Quantitative Analysis of Solidification Interface in Al-Cu Alloy using Time-Resolved X-ray Tomography

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Abstract: Accurate evaluation of permeability (K) in the mushy zone is essential for simulating macrosegregation during casting processes, yet it remains difficult due to the complex interface morphology. In this study, time-resolved X-ray tomography (4D-CT) was used to observe the solidification in Al－10mass%Cu alloys under various cooling conditions, enabling in situ three-dimensional reconstruction of dendritic structures. To enhance the quantitative analysis of solid-liquid interfaces, a phase-field-based image filter was applied to suppress high-frequency noise and accurately extract parameters such as interfacial area and curvatures. Based on these, machine learning models were trained to predict permeability from solid fraction and cooling rate, with the random forest model achieving the highest accuracy. This approach supports more reliable permeability estimation for casting simulations.

Keywords: dendritic structure, solidification interface; permeability; time-resolved X-ray tomography; machine learning; Al-Cu alloy; mushy zone; phase field model

1 Introduction

Macrosegregation caused by solute redistribution in the mushy zone severely affects the mechanical properties of cast alloys [1]. Accurate estimation of permeability ($\boldsymbol{K}$), which governs fluid transport in the dendritic networks, is critical for simulating and mitigating macrosegregation [2]. In this study, we employed time-resolved X-ray tomography (4D-CT) to visualize the solidification of Al-10 mass%Cu alloys under various cooling rates. A phase-field-based image filter was applied to reduce noise in the reconstructed images and improve the accuracy of morphological analysis. The extracted parameters were used to predict permeability using machine learning, contributing to the reliable simulation of solidification phenomena.

Since permeability is a key input for Darcy-based flow models in mushy zones, its accurate prediction enables more realistic numerical simulation of liquid flow through the dendritic network and solute transport during solidification, which are essential for assessing macrosegregation behavior.

2 Experimental Methods

2.1 Experimental Setup

Al-10mass%Cu samples (10 mm dia.) were solidified under various cooling conditions using time-resolved interior tomography (interior 4D-CT) at the BL20B2 beamline (SPring-8) [3-6] (Figs. 1 and 2) Phase-field filtering was applied to reduce artifacts induced in the reconstructed data. The morphological parameters, including solid fraction, specific interface area (interface area per unit volume), and curvatures were extracted for quantitative analysis of permeability using the Kozeny-Carman model [7,8]:

$$\boldsymbol{K} = \frac{(1-f_s)^3}{k_c S_s^2 f_s^2} \tag{1}$$

where $\boldsymbol{k_c}$ is a shape factor and $\boldsymbol{S_s}$ is the specific interface area of the solid-liquid interface. Evaluation of solid-liquid interface area, $\boldsymbol{S_s}$, as a function of solid fraction is advantageous because it is impossible to measure $\boldsymbol{S_s}$ from the microstructure observation after solidification. The reliable estimation through the advanced imaging technique and the prediction modeling is essential for accurate permeability prediction [9].

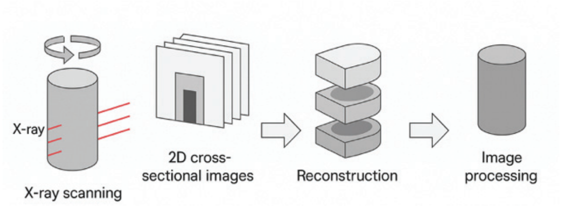


Fig. 1. Schematic of the experimental setup for time-resolved X-ray tomography

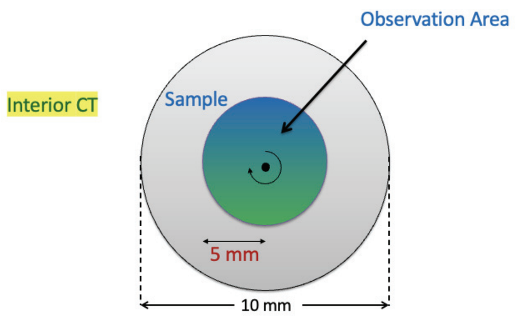


Fig. 2. Schematic of Interior CT [10-12]

The solidification processes under various cooling conditions were studied to investigate the effect of cooling conditions on the permeability and the interface morphology. The cooling scenarios included:

1. Continuous cooling at constant rates of 8 K/min, 16 K/min, 20 K/min, 30 K/min, and 40 K/min.
2. Multi-step cooling, where the cooling rate was adjusted during solidification (e.g., 16 K/min → 4 K/min → 16 K/min).

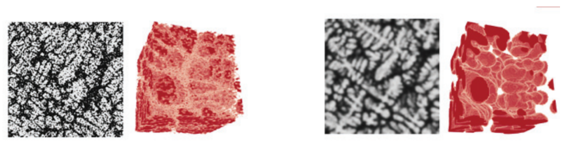
2.2 Phase-Field Filtering and Image Processing [13-15]

To improve the accuracy of interfacial property extraction, we adopted a phase-field model-based image processing technique (PFF). This method uses the curvature-driven evolution of the phase field variable φ to smooth noisy 3D reconstructions obtained from 4D-CT imaging. The evolution is governed by the following time-dependent equation [16, 17]:

$$\Delta\phi = -3\sqrt{2}\sigma\delta(M\Delta t)\left[\frac{2\sqrt{2}}{\delta r_0}\phi(1-\phi) + \frac{2}{\delta^2}\phi(1-\phi)(1-2\phi)w - \nabla^2\phi\right] \qquad (2)$$

This expression allows the computation of the temporal evolution of $\boldsymbol{\phi}$ by setting values for interfacial energy $\boldsymbol{\sigma}$, interface thickness $\boldsymbol{\delta}$, radius $\boldsymbol{r_0}$, interface mobility $\boldsymbol{M}$, and time step $\Delta\boldsymbol{t}$. Here $\boldsymbol{w}$ is a coefficient controlling the depth of the potential well.

As shown in Fig.3, this filtering procedures significantly reduced artifacts and enabled accurate curvature and interface area quantification.



(a) (b)

Fig.3 Example of 4D-CT observation of solidification in Al-Cu alloy (reconstructed image)
(a) Before PFF processing (b) After PFF processing

3 Results and discussion

3.1 Quantitative Analysis of permeability at different cooling conditions [18,19]

The permeability ($\boldsymbol{K}$) was evaluated using the Kozeny-Carman equation, incorporating the measured morphological parameters. Fig.4 shows the time-dependent changes in $\boldsymbol{K}$ for different cooling rates.

Higher cooling rates resulted in lower permeability due to the finer dendritic structures. This finding, obtained by the direct observation, agrees with the previous studies on the the relationship between cooling rate and microstructure.

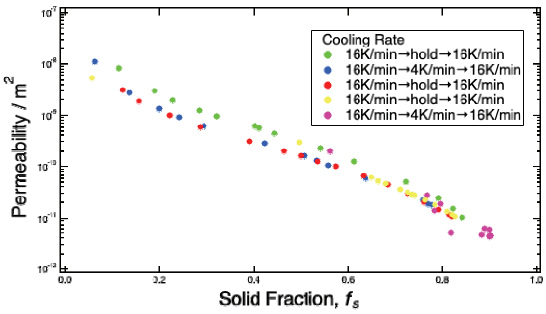


Fig.4 Permeability (K) as a function of solid fraction for various cooling rates

3.2 Machine Learning Model for Predicting Permeability

Our previous studies have attempted to model the time evolution of physical properties using empirical or semi-empirical time-evolution equations.

While this formulation fits experimental data, it requires many noise-sensitive parameters, especially in early stage of solidification.

In this study, to further improve the predictive understanding of permeability, a machine learning approach (Random Forest technique) was introduced [20]. It is known for its robustness against overfitting, ability to handle non-linear relationships, and low sensitivity to feature distribution. Using the time-series data extracted from 4D-CT observations, permeability ($\boldsymbol{K}$) was modeled as a function of solid fraction and morphological features.

The evolution of predicted and experimental permeability with solid fraction is shown in Fig.5. The model captures the sharp drop in $\boldsymbol{K}$ at low f_S and its gradual stabilization at higher f_S, which reflects the connectivity transition in the dendritic network.

As shown in the validation metrics, RF achieved high R^2 values for permeability across multiple folds (e.g., 0.992, 0.940), with very low mean absolute errors (on the order of 10^{-9} m²), confirming its predictive accuracy. The evolution of predicted and experimental permeability with solid fraction is shown in Fig.5. The model captures the sharp drop in $\boldsymbol{K}$ at low f_S and its gradual stabilization at higher f_S, which reflects the connectivity transition in the dendritic network.

In contrast to time evolution equations that require empirical parameter fitting, the machine learning model (RF) provides a flexible, data-driven solution adaptable to non-linear and multi-condition cases. The result suggests its applicability for enhancing macrosegregation simulations.

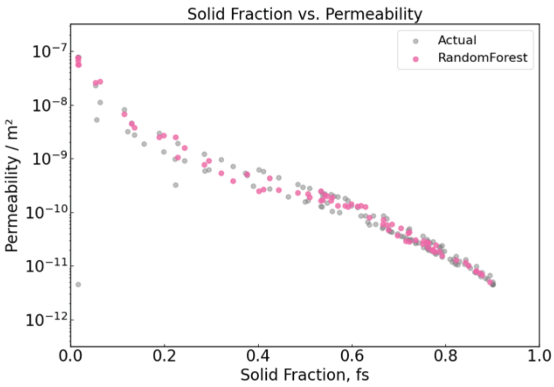


Fig.5 Model fitting result of permeability after Machine Learning

4 Conclusions

This study demonstrated the utility of the time-resolved X-ray tomography and the phase-field filtering for observing solidification morphology in Al-Cu alloys. By combining the quantitative morphological analysis? and machine learning, permeability under varying cooling rates was successfully predicted, supporting improved simulation accuracy in casting processes.

Conflicts of interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Declaration of generative AI and AI-assisted technologies in the writing progress

During the preparation of this work the authors used ChatGPT and DeepL to improve language. After using this tool, the authors reviewed and edited the content as needed and take full responsibility for the content of the publication.

References

[1] Hideyuki Yasuda. Fundamentals of Solidification Engineering: Understanding the Formation of Solidification Microstructures. 2022.

[2] Voller V R, Brent A D, Prakash C. The modeling of heat, mass and solute transport in solidification systems. Int. J. Heat Mass Transf. 1989, 32(9): 1719–1731.

[3] Landis E N, Keane D T. X-ray microtomography. Mater. Charact., 2010, 61(12): 1305–1316.

[4] Maire E, Withers P J. Quantitative X-ray tomography. International Materials Reviews, 2014, 59(1): 1–43.

[5] Maire, E., Withers, P. J. Quantitative X-ray tomography. International Materials Reviews, 2013, 59(1), 1–43.

[6] Stock, S.R. MicroComputed Tomography: Methodology and Applications (1st ed.). CRC Press, 2009.

[7] Bear J. Dynamics of Fluids in Porous Media. Courier Corporation, 1988.

[8] P.C. Carman. Flow of Gases Through Porous Media. London: Butterworths Scientific Publications, 1956.

[9] J.C. Heinrich, D.R. Poirier. Modeling of dendritic permeability in the mushy zone. Comptes Rendus Mécanique, 2004, 332

[10] Banhart J. Advanced tomographic methods in materials research and engineering. Oxford: Oxford University Press, 2008.

[11] Yoshio Waseda, Eiichiro Matsubara. X-ray Structure Analysis: Determining the Arrangement of Atoms. Tokyo: Uchida Rokakuho, 1998.

[12] C. Beckermann. Modeling of Macrosegregation: Past, Present and Future. In: Proceedings of the Merton C. Flemings Symposium on Solidification and Materials Processing, 2001: 297–310.

[13] Boettinger W J, Warren J A, Beckermann C, Karma A. Phase-field simulation of solidification. Annu. Rev. Mater. Res., 2002, 32: 163–194.

[14] M. Ohno. Modeling and analysis of grain refinement behavior. International Journal of Microgravity Science and Application, 2013, 30: 24–29.

[15] Karma A, Rappel W-J. Phase-field method for computationally efficient modeling of solidification with arbitrary interface kinetics. Phys. Rev. E. 1996, 53, R3017(R).

[16] H. Yasuda, et al. Characterization of dendritic growth in Fe–C system using time-resolved X-ray tomography and physics-based filtering. IOP Conf Ser Mater Sci Eng,

2019, 529, 012023.

[17] H. Yasuda, et al. Reconstruction of dendritic growth by fast tomography and phase field filtering. IOP Conf Ser Mater Sci Eng, 2023, 1281, 012064.

[18] Flemings M C. Solidification Processing. New York: McGraw-Hill, 1974.

[19] W. Kurz, D.J. Fisher. Fundamentals of Solidification, 4th ed. Switzerland: Trans Tech Publications, 1998.

[20] Mozaffar M., Bostanabad R., Chen W., et al. Deep learning predicts path-dependent plasticity. Proceedings of the National Academy of Sciences, 2019, 116(52): 26414–26420.