Phase-field-crystal (PFC) modeling of defect-mediated precipitation in Al–Si alloys for additive manufacturing

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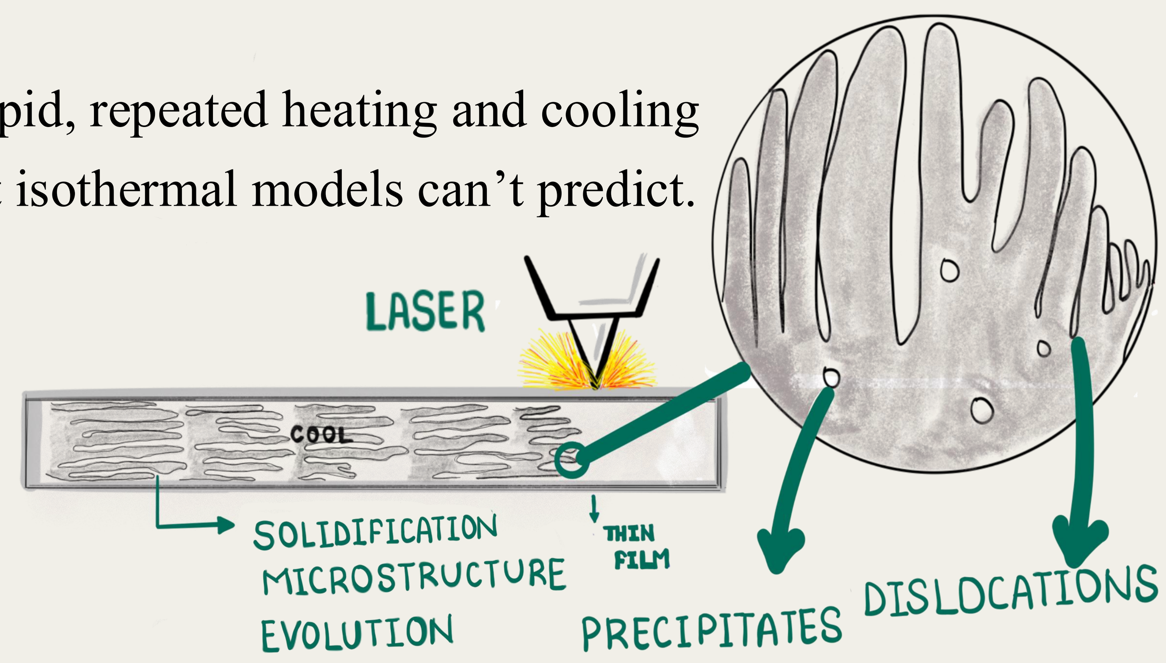
1 MOTIVATION

- Precipitates set the strength and ductility of 3D-printed parts and they form preferentially at crystalline defects.
- Additive manufacturing's rapid, repeated heating and cooling produces microstructure that isothermal models can't predict.
- We resolve how defects and precipitates interact under realistic AM thermal histories.



2 METHODOLOGY

- The Binary PFC model [1] is used to model the phase transformation between solid and liquid phase using the direct two-point correlation function.

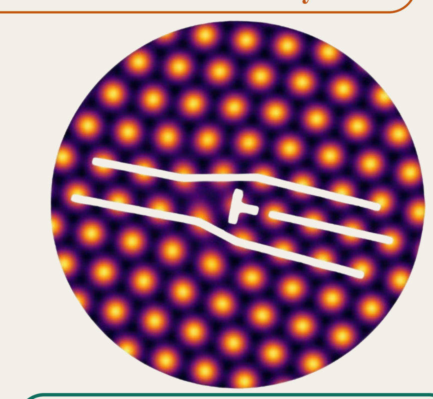
$$\mathcal{F} = \tau \int dr \left\{ \underbrace{\frac{1}{2} n(r) C_{nn}(r,r') * n(r') + \frac{W_c}{2} |\nabla c(r)|^2}_{\text{excess term}} + \underbrace{\omega \sum_{a,b} \Gamma_{a,b} n^a c^b}_{\text{ideal term}} \right\}$$

Free energy functional

$$\frac{\partial n/c}{\partial t} = \nabla \cdot M_{n/c} \nabla \frac{\delta \mathcal{F}}{\delta n/c}$$

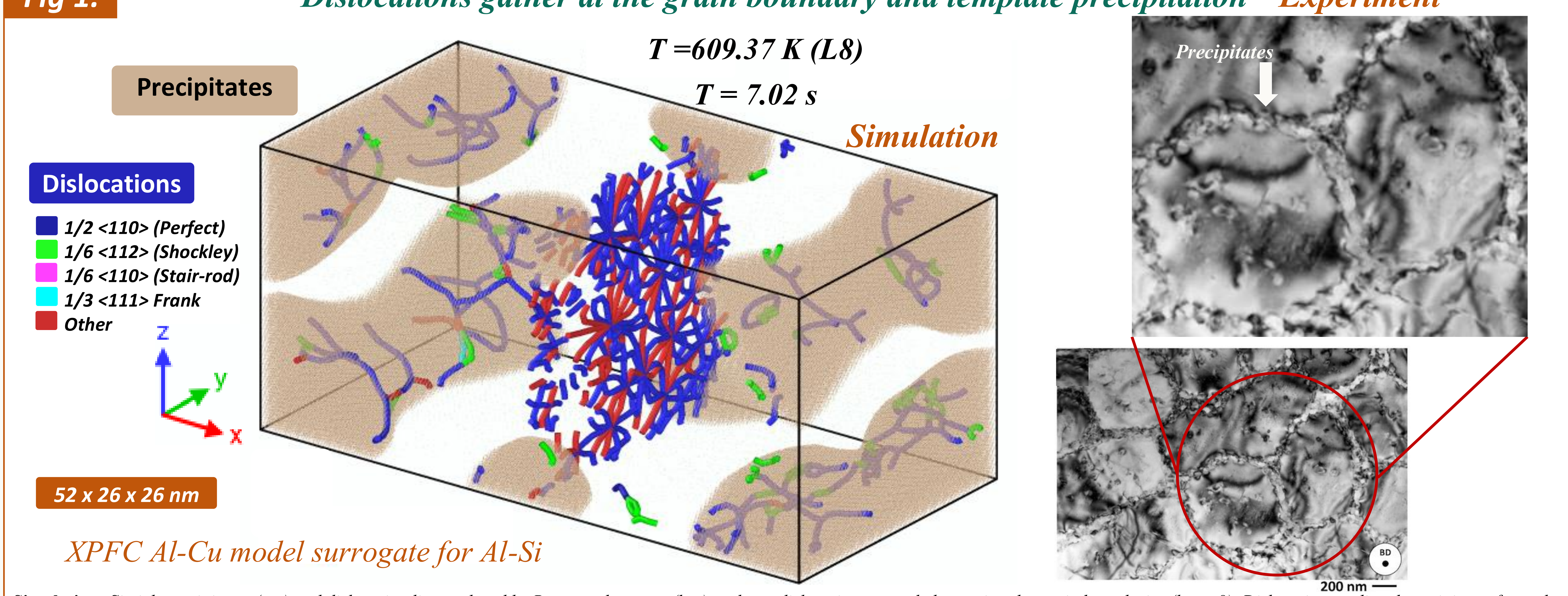
Model Dynamics

- The density (n) and concentration (c) field evolve by dissipative dynamics that minimized this binary. XPFC free energy; two-point correlation C_{nn} sets the crystalline order, and ideal term f_{ideal} drives Si precipitates.
- Binary XPFC model for Al-Si, run on *OpenPFC* – an open-source High Performance Computing PFC framework.
- Initialized by two solid slabs divided and surrounded by incoherent high angle grain-boundaries.



PFC resolves the atomic lattice and individual dislocations – Image by Daniel Coelho

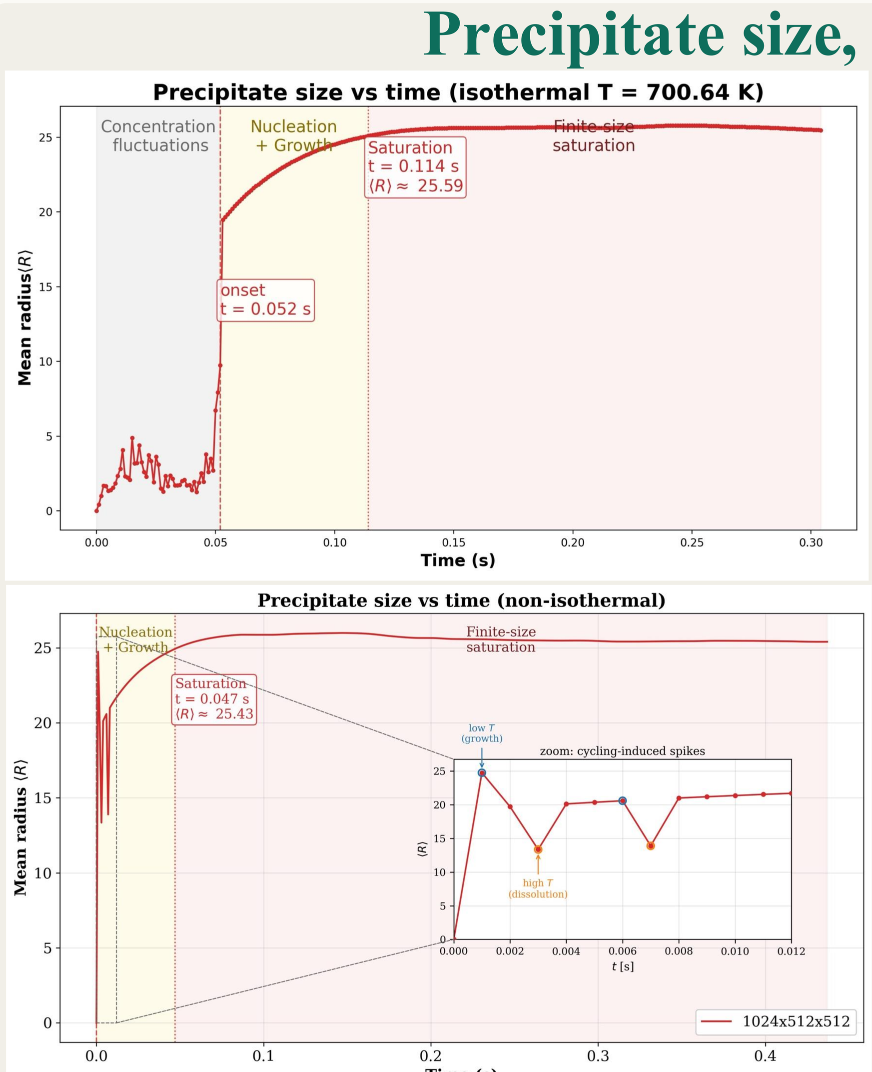
Fig 1. *Dislocations gather at the grain boundary and template precipitation*



Simulation: *Si-rich precipitates (tan) and dislocation lines colored by Burgers character (key); a dense dislocation network decorating the grain boundaries (layer 8). Dislocation-mediated precipitates form along the grain-boundaries.* **Experiment:** *AM Al-Si-Mg (dilute Mg) from our collaborators [2]; (a) top and (b) bottom of the AM build. Eutectic Si forms as precipitates due to dislocation along the grain boundaries.*

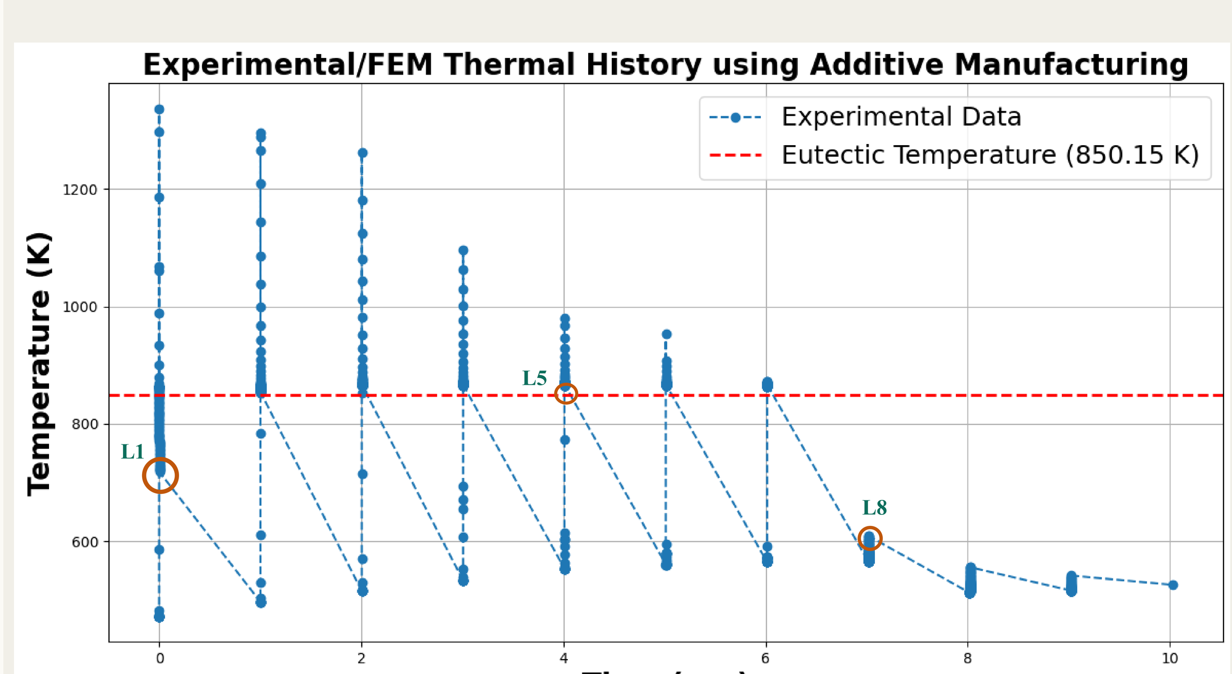
RESULTS

Precipitate size, R(t)



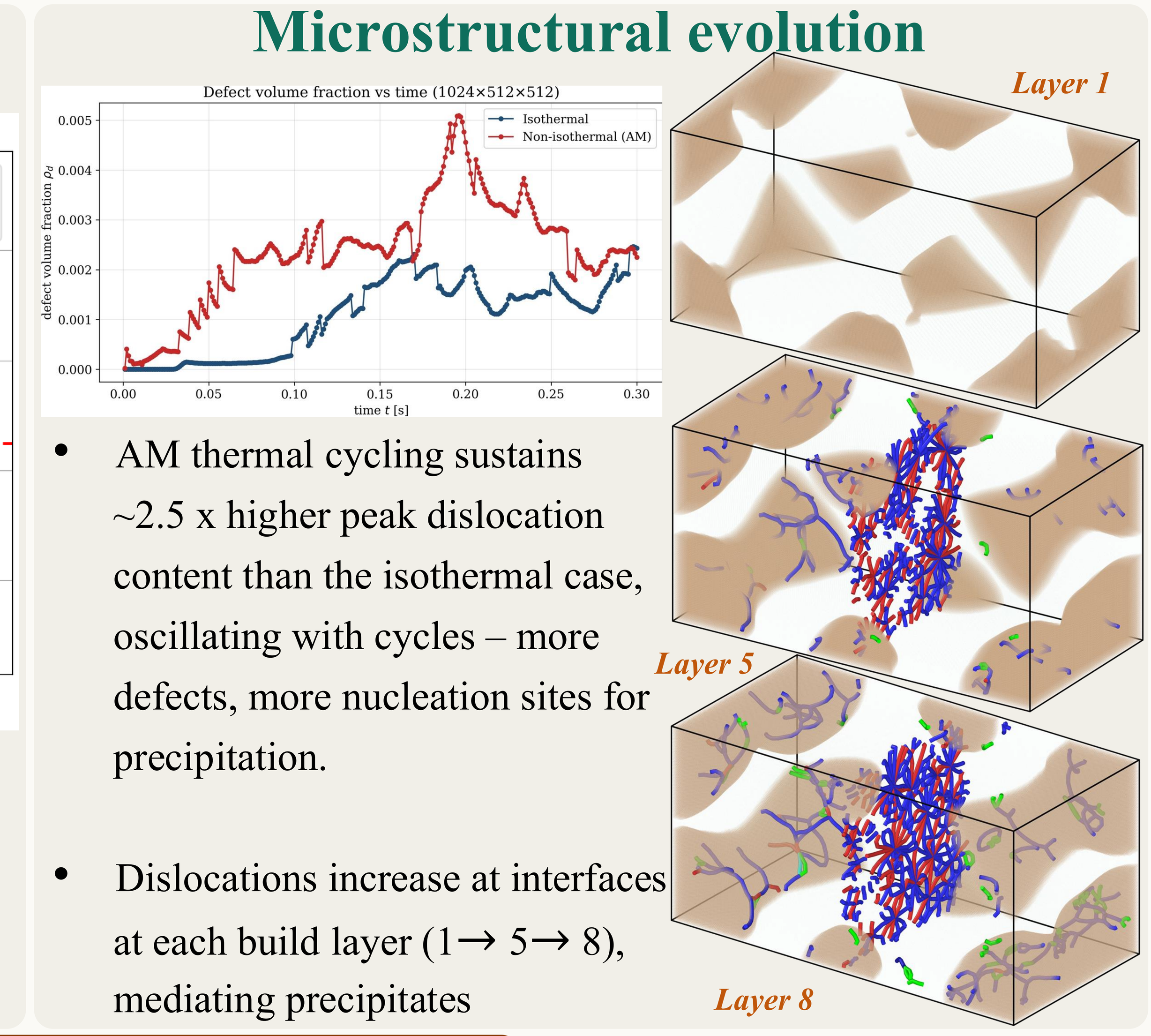
1. For isothermal and non-isothermal conditions saturates near $< R > \approx$ 25.5 (finite 52 x 26 x 26 nm box).
2. AM cycling reaches saturation ~2 x faster (0.047 s vs 0.114 s)
3. Growth/dissolution spikes on each thermal swing.

AM Thermal Cycling Profile



Layer 1: T = 718.40 K t = 0.0025 s
Layer 5: T = 866.43 K t = 4.0125 s
Layer 8: T = 609.37 K t = 7.02 s

Microstructural evolution



- AM thermal cycling sustains ~2.5 x higher peak dislocation content than the isothermal case, oscillating with cycles – more defects, more nucleation sites for precipitation.
- Dislocations increase at interfaces at each build layer (1→ 5→ 8), mediating precipitates

CONCLUSION

- Precipitates nucleate on dislocation cores – a one-to-one link between defects and precipitation.
- In isothermal quenches, dislocations number relatively fixed, while thermal cycling in AM's increases their density, promoting more precipitation.
- Dislocations are not passive defects instead, they actively guide where precipitates form, and the process thermal history is an essential part of the final microstructure.

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[2] M.H. Ghoncheh, A. Asgari, B. Shalchi Amirkhiz, B. Langelier, A. Hadadzadeh, A. Lloyd, and M. Mohammadi, "Solute-induced transition in Poisson's ratio and strength: A phenomenon in additively manufactured Al-Si-Mg alloys," Materials Characterization (2024).

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