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Measuring Material Parameters by Comparing Phase-Field Simulations with 4D Tomography

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Summary: Accurate material parameters are essential for materials design. In this work, we propose an approach to characterize material parameters by direct comparison between two 3D movies, one acquired by synchrotron experiments and one calculated by phase-field simulations. The proposed method is demonstrated by determining the liquid diffusion coefficient in an Al-Cu alloy.

1. INTRODUCTION

Accurate material parameters are essential for optimizing material process-microstructure-properties [1]. Traditionally, material parameters are measured one at a time with idealized samples. Such measurements may not be representative of the materials used in processing which generally exhibit complex heterogeneous microstructures. This study provides an approach for determining material parameters directly from structural studies of bulk samples acquired during synthesis or processing. 3D movies of structural evolution are acquired during processing by means of an x-ray tomographic method. The experimentally determined structure is used as input to a 3D phase-field model. The phase-field simulation provides a second 3D movie for a given set of materials parameters. Using optimization techniques, the optimal resemblance between the two movies is determined, thereby providing a best-fit value of the material parameters.

Liquid diffusion coefficients are known to be difficult-to-measure material parameters. It has been measured several times for Al-Cu alloys [2, 4, 3] and the measured values show a significant spread. As shown by Lee *et al.* [2], convection in the liquid phase is not negligible in a capillary tube experiment if the diameter of the tube is large and this will result in a larger measured liquid diffusion coefficient. Moreover, experiments that determine diffusion coefficients by composition measurements on quenched samples following directional solidification involve a large temperature gradient [2], which can result in uncertainty in the temperature and composition at which the liquid diffusion coefficient is determined. In addition, microstructure evolution during quench may alter the composition profile, which will influence the measured diffusion coefficient. In the current work, the imaged microstructure has features at a micrometer scale so the Rayleigh number is very small, hence convection can be neglected. The experiment is performed under isothermal conditions, so the uncertainty caused by the temperature gradient is prevented. Moreover, the quenching process intrinsic to many experimental approaches is avoided in the present study since the measurements are *in situ*.

2. METHOD

The optimization process is shown in Fig. 1. Firstly, time-resolved tomography is used to acquire a 3D movie of the evolving microstructure during coarsening [5]. One time frame of the experimental movie is then input to the phase-field model [6]. Together with an initial guess of the material parameters $\mathbf{p}_0$, the phase-field model is solved to a time t corresponding to a later time frame of the experimental movie. The experimental and simulated microstructures are compared to calculate a cost function f_{cost}, which measures the dissimilarity between experiment and simulation. An optimization algorithm is used to update the material parameters $\mathbf{p}$,

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with which the phase-field simulation is repeated until convergence. The material parameters $\mathbf{p}^{\mathrm{fit}}$ which provide a best match between experiment and simulation are regarded as the physically correct ones.

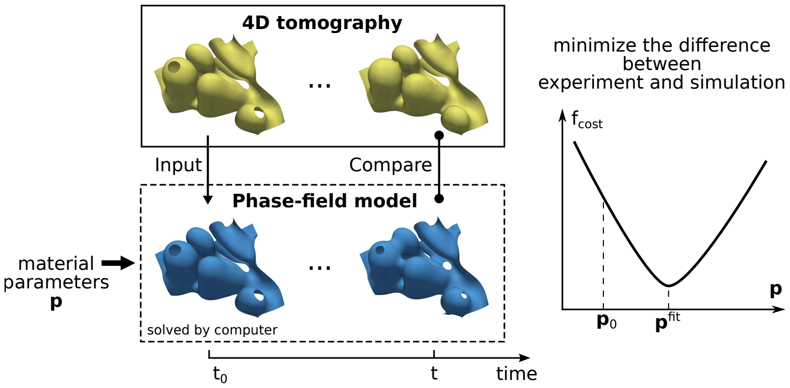

Figure 1: Schematic diagram of the proposed method to determine material parameters.

3. RESULTS

For a given time frame of the experimental input t_0, the liquid diffusion coefficient D^{L} is fitted at different t. The mean value and standard deviation (shown in Fig. 2) are calculated from the best-fit values (fitting with different t and interfaces at different parts within the sample). The process is repeated with different experimental input t_0. Taking into account the results with all combinations of t_0 and t, the measured liquid diffusion coefficient is $D^{\mathrm{L}} = 8.33 \pm 0.24 \times 10^{-10}\ m^2/s$ (orange line in Fig. 2).

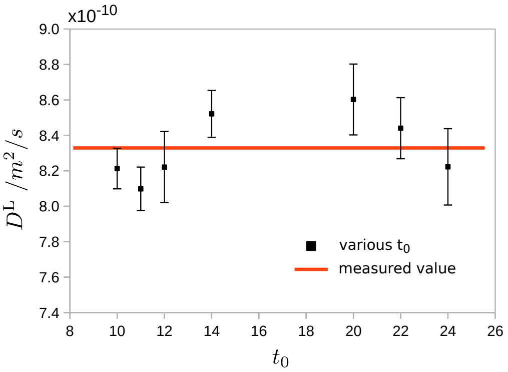

Figure 2: The best-fit liquid diffusion coefficient. The black dots correspond to the mean value of the best-fit D^{L} with given experimental input t_0. The error bars indicate standard deviation.

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