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静電浮遊中の Fe-Cu 液滴の相形成における液相分離と熱流動のシミュレーション

Modeling of liquid phase separation and thermofluidics in levitated Fe-Cu droplets

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1. Introduction

For reliable and stable supply of renewable energy, various energy storage systems are being developed. One method is using phase change materials (PCMs) for the Thermal Energy Storage (TES); the use of immiscible alloys as PCMs can increase energy efficiency and sustainability. The purpose of the *Thermal Storage* Project is to obtain accurate thermophysical properties of alloys, necessary for the comprehensive engineering design of TES. In the *TS* project, experiments were conducted to measure the thermophysical properties of immiscible Fe-Cu alloys melted in the Electrostatic Levitation Furnace (ELF) on the International Space Station. The supercooled immiscible Fe-Cu alloy separates into two liquid phases, an Fe-rich phase and a Cu-rich phase. Supercooling has been confirmed in ELF experiments from recorded camera images and temperature history. The thermophysical properties obtained strongly dependent on which phase is exposed on the surface of the droplet. As it is not feasible to identify the phase during the experiment due to opaqueness, it is imperative to predict the phase separation state through simulation.

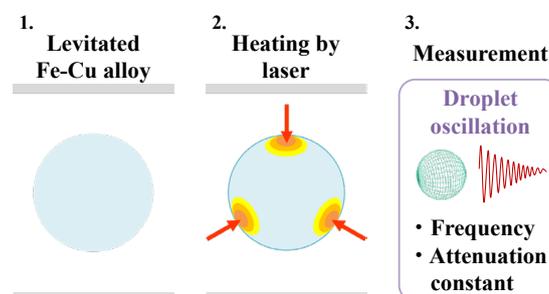


Fig 1. ELF Experiment Overview

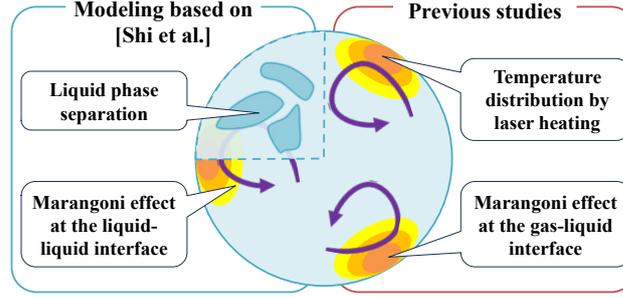


Fig 2. Four elemental models

2. Model formulation

For simulations of ELF experiments, the physical model must involve heat transfer based on laser heating, the Marangoni effect at the gas-liquid interface, the Marangoni effect at the liquid-liquid interface, and liquid phase separation by spinodal decomposition. Regarding the heat transfer with laser heating and the Marangoni effect on the gas-liquid interface, physical models have been developed in previous studies by author's research group ¹⁾. In contrast, the models for liquid-liquid phase separation and the Marangoni effect at the liquid-liquid interface are newly developed in the present study, according to the work done by Shi et al. ²⁾. The following governing equations are considered in this study.

$$\nabla \cdot \mathbf{u} = 0, \quad (1)$$

$$\rho \frac{\partial \mathbf{u}}{\partial t} + \nabla \rho \cdot (\mathbf{u}\mathbf{u}) = \rho \mathbf{g} + \nabla^2(\mu\mathbf{u}) + \nabla \cdot \boldsymbol{\tau}, \quad (2)$$

$$\frac{\partial T}{\partial t} + \nabla \cdot (\mathbf{u}T) = \nabla \cdot (\alpha \nabla T), \quad (3)$$

$$\frac{\partial c}{\partial t} + \nabla \cdot (\mathbf{u}c) = M_c \nabla^2 \left(\frac{\partial G_m^{liq}}{\partial c} - 2\kappa \nabla^2 c \right) + \zeta_c, \quad (4)$$

where \mathbf{u} is velocity, ρ is density, $\boldsymbol{\tau}$ is stress tensor acting at the liquid-liquid interface, T is the temperature, α is the thermal diffusivity, c is the concentration of Cu, M_c is the mobility of atomic diffusion, κ is the concentration gradient energy coefficient, and ζ_c is the thermal fluctuation. The aforementioned physical model was implemented in OpenFOAM, an open-source computational fluid dynamics framework.

3. Simulation results

Figure 3 shows three snapshots extracted from the calculation results. The simulation conditions for the ELF experiment were set to an initial concentration of $c_0 = 0.5$ and a droplet diameter of 2 mm, and the boundary conditions of laser heating and the Marangoni effect at the gas-liquid interface were considered in the simulation. From the simulation results, it is predicted that the Cu-rich and Fe-rich phases may exhibit complex time evolution of separation and merging.

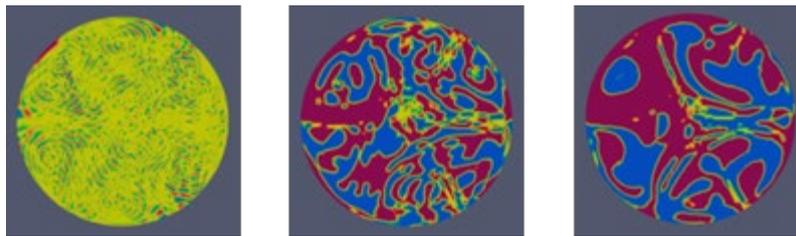


Fig 3. Simulation for ELF experiment

References

- 1) R.P. Shi et al., Acta Mat. 61(4), p.1229 (2013). DOI: [10.1016/j.actamat.2012.10.033](https://doi.org/10.1016/j.actamat.2012.10.033)
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