Designing a Phase Field Model of a Spiral Eutectic

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Abstract

When a liquid mixture of Mg and Zn that is 97wt.% Zn is cooled past a critical point it unexpectedly forms an MgZn2-Zn spiral eutectic. Understanding how this spiral eutectic forms is essential for scaling up its manufacture, opening up the mass production of a new form of metamaterials. Previous studies indicated that the mechanism occurred at longer time and length scales than are accessible through molecular dynamics. This project designs and implements a phase field model (PFM) that accesses these time and length scales, which will enable future studies of spiral eutectics.

Introduction and Background

- Spiral eutectics are able to act as metamaterials, which are materials that bend EM waves backwards.
- A mixture of 97wt.% Zinc and 3wt.% Magnesium would theoretically crystalize into a eutectic of $Zn_{11}Mg_2$ and Zn. [1]
- Ultimately, the goal of this project is to determine if a proposed growth mechanism of the spiral eutectic is accurate.

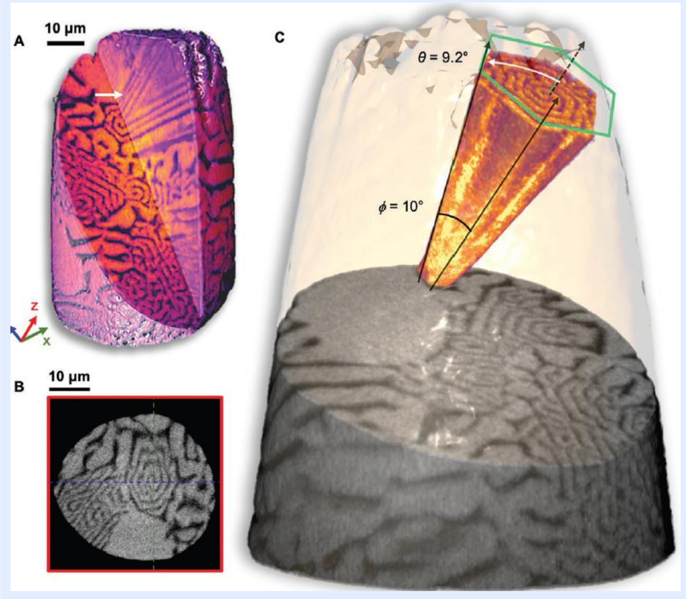
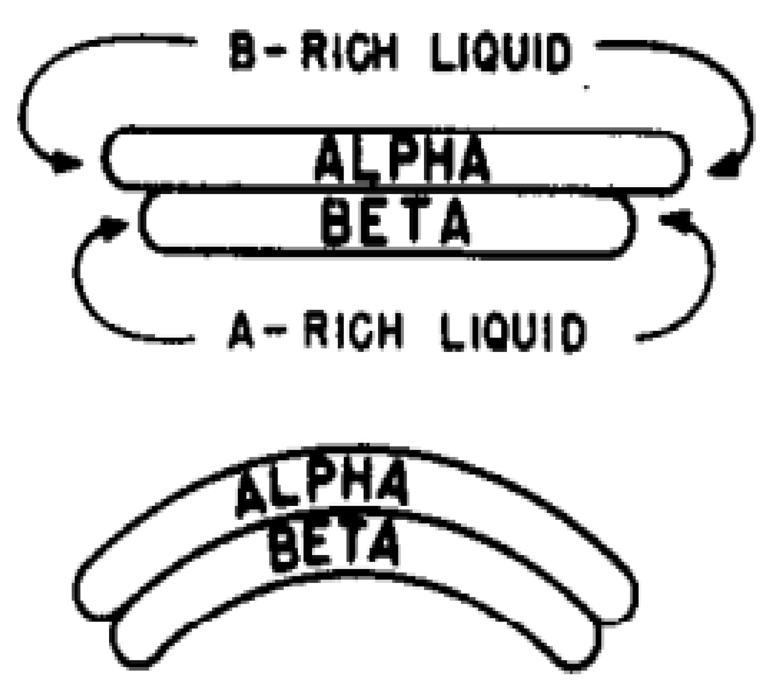


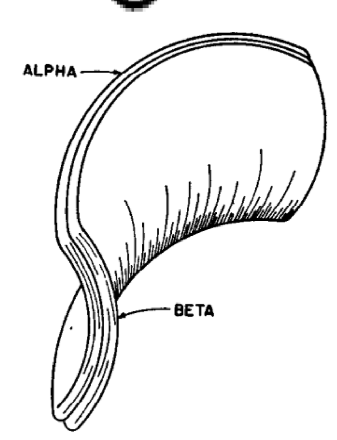
Figure 1: X-ray topography of Spiral Eutectic [2]

Proposed Mechanisms

- Moniri et al. provided evidence from in situ microscopies that a Zn-Mg alloy system exhibits phase separation and metastable crystal nucleation in ways that lead to spiral microstructures of a MgZn2 eutectic with Zn forming on the ledges of the steps of the spiral. [2]



- A previous study out of the 1950s studied the Mg-Zn spiral eutectic in depth, where they proposed that a different in growth rates at different angles between two phases could lead to spiral growth. [3]



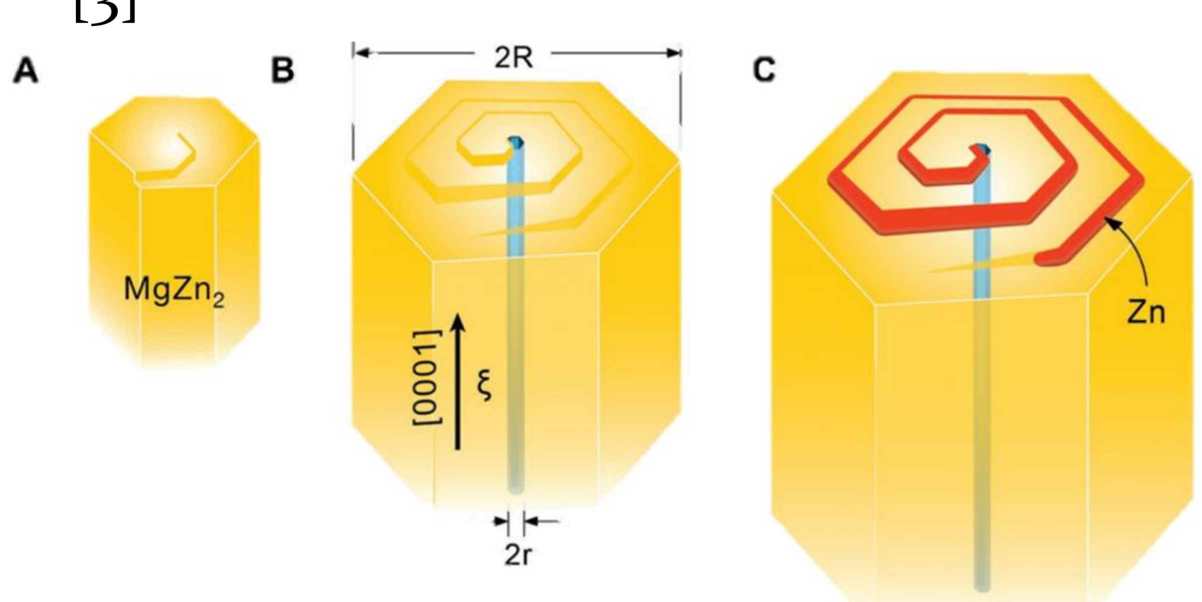


Figure 1: Proposed mechanisms for $MgZn_2$-Zn spiral eutectic formation from [2] (left) and [3] (above).

Phase Field Model

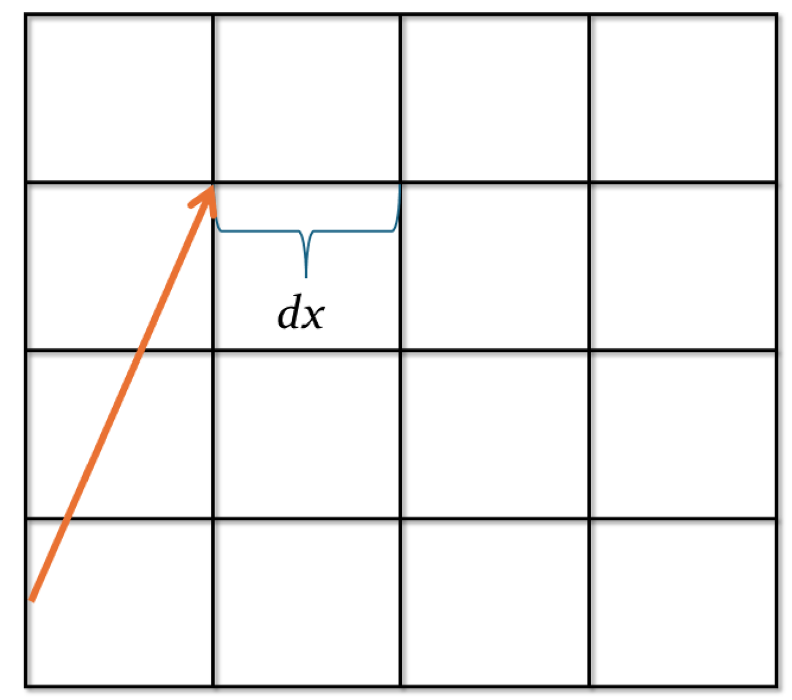
Setup:

- Grid of initial conditions for $\tilde{c},u$
- Some spacing of dx
- Some timestep dt

(Right) Representation of the setup

Some position x,y

Has values for $\tilde{c},u$



Algorithm 1 Cahn Hilliard Evolution

```
dt = timestep
size = dimension of grid
grid[0][size][size] = c initial values
grid[1][size][size] = u initial values
for time = 0 to final timestep do
    for x,y = all spaces in grid do
        time derivative c[x][y] = Cahn Hilliard c(grid)
        time derivative u[x][y] = Cahn Hilliard u(grid)
    end for
    grid[0] = grid[0] + time derivative c * dt
    grid[1] = grid[1] + time derivative u * dt
end for
```

Equations and Algorithm

$$f_{sol} = \frac{1}{8}(u^2-1)^2 + (\tilde{c}ln(\tilde{c}) - \tilde{c}) - ln(K)\tilde{c} - \frac{\Delta T}{T_E}$$

$$f_{liq} = \frac{1}{2}u^2 + (\tilde{c}ln(\tilde{c}) - \tilde{c})$$

$$f = h(\phi)f_{sol} + (1-h(\phi))f_{liq}$$

Equation 1: Free Energy for Solid, Liquid, and Overall [4]

$$\frac{\partial u}{\partial t} = \nabla \cdot \left[M\nabla\left(\frac{\partial f}{\partial u} - W_u^2\nabla^2 u\right)\right]$$

$$\frac{\partial \tilde{c}}{\partial t} = \nabla \cdot \left[\tilde{M}\nabla\left(\frac{\partial f}{\partial \tilde{c}}\right)\right]$$

Equation 2: Cahn-Hilliard Equation [4]

Future Work

- Refine starting conditions and determine reasonable ranges for grid size, undercooling, and timestep.
- Build out visualization tools, including individual time step visualizers of different phase parameters, difference mappings, and movies showing evolving parameters.

Figure 2: Examples of Eutectic Growth in PFM [4]

Left: Scan the QR code for the updated GitHub repository.

Citations

[1] P Ghosh, M Mezbahul-Islam, and M Medraj. Critical assessment and thermodynamic modeling of mg–zn, mg–sn, sn–zn and mg–sn–zn systems. Calphad, 36:28–43, 2012.

[3] Saman Moniri, Hrishikesh Bale, Tobias Volkenandt, Yeqing Wang, Jianrong Gao, Tianxiang Lu, Kai Sun, Robert O Ritchie, and Ashwin J Shahani. Multi-step crystallization of self-organized spiral eutectics. Small, 16:1906146, 2020.

[3] R. L. Fullman and D. L. Wood. Origin of spiral eutectic structures. ACTA METALLURGICA, 2:188–193, 3 1954.

[4] Arka Lahiri, Chandrashekhar Tiwary, Kamanio Chattopadhyay, and Abhik Choudhury. Eutectic colony formation in systems with interfacial energy anisotropy: A phase field study. Computational Materials Science, 130:109–120, 4 2017. 2