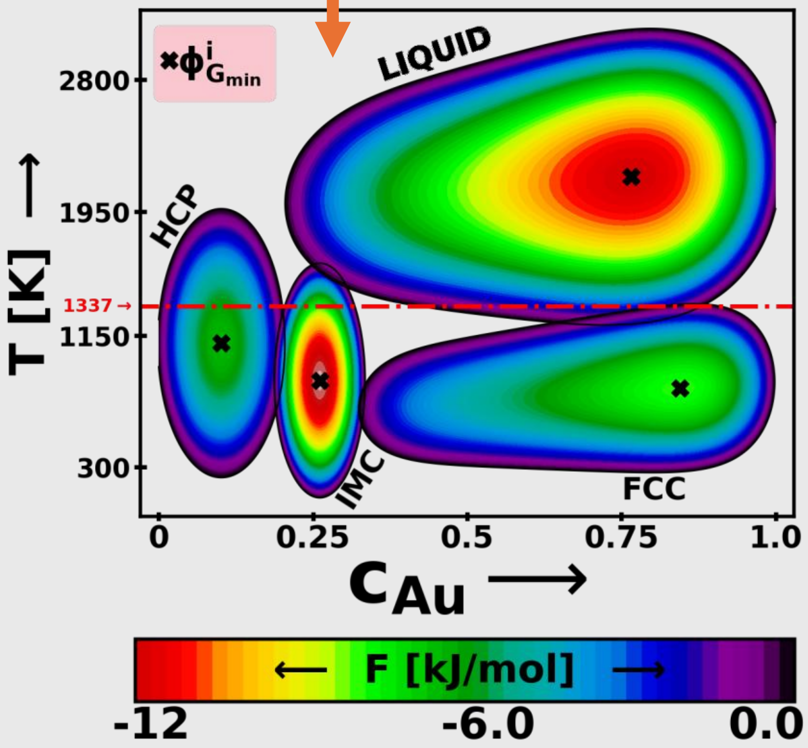

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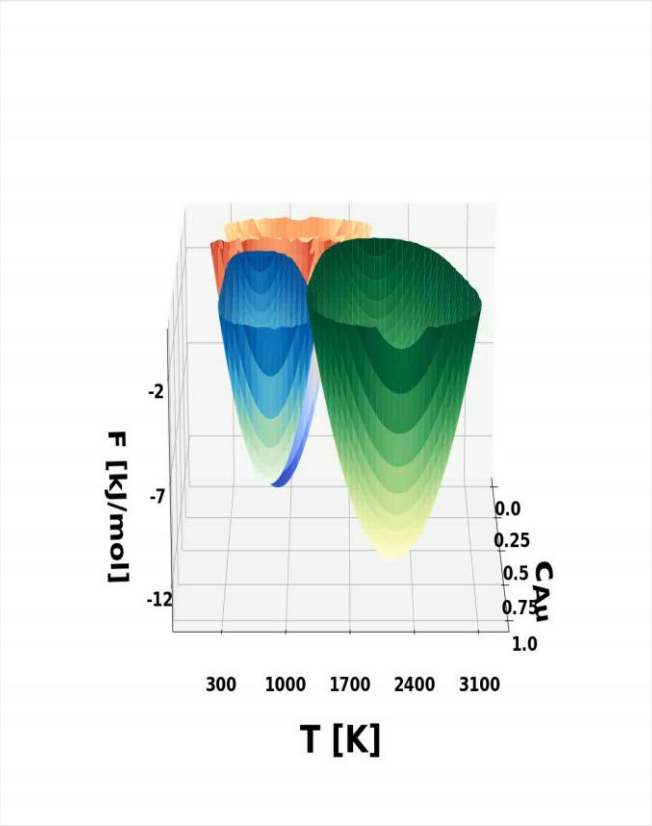
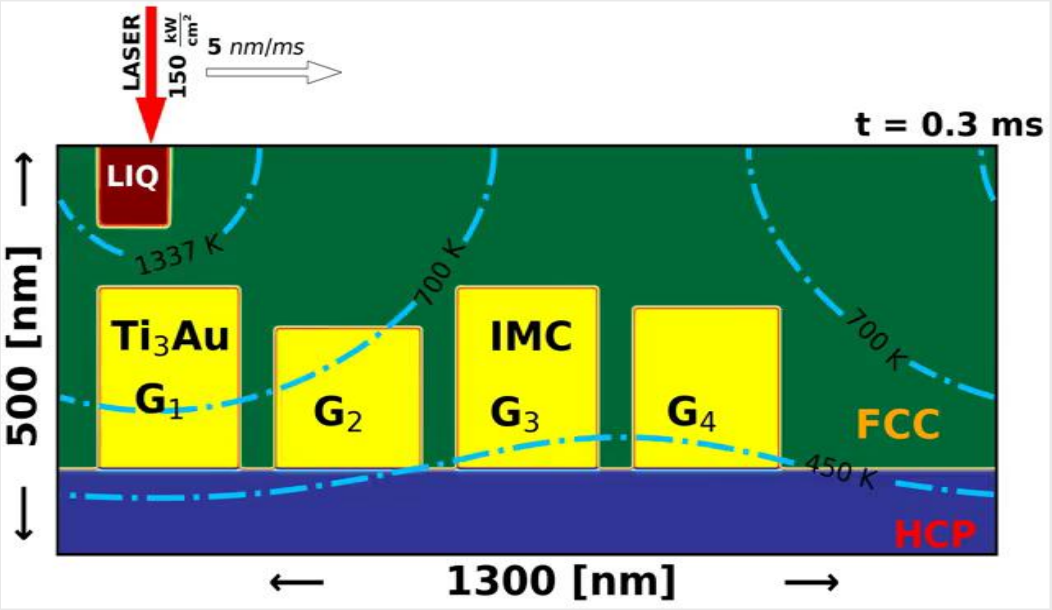




.TDB file Source: Xiong et. al, Calphad 66 (2019), https://doi.org/10.1016/j.calphad.2019.101629

(B) 4 Phase 7 η Binary “Au-Ti” System

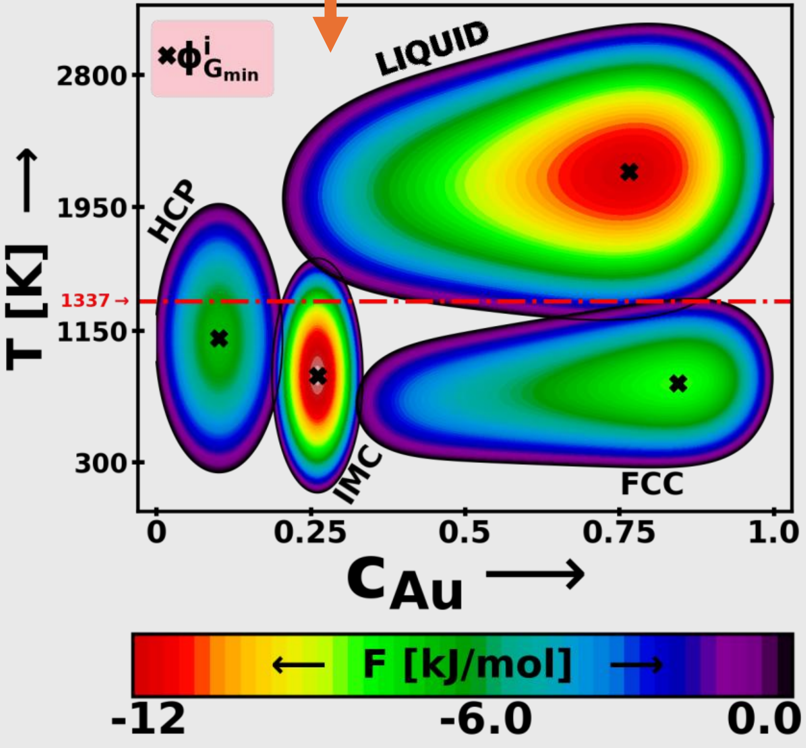
Au rich FCC

Ti rich HCP

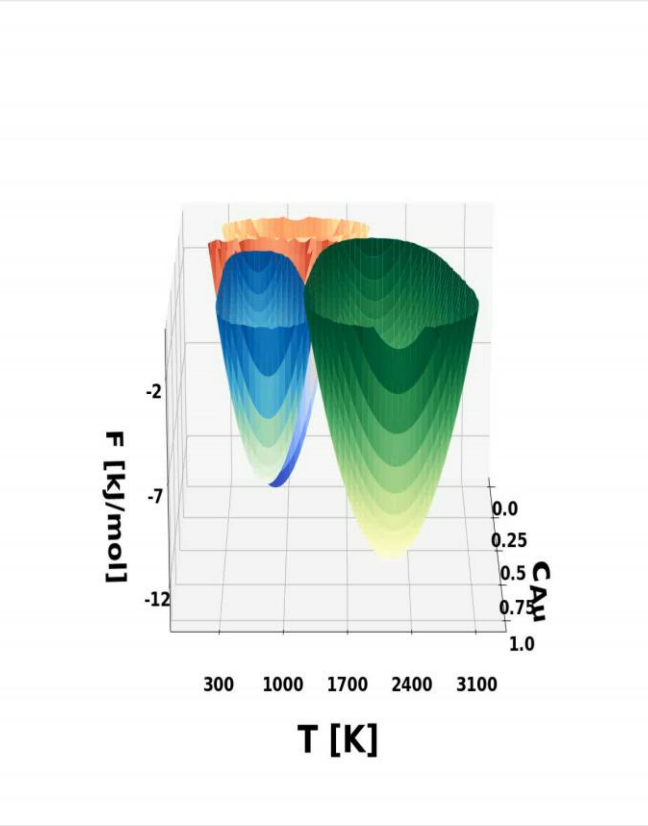
Ti3Au IMC

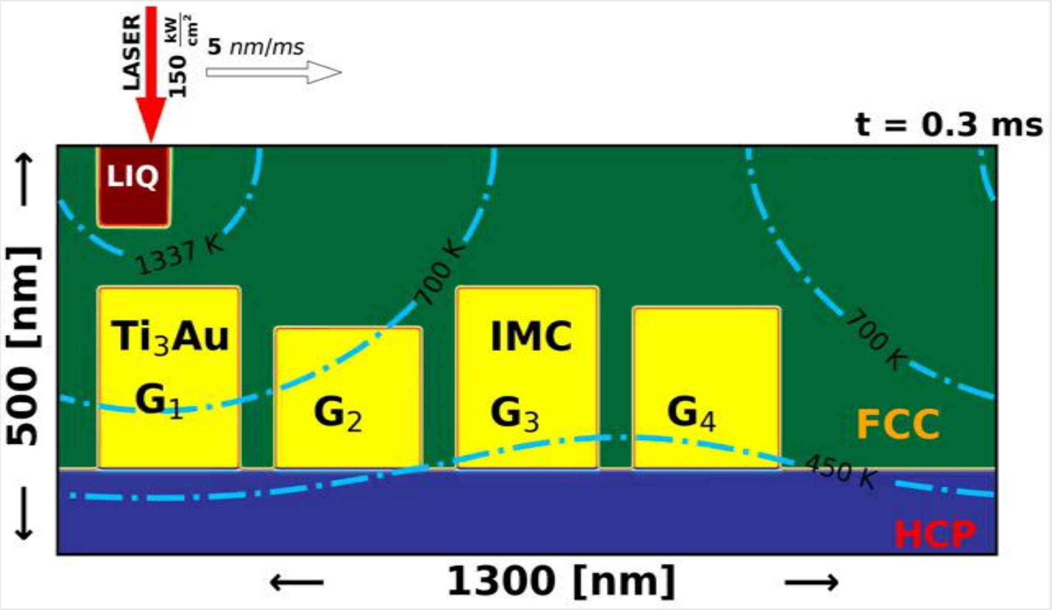
LIQUID

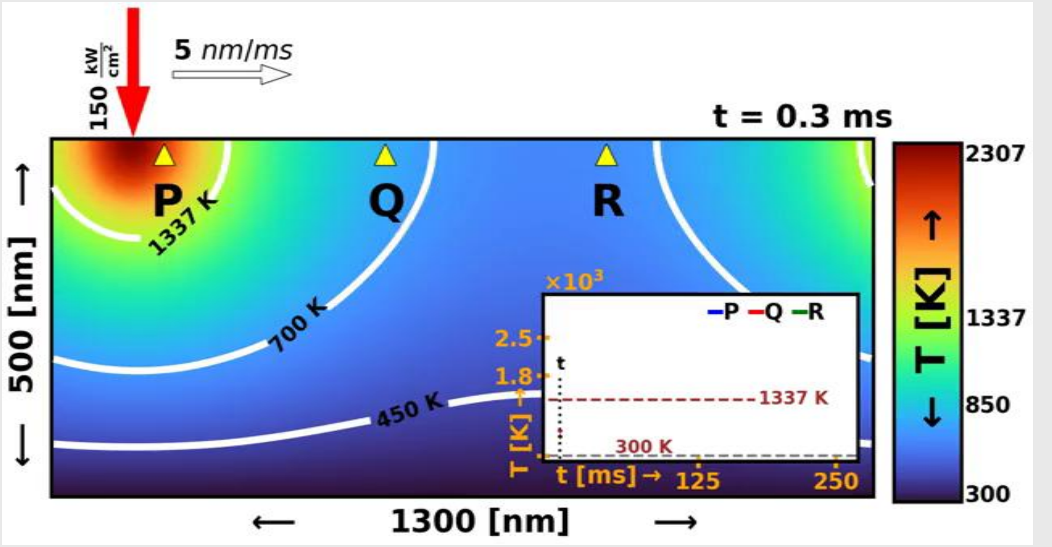
$$F^i = f(c_{Au}, T)$$



i → FCC, HCP, LIQ, IMC







.TDB file Source: Xiong et. al, Calphad 66 (2019), https://doi.org/10.1016/j.calphad.2019.101629

(B) 4 Phase 7 η Binary "Au-Ti" System

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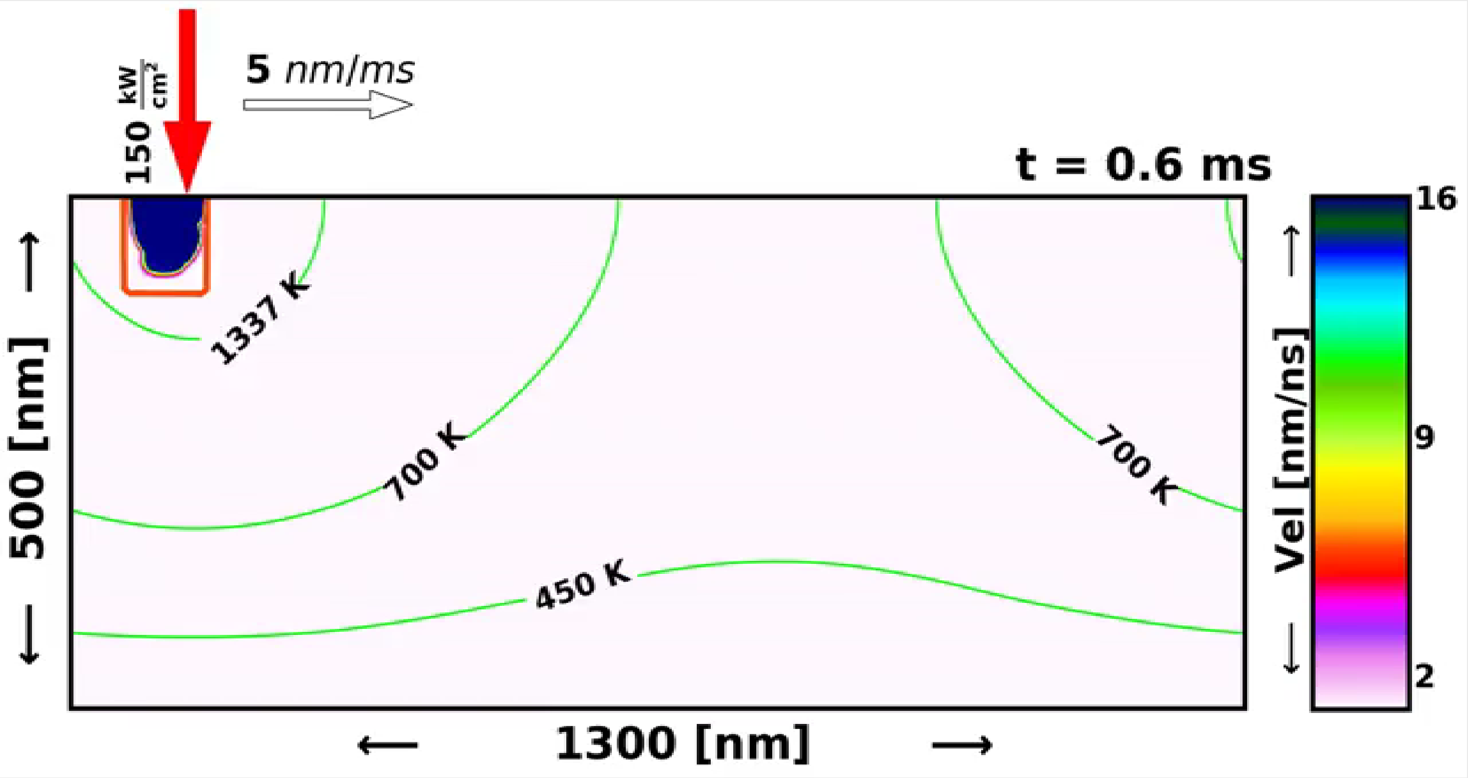
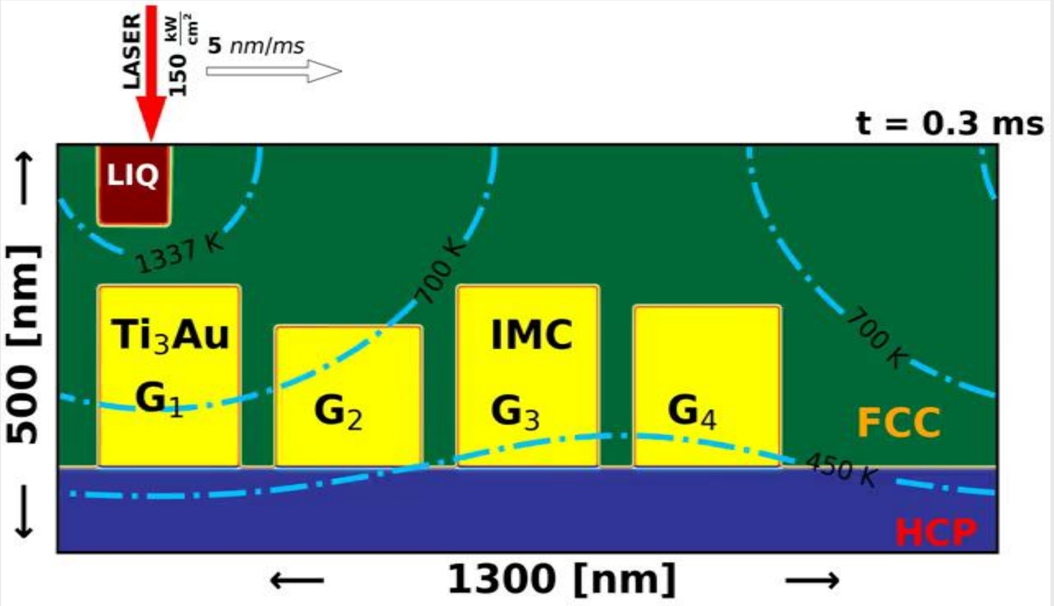
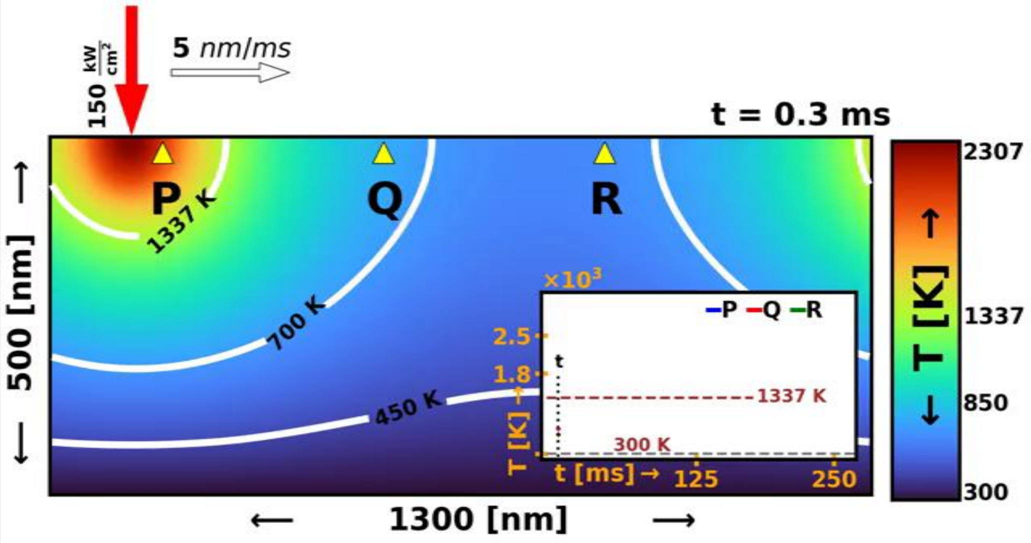
Ti rich HCP

Ti3Au IMC

LIQUID







.TDB file Source: Xiong et. al, Calphad 66 (2019), https://doi.org/10.1016/j.calphad.2019.101629

(C) 5 Phase 10 η Ternary “Cu-Sn-Gas” System

(C) 5 Phase 10 η Ternary "Cu-Sn-Gas" System

Cu rich FCC
Sn rich BCT

Cu6Sn5 IMC
LIQUID

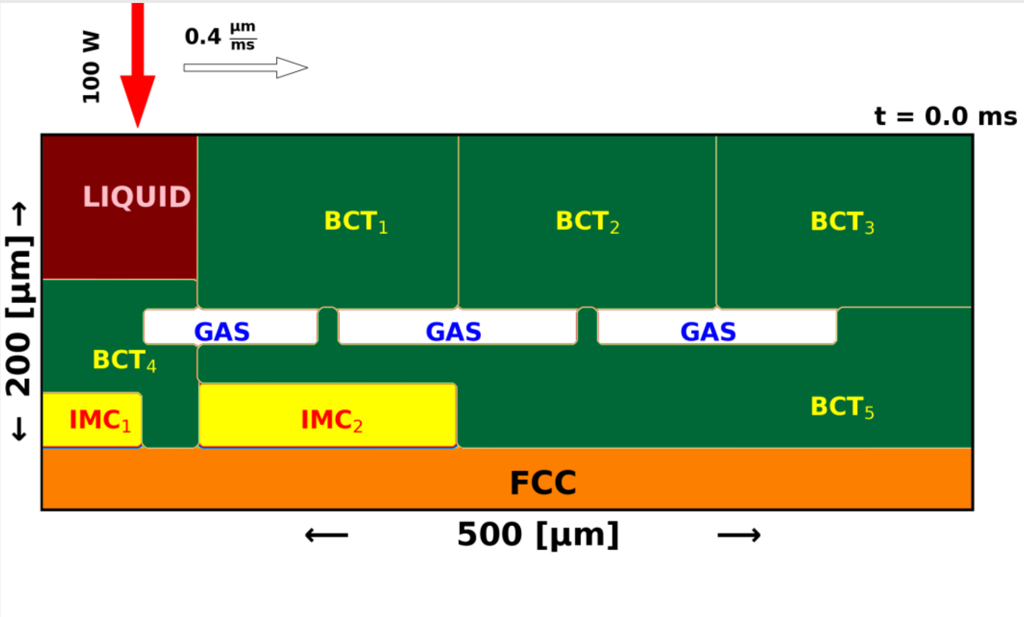
AIR / GAS

(C) 5 Phase 10 η Ternary "Cu-Sn-Gas" System

Cu rich FCC
Sn rich BCT

Cu6Sn5 IMC
LIQUID

AIR / GAS



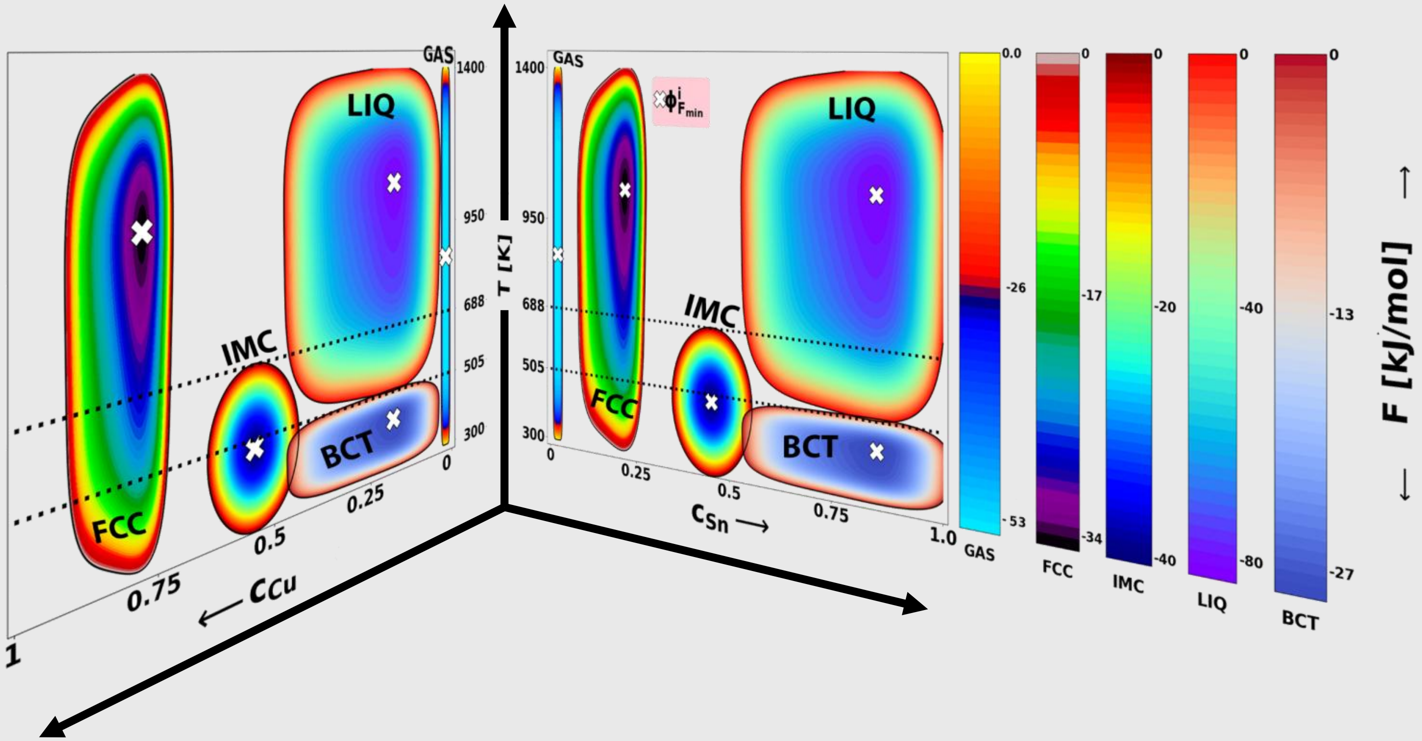
(C) 5 Phase 10 η Ternary "Cu-Sn-Gas" System

Cu rich FCC
Sn rich BCT

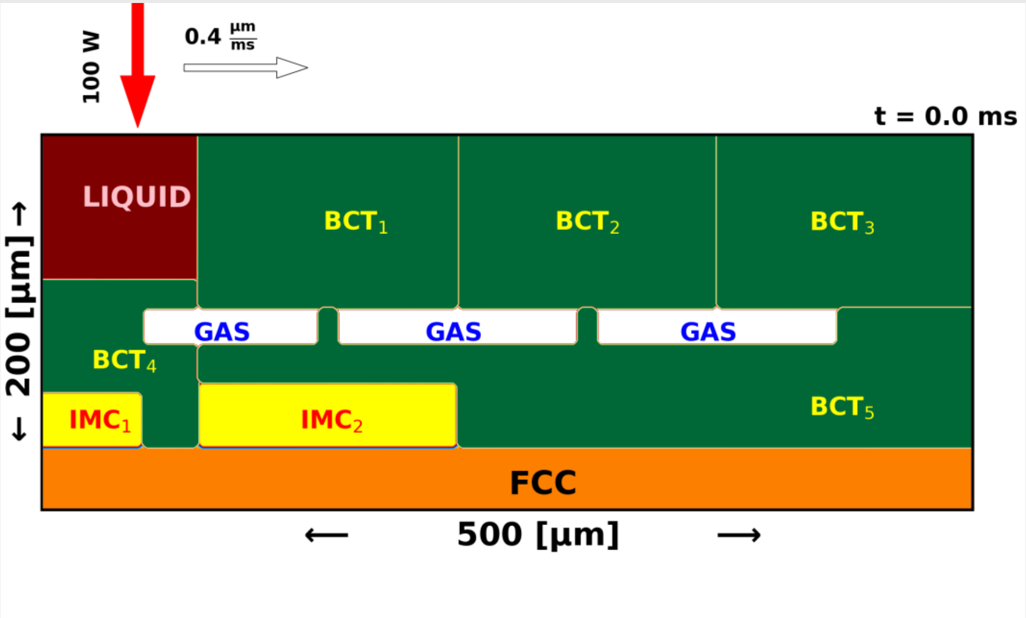
Cu6Sn5 IMC
LIQUID

AIR / GAS

$$F^{i} = f(c_{Cu}, c_{Sn}, T)$$



i → FCC, BCT, LIQ, IMC, AIR



.TDB file Source: Li et. al, Calphad 43 (2013), https://doi.org/10.1016/j.calphad.2013.04.003

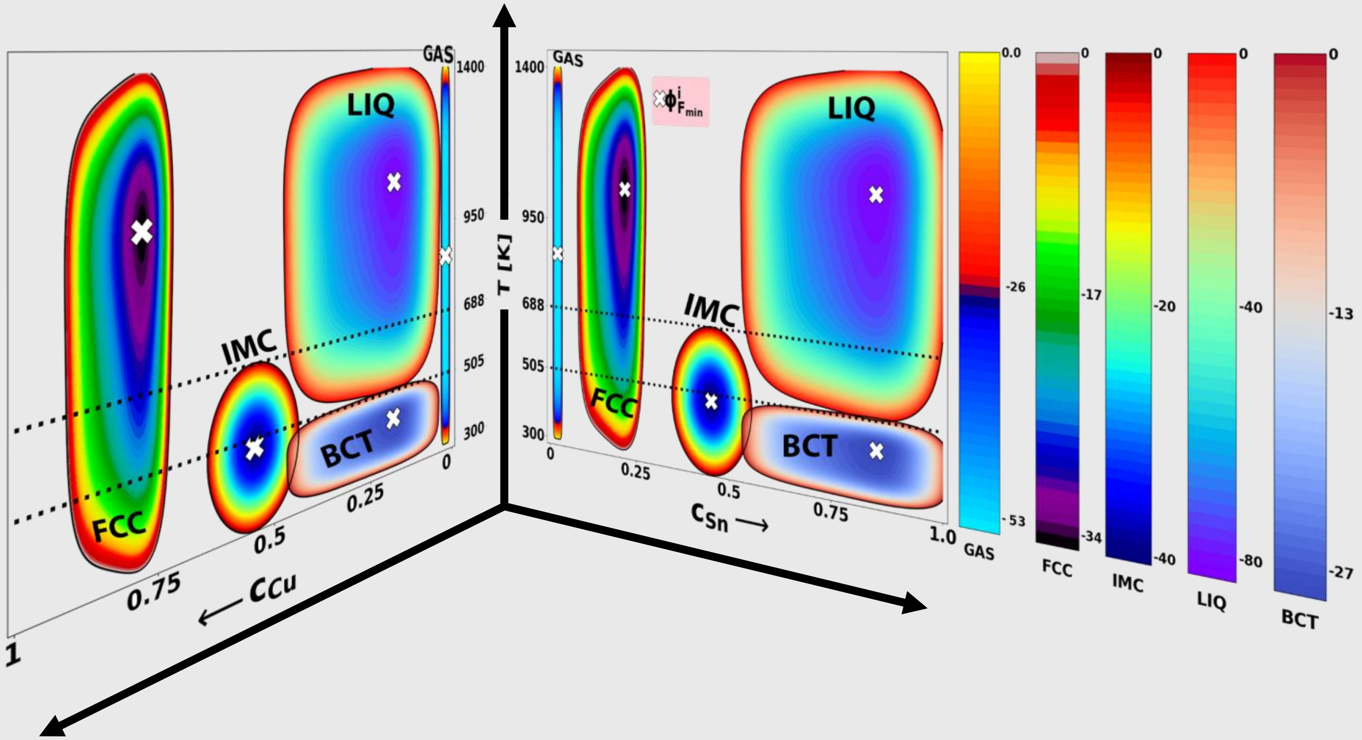
(C) 5 Phase 10 η Ternary "Cu-Sn-Gas" System

Cu rich FCC
Sn rich BCT

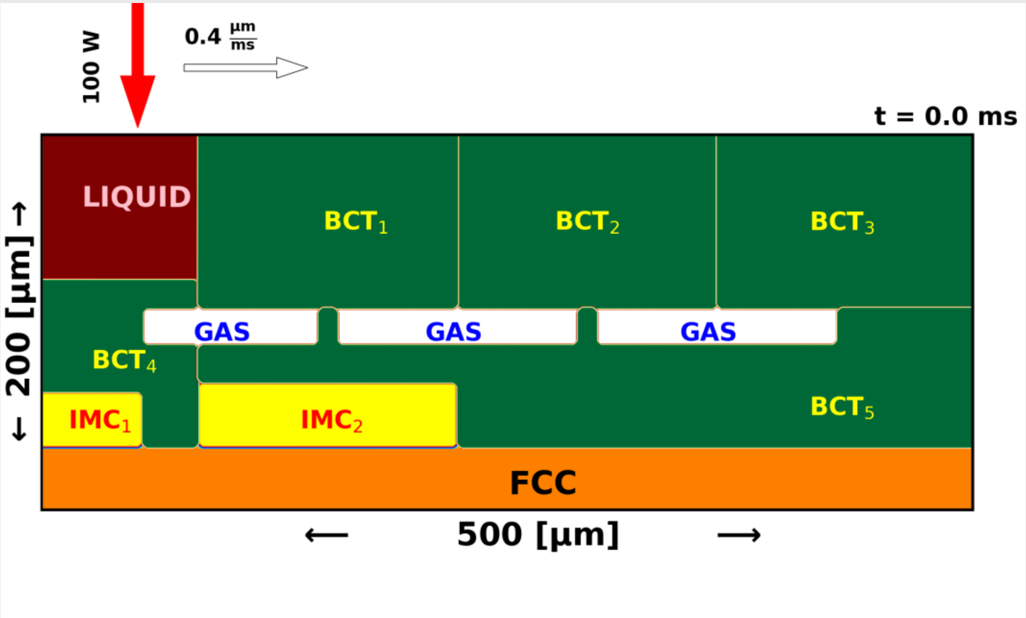
Cu6Sn5 IMC
LIQUID

AIR / GAS

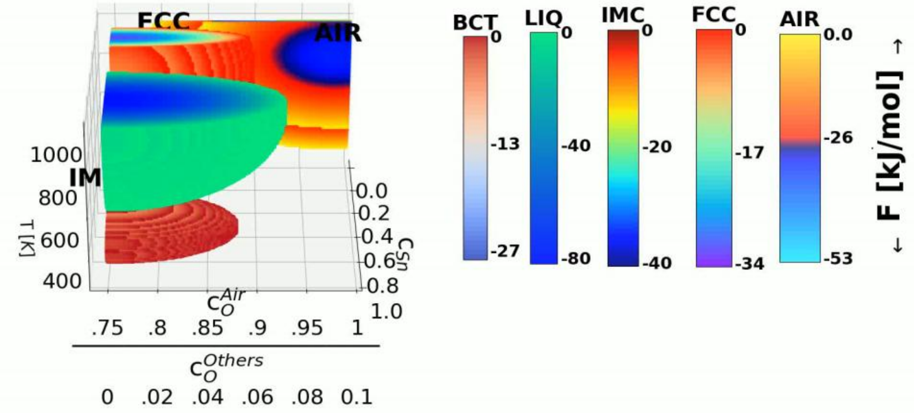
$$F^i = f(c_{Cu}, c_{Sn}, T)$$



i → FCC, BCT, LIQ, IMC, AIR



$$F^i = f(c_{Air}, c_{Sn}, T)$$

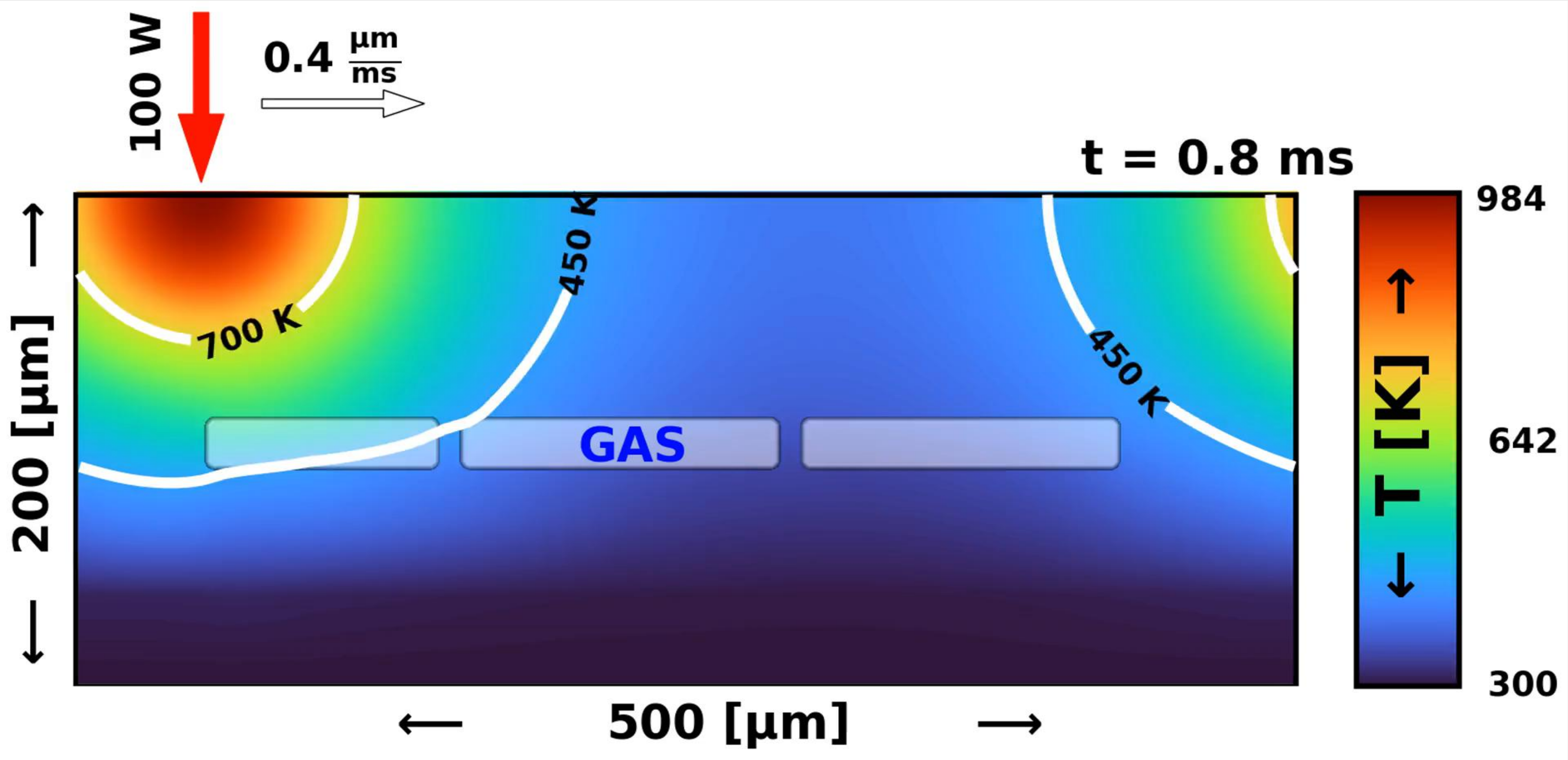


.TDB file Source: Li et. al, Calphad 43 (2013), https://doi.org/10.1016/j.calphad.2013.04.003

Simulation Result

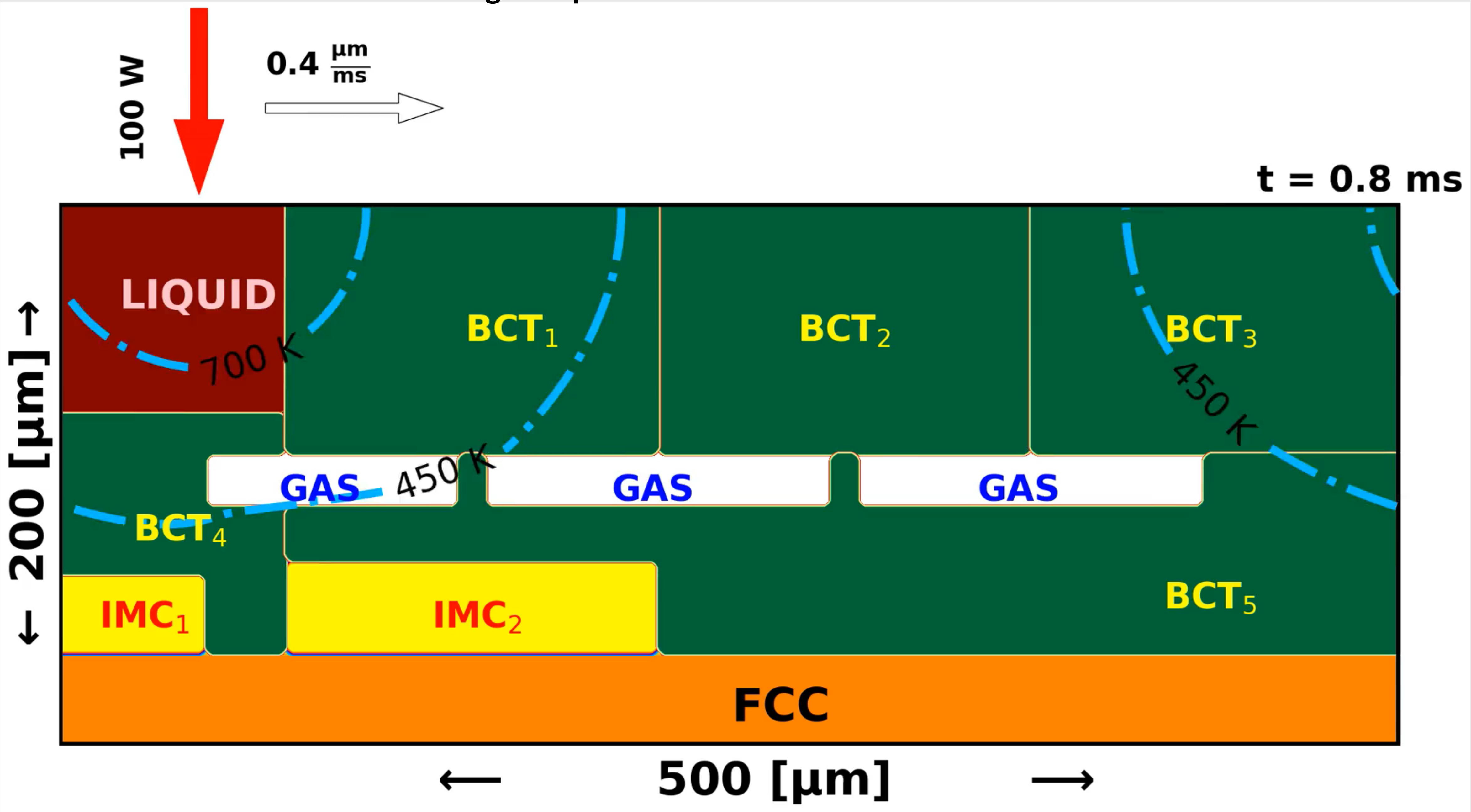
Simulation Result

Fig. Transient Temperature Distribution



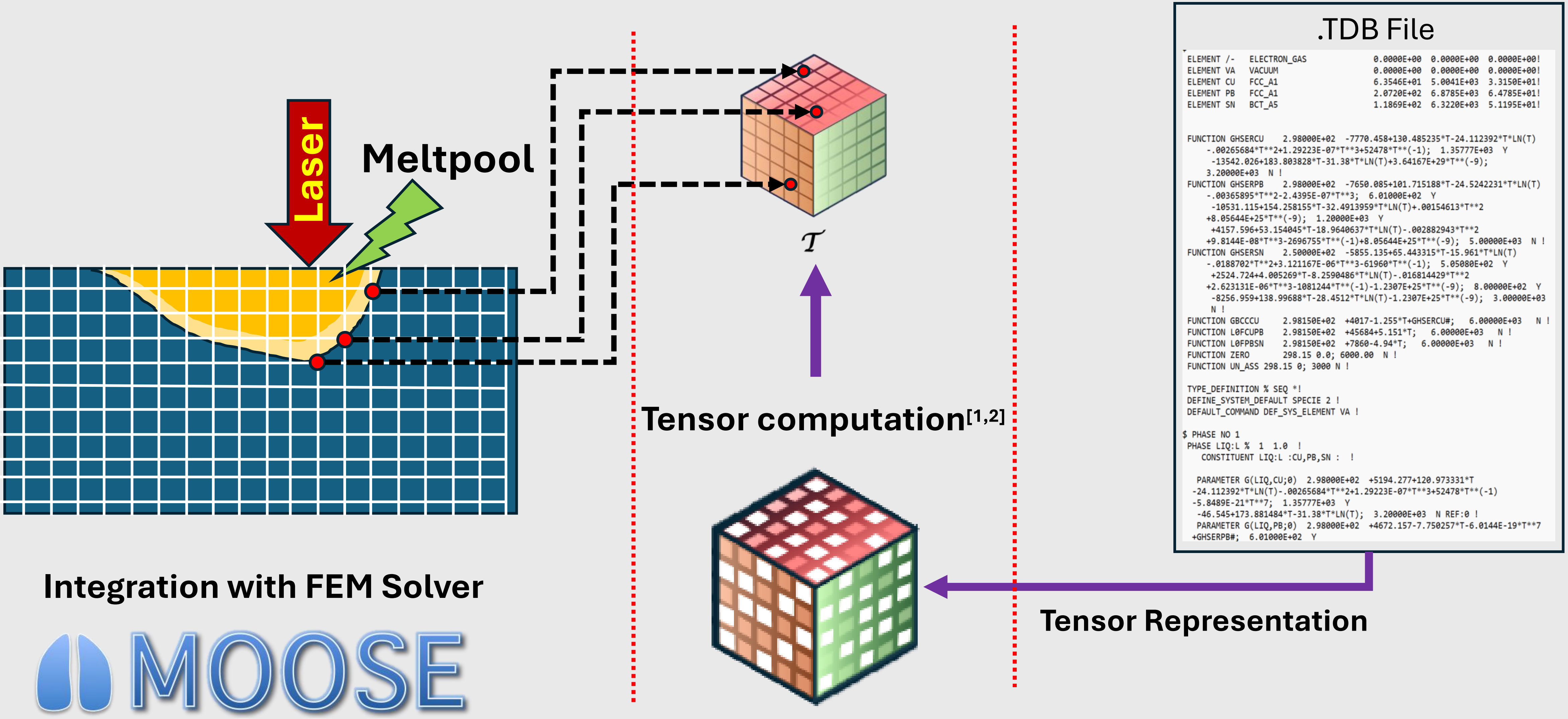
Simulation Result

Fig. Temporal Phase Evolution



Thermodynamic Data Tensor

Free Energy for higher component system (Work in Progress ...)



[1] Coutinho et. al., npj Comput Mater 6, 2 (2020). https://doi.org/10.1038/s41524-019-0268-y
[2] Subedi et. al., Scripta Materialia, 244, (2024). https://doi.org/10.1016/j.scriptamat.2024.116027