Comparison of three-dimensional *in situ* observations and phase-field simulations of microstructure formation during directional solidification of transparent alloys aboard the ISS

Kaihua Ji[1], F.L. Mota[2], Y. Song[1], J. Pereda[2], T. Lyons[3], L.L. Strutzenberg[4], R. Trivedi[3], N. Bergeon[2], A. Karma[1]
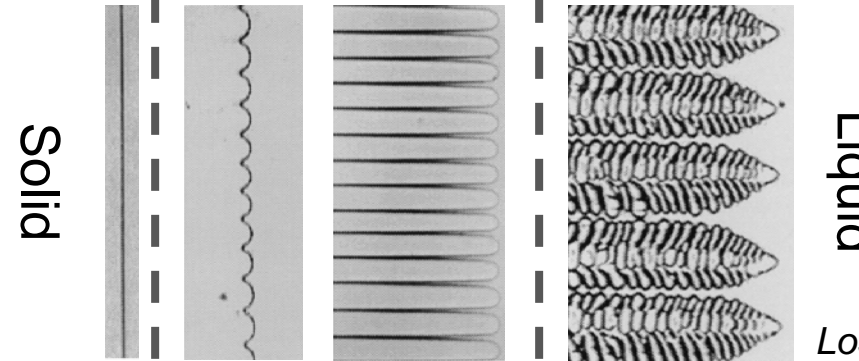
[1]Northeastern University
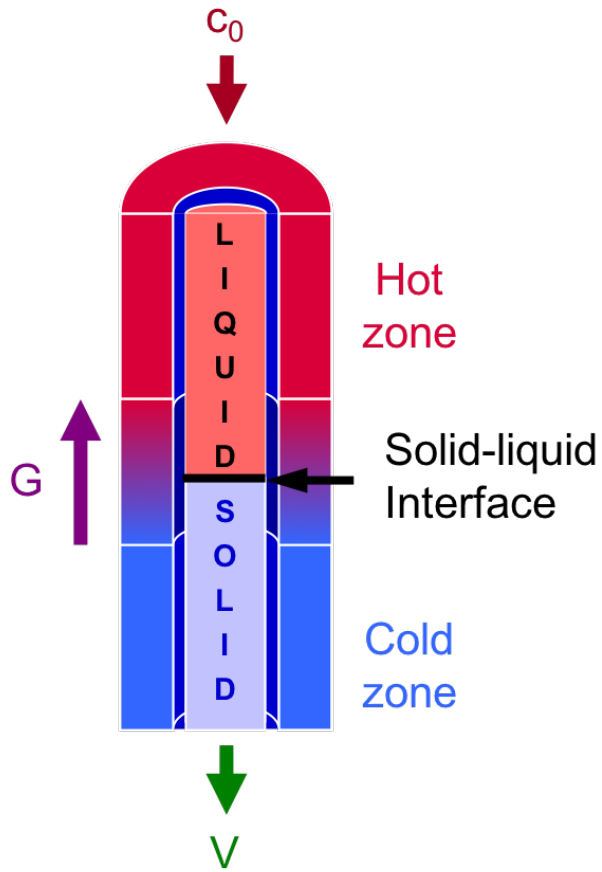[2]IM2NP, Aix-Marseille Université
[3]Iowa State University
[4]Marshall Space Flight Center

THE WORLD COMES HERE
TMS 2020
149th Annual Meeting & Exhibition
CO-LOCATED INTERNATIONAL CONFERENCE
PbZn 2020
February 23-27, 2020
San Diego, California, USA
#TMSAnnualMeeting
1

The system – directional solidification

- Microstructure formation under well-controlled growth conditions (G, V, C_0)

*http://www.rksteel.com.pk/*

David et al. Science (1992)

Temperature gradient G

Growth velocity V

Solute concentration C_0

Solid   Liquid
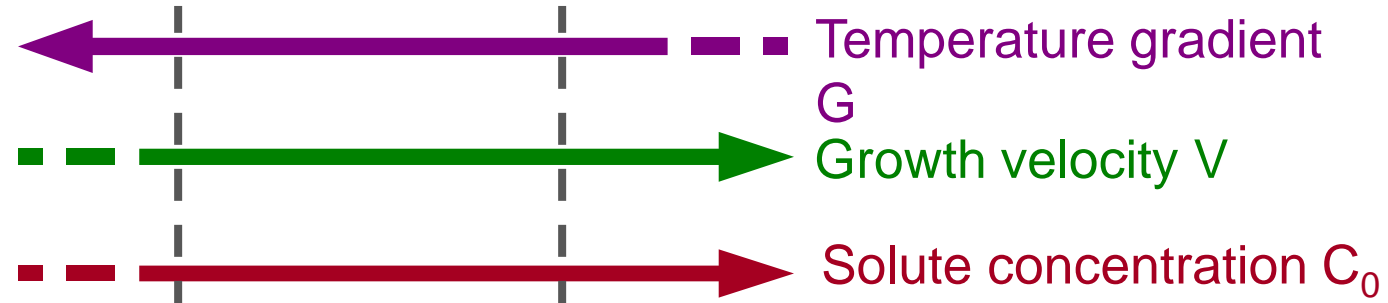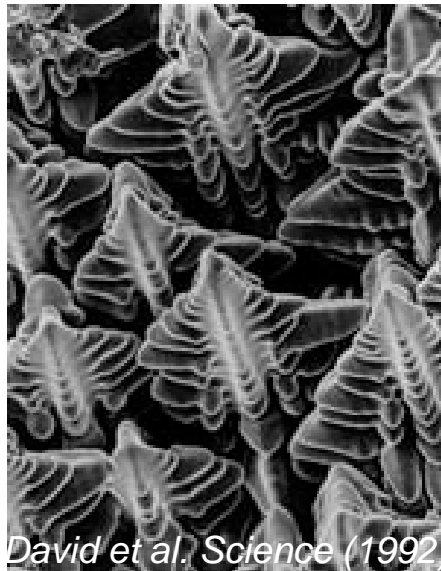
Losert, Shi, and Cummins (1998)

Constitutional supercooling

$$V > \frac{kDG}{mC_0(1-k)}$$

THE WORLD COMES HERE

TMS 2020
149th Annual Meeting & Exhibition

CO-LOCATED INTERNATIONAL CONFERENCE

PbZn 2020

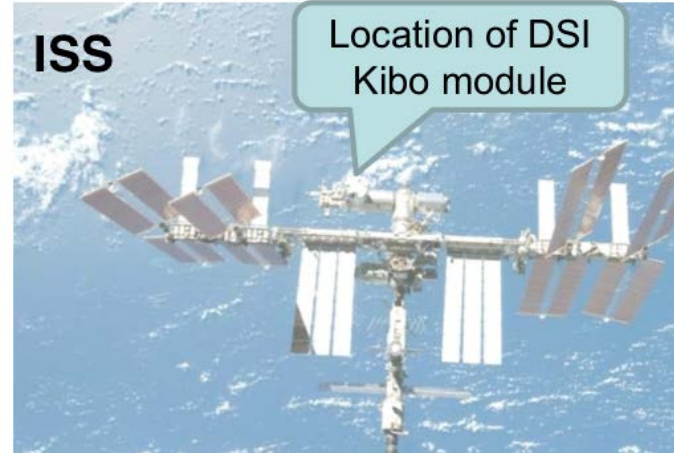February 23-27, 2020
San Diego, California, USA
#TMSAnnualMeeting

2

Microgravity experiments – diffusive regime

Gravity-induced convection

Microstructure heterogeneities

Microgravity experiment

Location of DSI Kibo module
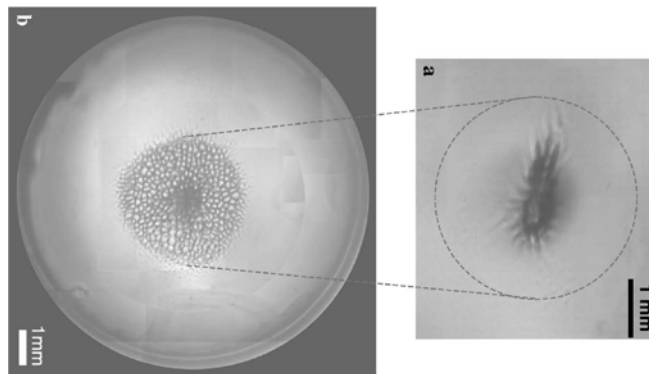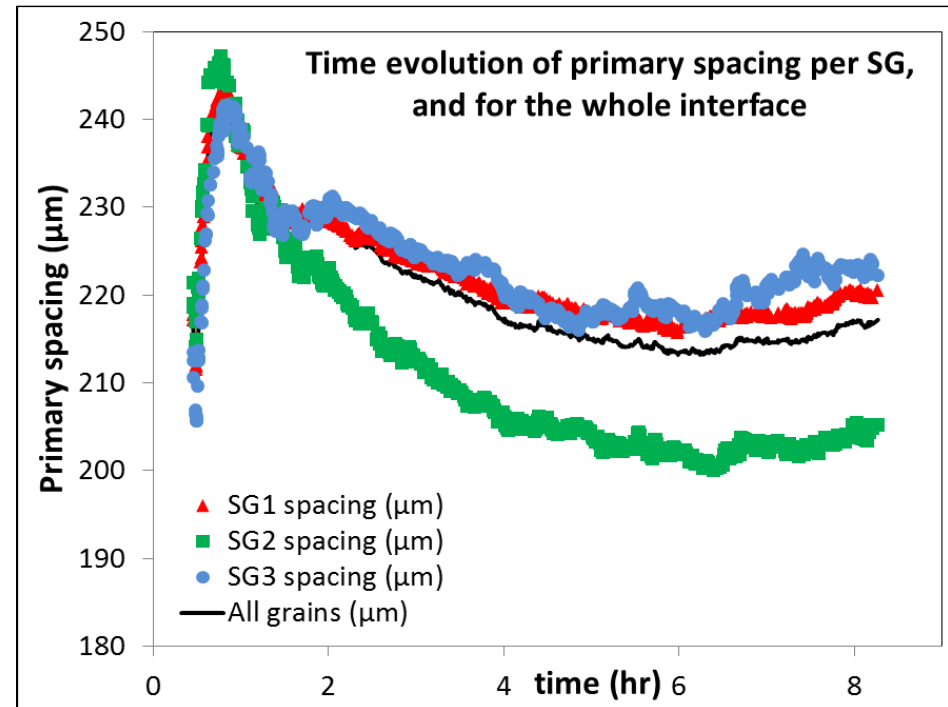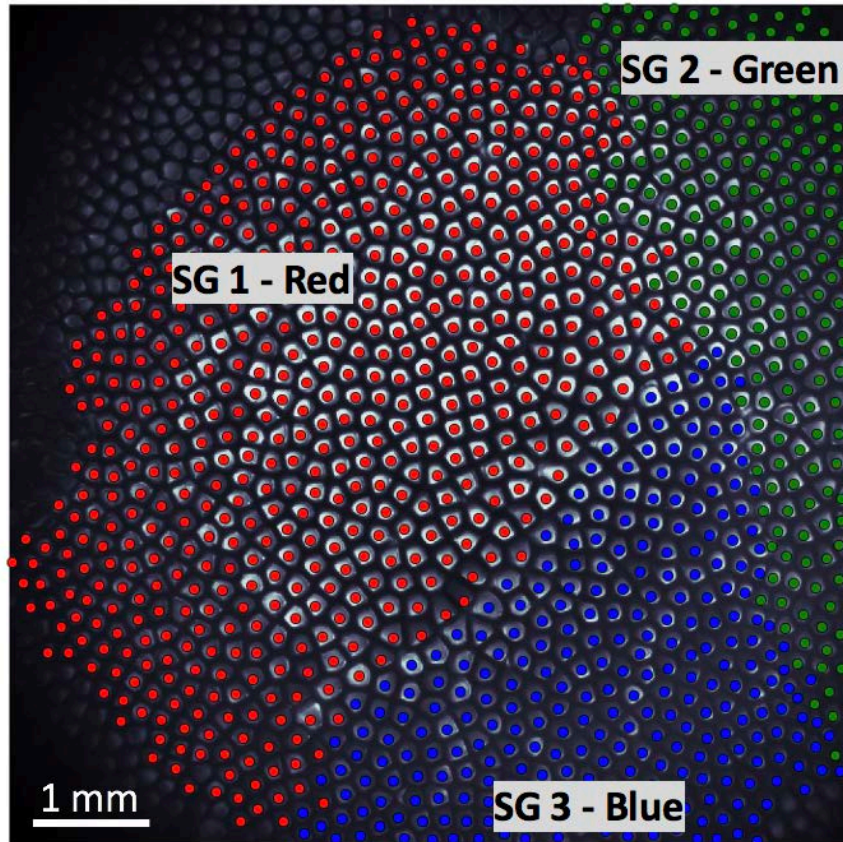
ISS
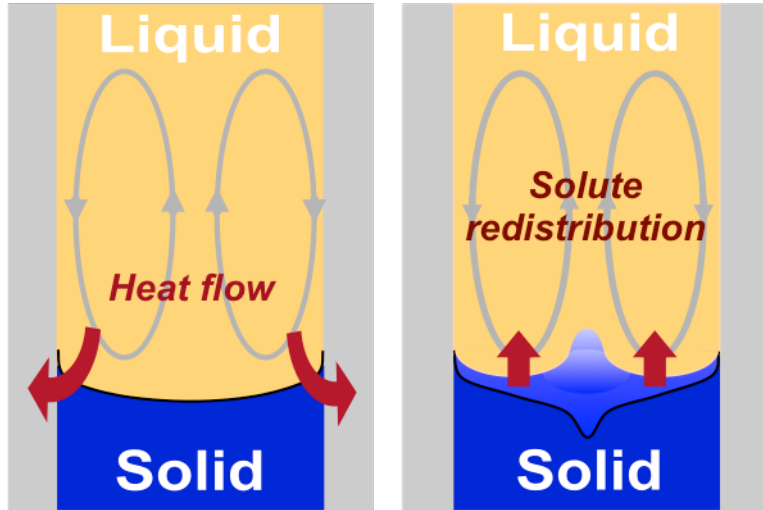
Two campaigns:
- Microgravity experiments from 2009-2011 dedicated to cellular regime.
- Microgravity experiments from 2017-2018 dedicated to dendritic regime.

DSI
(**D**irectional **S**olidification **I**nsert)

DECLIC

THE WORLD COMES HERE
TMS2020
149th Annual Meeting & Exhibition

CO-LOCATED INTERNATIONAL CONFERENCE
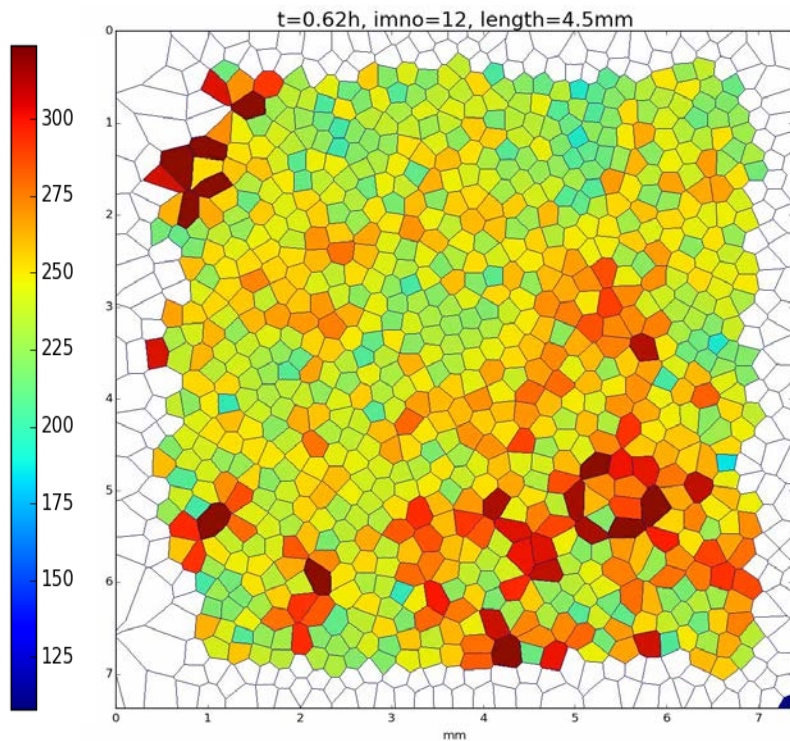PbZn 2020

February 23-27, 2020
San Diego, California, USA
#TMSAnnualMeeting

3

Polycrystalline solidification
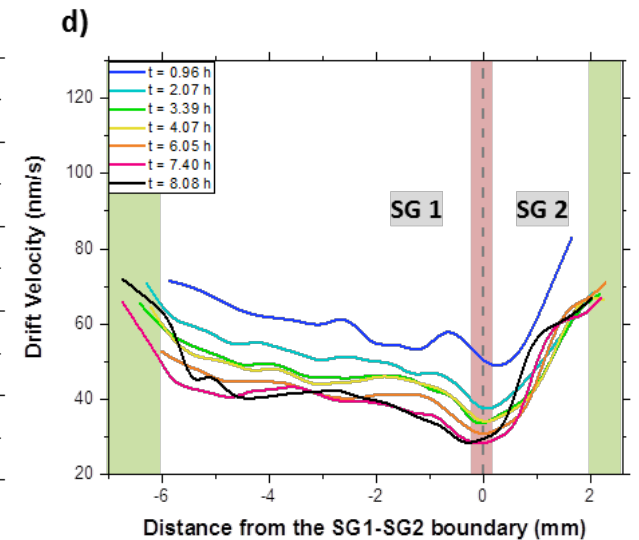

SCN-0.24wt% Camphor, G = 19 K/cm, V = 2 μm/s


- Noticeable primary spacing evolution depending on sub-grain.

- Cannot be attributed to the misorientation ($1.4° < \theta_g < 1.9°$)

THE WORLD COMES HERE
TMS 2020
149th Annual Meeting & Exhibition

CO-LOCATED INTERNATIONAL CONFERENCE

PbZn 2020

February 23-27, 2020
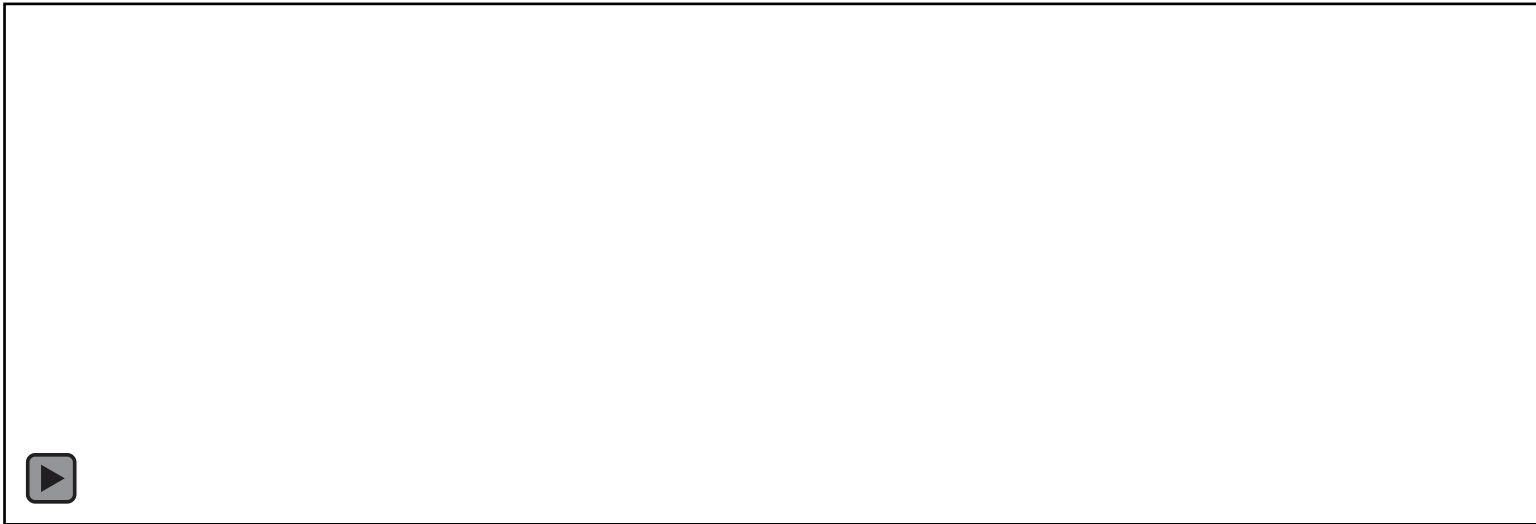San Diego, California, USA
#TMSAnnualMeeting
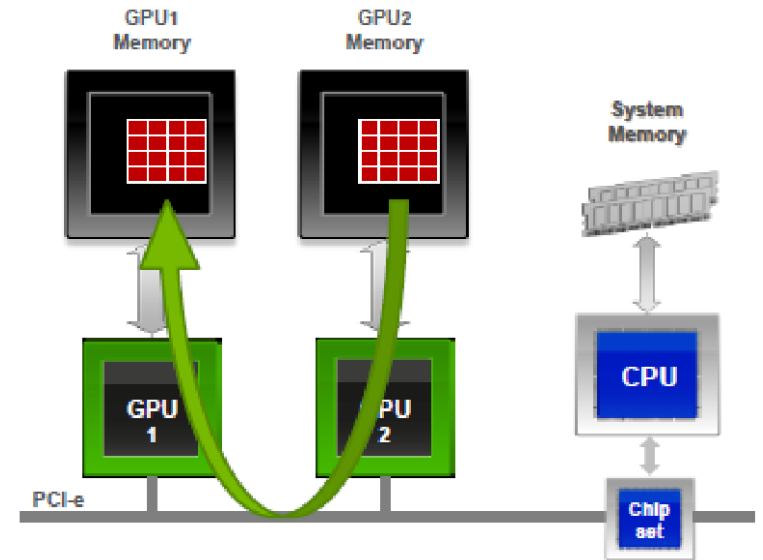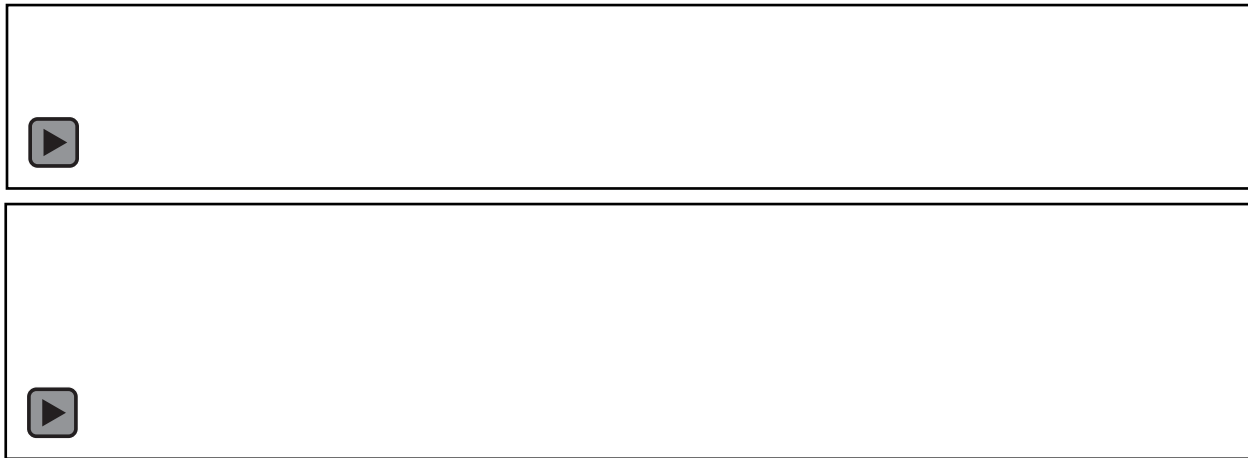
4

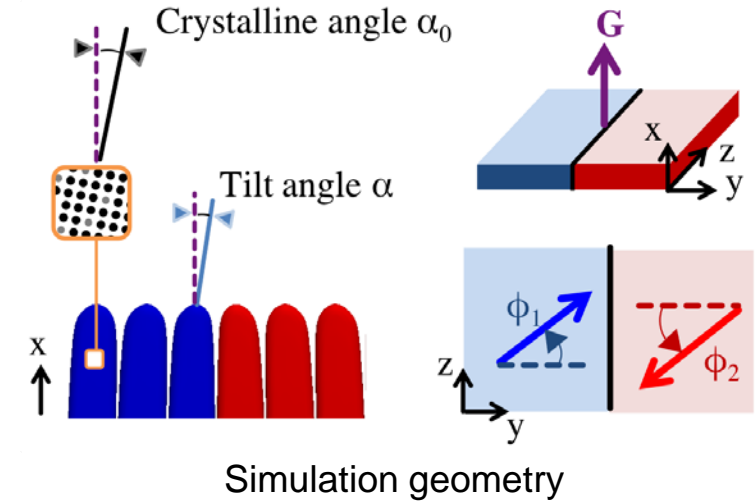# Effects of sub-grain boundaries

- Initially: large spacing with homogeneous distribution.
- With time: global decrease of spacing except at a divergent sub-grain boundary.
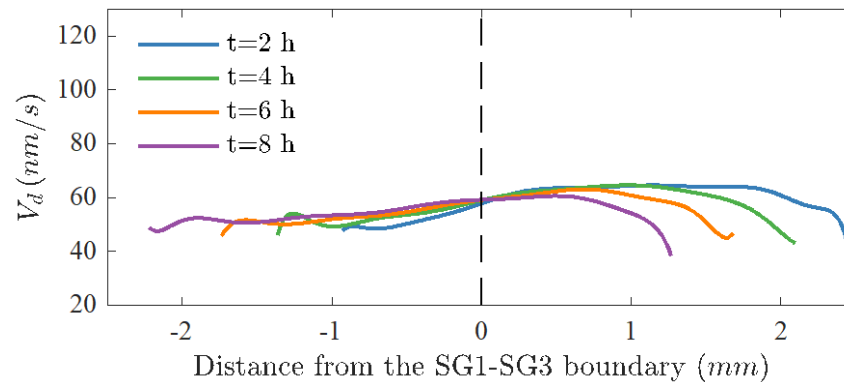
Phase-field simulation

60 μm

Simulation geometry
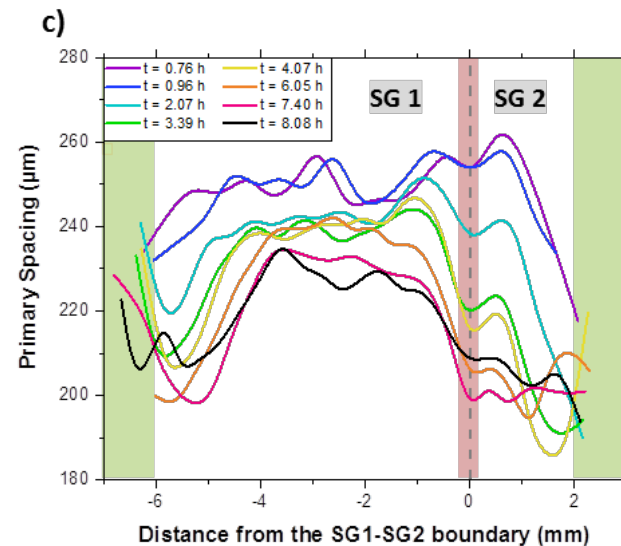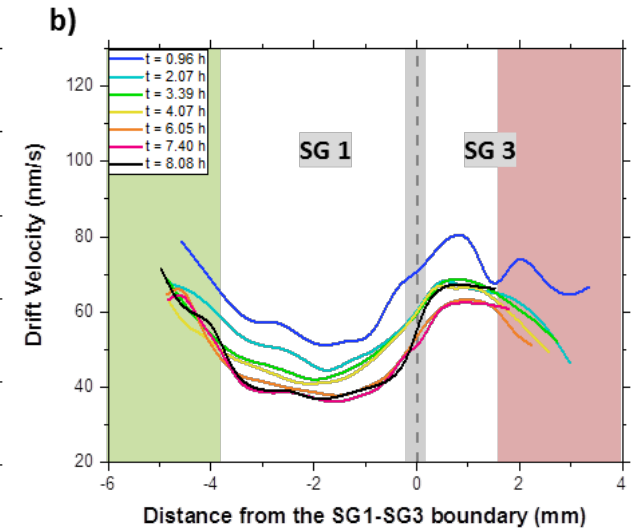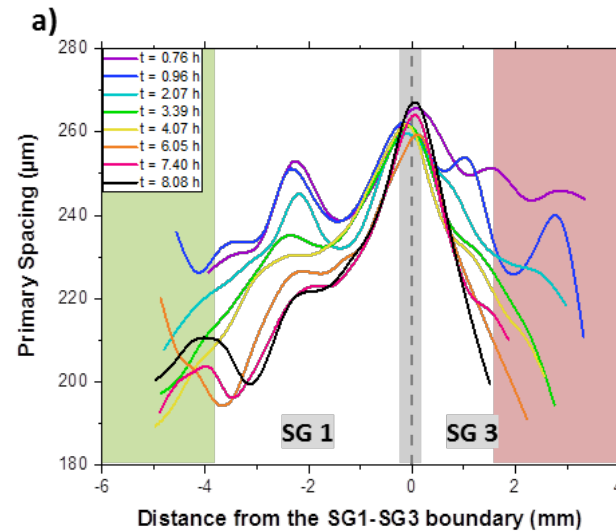
Multi-GPU intra-node communication

Simulation of SCN-0.24wt% Camphor, G = 19 K/cm, V = 2 μm/s over 4 hours
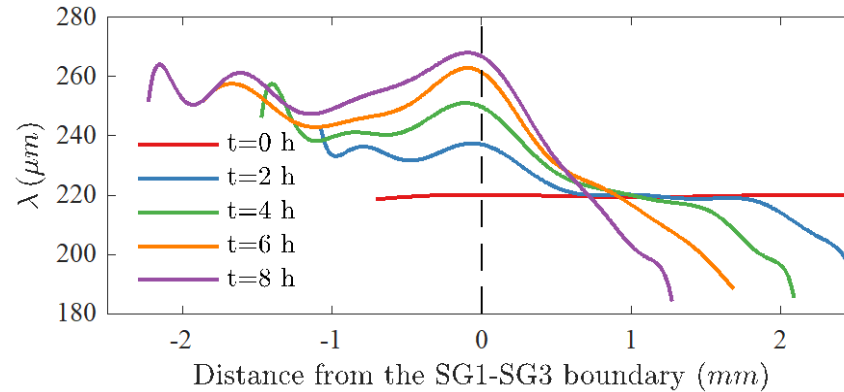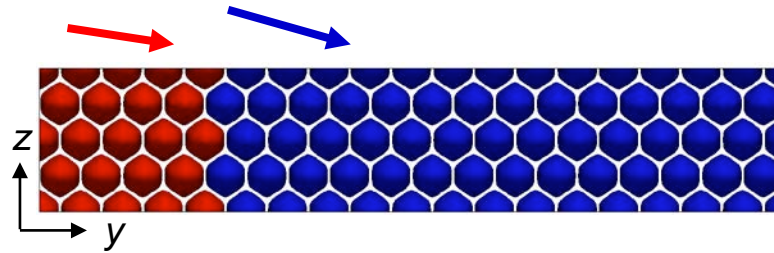
Divergent sub-grain boundary

- Peak of primary spacing at the divergent sub-grain boundary (*same as experiments*).

- A plateau with the increasing spacing (*different from experiments*).

- A source on the left that produces larger cells.

Regular hexagonal array

Irregular hexagonal array

Effect of a source

Spacing distribution · **Drifting velocity** · **Microstructures**

Master curve

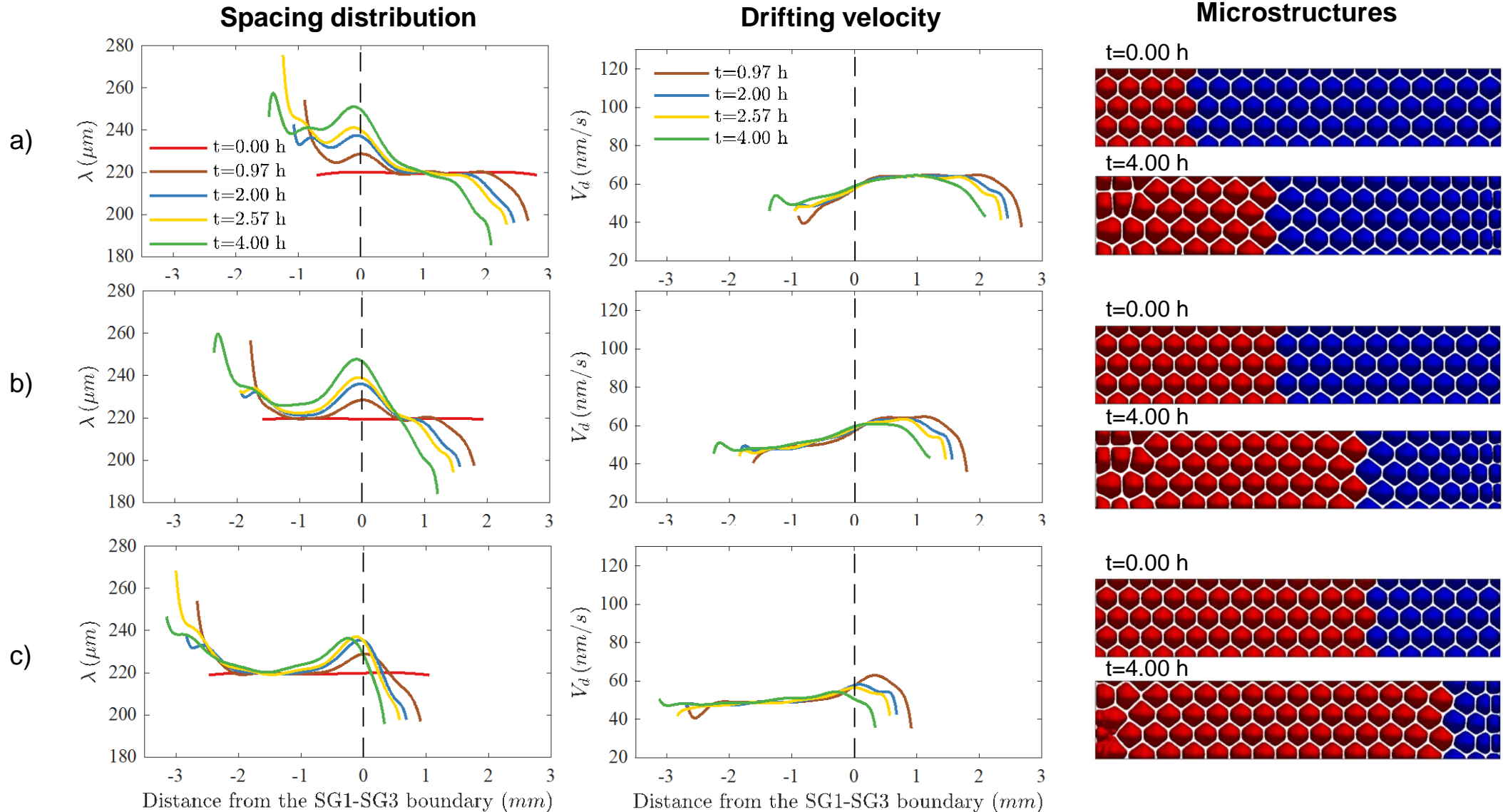- The ratio θ_g/θ_0 between the cell-tilt angle and the misorientation angle is a function of the Péclet number Pe (**master curve**).

- The master curve is independent of the misorientation angle θ_0.

- The master can be fitted by a phenomenological function with constants f an g.

$$\frac{\theta_g}{\theta_0} \equiv F(\mathrm{Pe}) = 1 - \frac{1}{1 + f\mathrm{Pe}^g}$$

Misorientation angle θ_0

Tilt angle θ_g

z

y

x

y *Song el al. Phys Rev Mat (2018)*
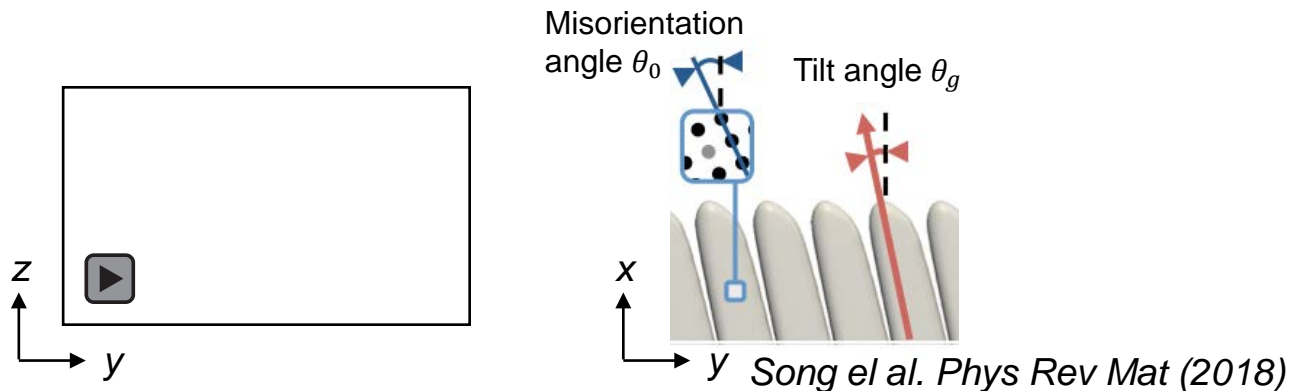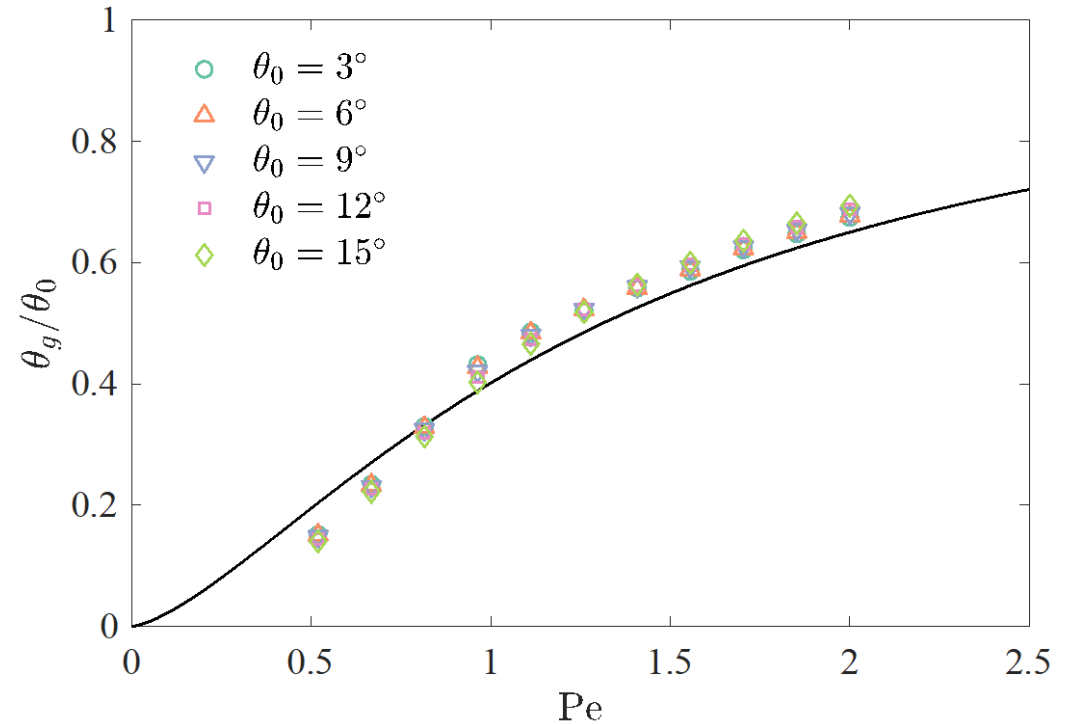
Deschamps, Georgelin and Pocheau, PRE (2008)

Plot legend:
- $\theta_0 = 3°$
- $\theta_0 = 6°$
- $\theta_0 = 9°$
- $\theta_0 = 12°$
- $\theta_0 = 15°$

θ_g/θ_0 vs Pe

Effect of a divergent sub-grain boundary

- The divergent sub-grain boundary can damp the drifting velocities of nearby cells in SG 3 (blue), which have large *Pe* and are placed below the master curve.

- The divergent sub-grain boundary can boost the drifting velocities of nearby cells in SG 1 (red), which have large *Pe* and are placed above the master curve.

- The phase diffusion generically relaxes spatially modulated nonequilibrium patterns towards a spatially uniform spacing:

$$\frac{\partial \lambda}{\partial t} = D_\lambda \frac{\partial^2 \lambda}{\partial y^2}$$
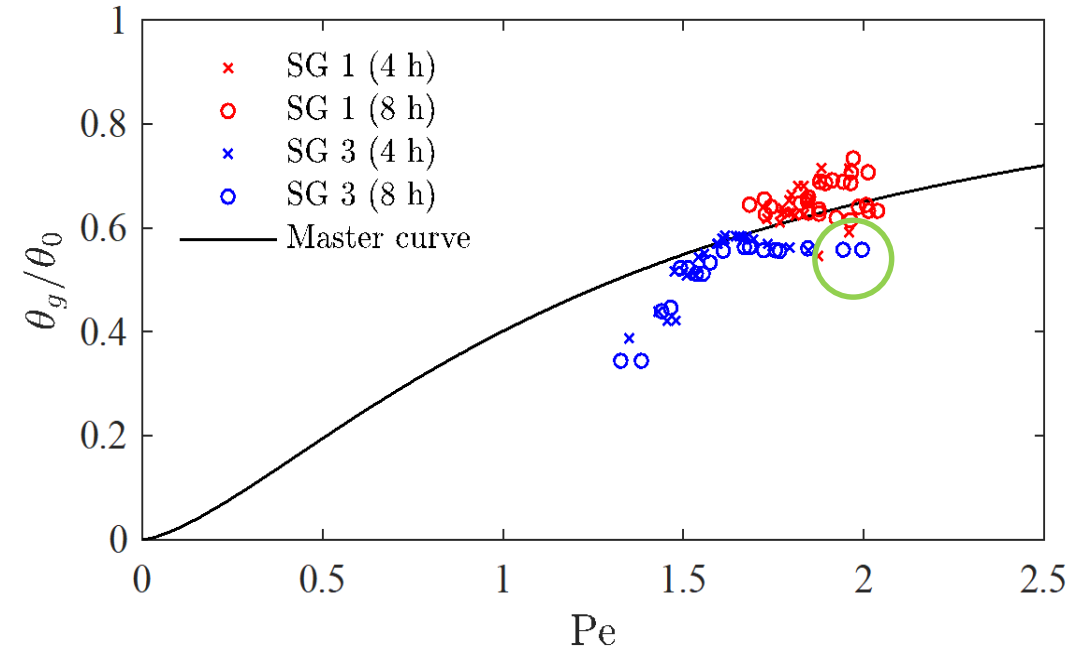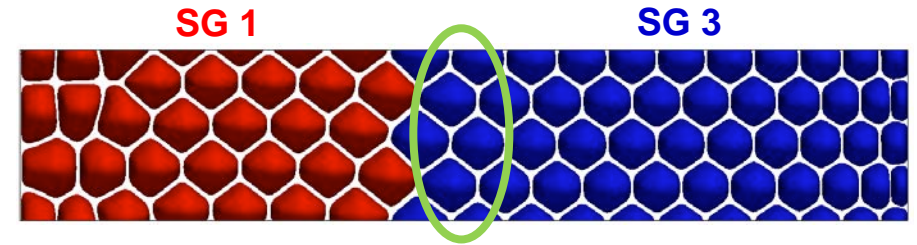
Effect of a convergent sub-grain boundary
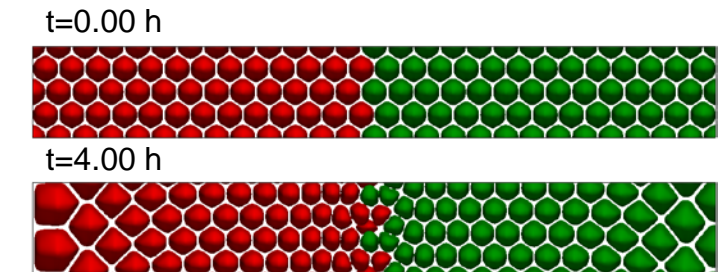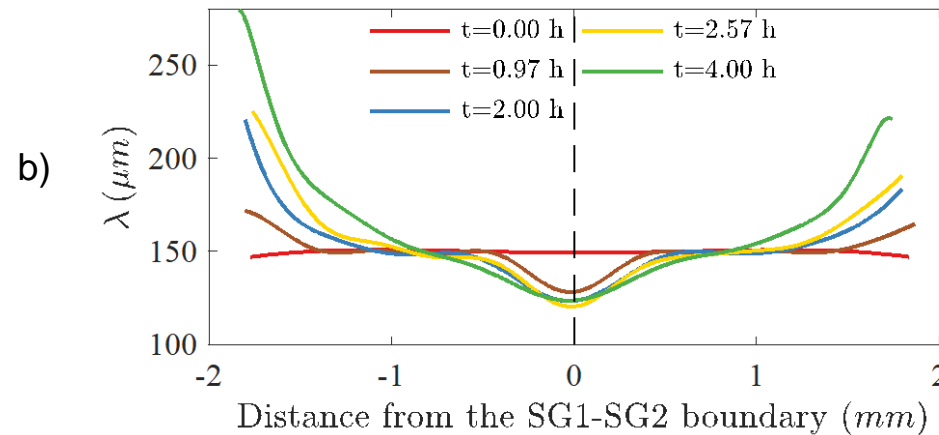
- The primary spacing decreases about 60 µm at a convergent sub-grain boundary in simulation, whereas 30 µm in experiments.

- Different stable spacing ranges.

- Different types of grain competition, elimination or invasion.

Spacing distribution

Microstructures
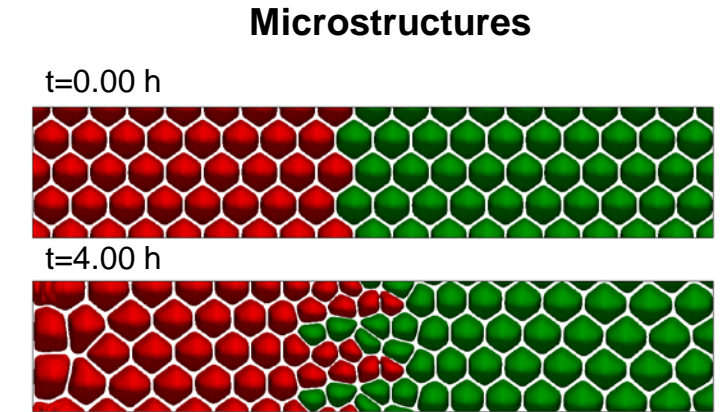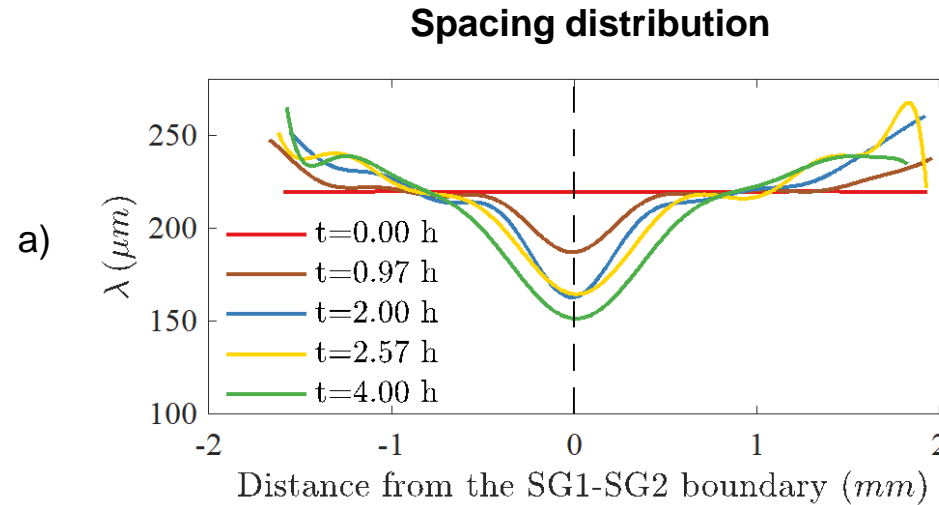
DSI-R: dedicated to the dendritic regime

- Increase the concentration from SCN-0.24wt% Camphor to **SCN-0.46wt% Camphor**. Dendrites form at lower pulling velocity.
- Study of the formation of well-developed dendritic array structures.

V = 1.5 µm/s, G = 12 K/cm

Camera : HR2

V = 6 µm/s, G = 12 K/cm

Camera : HR2
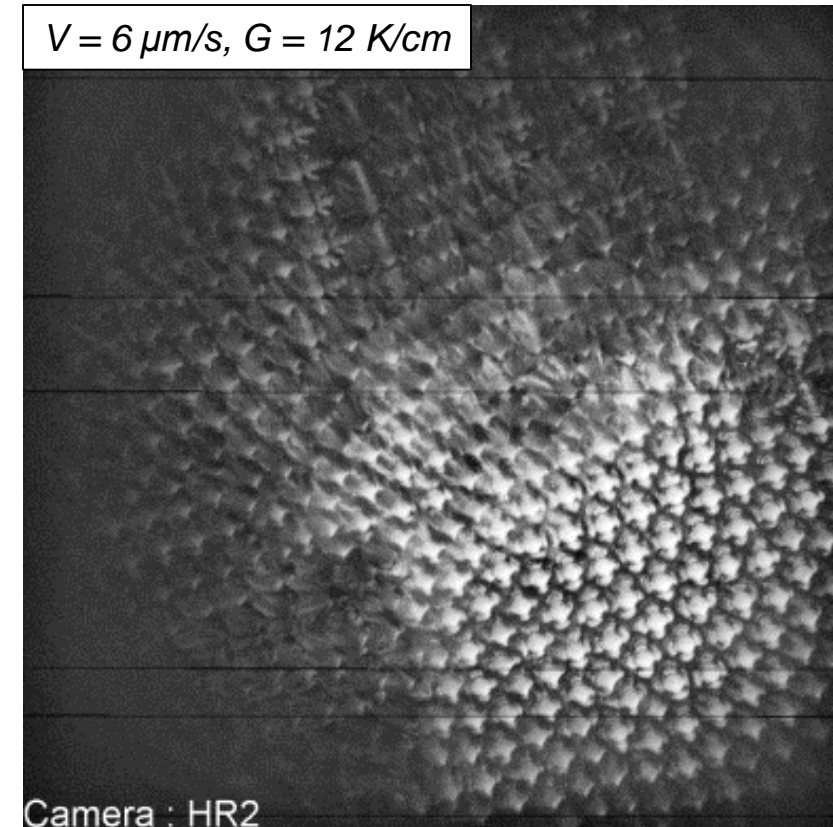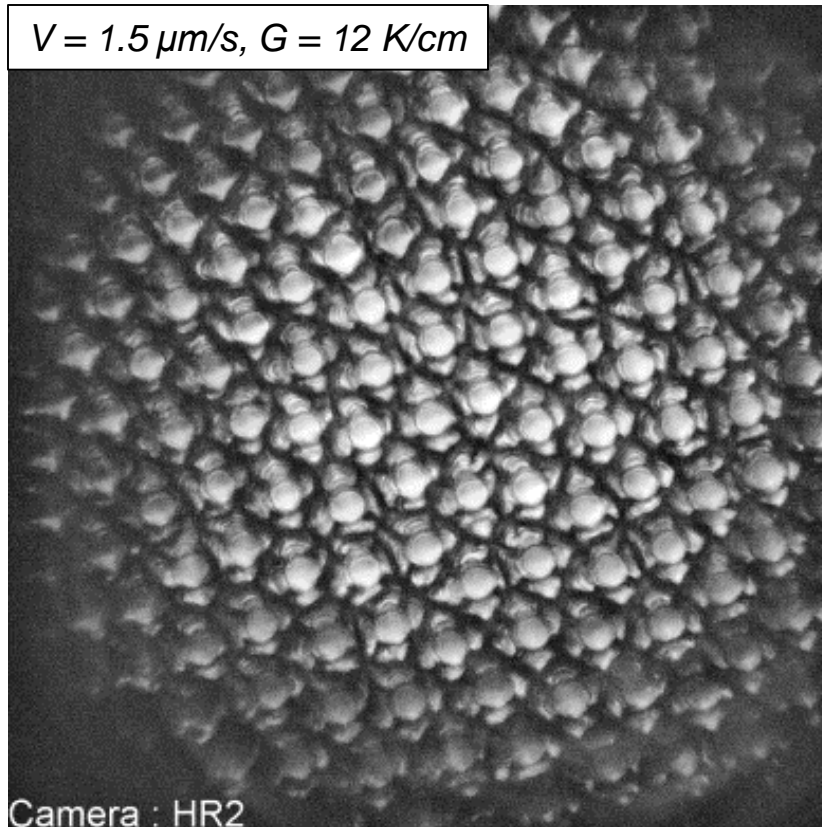
Summary

- Both the divergent and convergent sub-grain boundaries can affect the microstructure evolution during directional solidification of binary alloys, including the primary spacing distribution and the drifting velocity profile.

- Phase-field simulations at experimentally relevant length and time scales show similar results as experiments for a divergent boundary, including the peak and distribution of primary spacing.

- The differences between simulations and experiments are because of a source of cells. In the simulation, a source can produce large cells and lead to an increasing plateau; in the experiment, the small cells are generated near the crucible boarder and leads to a decreasing plateau.

- Near a convergent sub-grain boundary, the differences between simulations and experiments stems from the difference in stable ranges of cell spacings, which leads to different types of grain competition (elimination versus invasion).

THE WORLD COMES HERE
TMS 2020
149th Annual Meeting & Exhibition

CO-LOCATED INTERNATIONAL CONFERENCE
PbZn 2020

February 23-27, 2020
San Diego, California, USA
#TMSAnnualMeeting

13

Outlook

- Investigate the pulling velocity jump and the history dependence of a dendritic pattern.

- Investigate the thermal diffusivity that varies with the distance from the crucible wall. The spatial dependent thermal diffusivity could affect primary spacing selection and the evolution of an interface curvature in the experiments.

- Experimental observations and phase-field simulations reveal that the selected pattern at a divergent sub-grain boundary is different from the initially selected pattern near the center region of the crucible. The pattern adjustment could come from the drifting dynamics of misoriented grains.
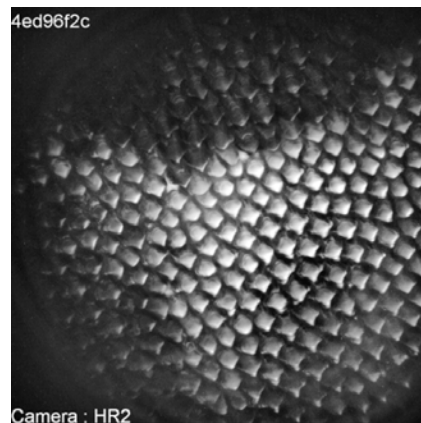
SCN-0.46wt% Camphor, G = 12 K/cm, V = 2 μm/s
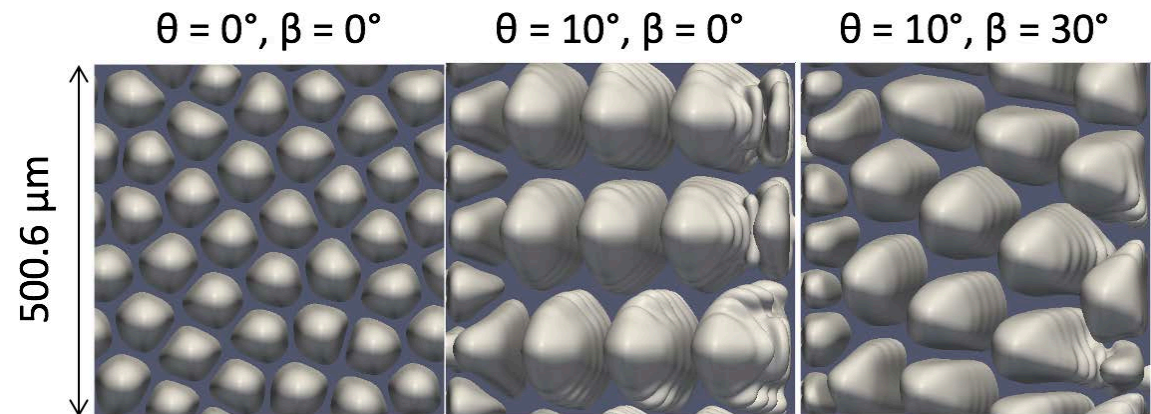
Acknowledgement

Kaihua Ji, Y. Song*, A. Karma
Northeastern University

F.L. Mota, J. Pereda,
N. Bergeon
Aix-Marseillé Université

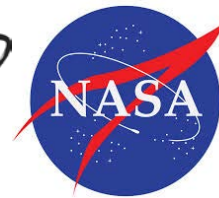T. Lyons, R. Trivedi
Iowa state University

L.L. Strutzenberg
Marshall Space Flight Center

*Current address: Oak Ridge National Laboratory

THE WORLD COMES HERE
TMS 2020
149th Annual Meeting & Exhibition

CO-LOCATED INTERNATIONAL CONFERENCE
PbZn 2020

February 23-27, 2020
San Diego, California, USA
#TMSAnnualMeeting

15

Thank you
for your attention