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Extraction of reduced-order process-structure linkages from phase-field simulations

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ABSTRACT

Phase-field simulations have achieved notable success in capturing characteristic details of micro-structure evolution in directional solidification of ternary eutectic alloys. In spite of the impressive advances in high performance computations, phase-field simulations for most practical problems in materials design are resource intensive because of the need to incorporate multiple physical fields over large-scale three-dimensional domains. There is, therefore, a need to learn and capture the underlying materials knowledge embedded in the results produced by such expensive simulations, and facilitating an easy transferability to new problems of interest. This paper demonstrates the viability of extracting the salient process-structure linkages from phase-field simulations, while casting them in forms amenable for a rapid and efficient exploration of a relatively large process space. The presented framework is based on low dimensional representation of material structure obtained through principal component analysis (PCA) of 2-point spatial correlations.

1. Introduction

New and improved materials have been at the core of almost all of the advanced technologies introduced throughout human history. However, the pace of materials innovation lags significantly behind the rate of innovation in many other fields. Today, introducing a new material takes around 20 years from its discovery to its deployment in a commercial product [1–4]. The central impediment comes from the need to understand and utilize the important relationships between the material structure at multiple length scales, its evolution through different manufacturing processes, and the associated macroscale properties. These are generally referred as process-structure-property (PSP) linkages [5–17]. The conventional approaches used for extracting the important PSP linkages needed in materials innovation have proven to be slow, expensive and effort intensive. Integrated Computational Materials Engineering (ICME) [4] paradigm and Materials Genome Initiative (MGI) [1] propose to dramatically accelerate material innovation through utilization of data science tools in conjunction with multiscale experiments and multiscale simulations.

Phase-field simulations have played a pivotal role in simulating the microstructure evolution in several phenomena such as thin film growth [18], grain growth [19,20], recrystallization [21], and directional solidification [22–24]. In this study, we focus on building process-structure linkages from phase-field simulations of directionally solidified ternary eutectic alloys. During the directional solidification of a eutectic system, two or more solid phases evolve simultaneously from the melt. In ternary eutectic alloys, three phases form, resulting in various spatial patterns, depending on the process parameters. The overall (effective) mechanical properties are indeed influenced by these spatial patterns [25–27]. Therefore, it is of interest to quantify the influence of the process parameters on the evolving microstructure. One alloy of scientific interest is the ternary eutectic system Al-Ag-Cu [28–32], due its favorable physical properties. As an example, the influence of sedimentation in directional solidification is being studied in experiments conducted on the international space station (ISS) as

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part of the Solidification along a Eutectic path in Ternary Alloys (SETA) program [33]. Phase-field models have been used successfully for simulating these experiments. Several investigations of the pattern formation process in the Al-Ag-Cu system have been conducted with the phase-field method [24,34–38], which include three-dimensional simulations [34] as well as large-scale simulations [24,35]. The influence of the melt concentration in the vicinity of the ternary eutectic point on the pattern formation was also investigated [36]. Although the influence of the process parameters on the microstructure pattern formation has been studied in Al-Ag-Cu, there do not yet exist low cost surrogate models (also called metamodels or linkages) capturing these relationships.

A rigorous quantification of the microstructure is central to extracting a high value process-structure linkage. Although a number of measures such as volume fraction [39], average grain size [40], number of nearest neighbors [24], and pair correlations [41] have been employed in literature to quantify the material structure, only n-point spatial correlations (also referred as n-point statistics) [42–44] give the most systematic and complete information about the material internal structure. For example, one-point statistics reflect the probability density of finding a local state of interest at any single location selected in the representative volume of the material microstructure. At the next level, two-point statistics describe the probability density of finding local states h and h' separated by a prescribed vector r. In prior work [14,37,38,45,46], two-point statistics were demonstrated to be successful in objective classification of microstructure. Higher-order statistics can be defined in a similar manner. However, the number of measures included in these representations (which reflects the dimensionality of structure representation) increases exponentially. Hence, a reduced-order representation of microstructure is required. For this purpose, principal component analysis (PCA) is used [14,37,38,45,46]. PCA essentially involves a linear transformation of the coordinate frame, where the available data could be viewed to capture the salient differences in the datapoints

generating the calibration datasets (red box), (ii) reduced order representation of the microstructure (green box), and (iii) building the process-structure linkages (blue box). In many respects, this workflow has the same main components as the workflow presented in our prior work for establishing structure-property linkages [14]. One of the main benefits of such workflow templates is that they provide modularity (for example, the individual components in Fig. 1 can employ any of the different options available for that component), while promoting higher levels of interoperability needed for standardization, automation, and scale-up. Briefly, these templated workflows start by identifying (or specifying) the process parameters of interest and their ranges. This information is then utilized to generate a suitable calibration dataset using a previously established approach in the domain of practice (in the present case, these are the phase-field models [24,37]). After generating the calibration dataset, the microstructure is quantified through spatial statistics and this information is projected onto a reduced-order space to obtain a low dimensional representation. In the final step, the process space and the reduced order representation of microstructure are mapped to arrive at the needed process-structure linkages through machine learning approaches and cross validation techniques.

2. Phase-field model and calibration data sets

2.1. Phase-field model

To model the microstructure evolution of ternary eutectics during directional solidification, a thermodynamically consistent phase-field model based on the Grand potential approach is employed [47,48]. The evolution equations for the N phase-fields ϕ_α in the vector ϕ are calculated from the total energy in the system. Based on the Grand potential functional [47,48] and applying an Allen-Cahn type approach, the evolution equations of the form

$$\tau\varepsilon\frac{\partial\phi_\alpha}{\partial t}=\underbrace{-\varepsilon T\left(\frac{\partial a(\phi,\nabla\phi)}{\partial\phi_\alpha}-\nabla\cdot\frac{\partial a(\phi,\nabla\phi)}{\partial\nabla\phi_\alpha}\right)}_{:=\text{rhs1}_\alpha}\underbrace{-\frac{1}{\varepsilon}T\frac{\partial\omega(\phi)}{\partial\phi_\alpha}-\sum_{\beta=1}^{N}\psi_\beta(\boldsymbol{\mu},T)\partial\frac{h_\beta(\phi)}{\partial\phi_\alpha}}_{:=\text{rhs2}_\alpha}-\lambda. \tag{1}$$

in the minimum number of dimensions. In other words, a data-driven reduced-order representation of the microstructure can be obtained by retaining only a small number of components. PCA was successfully implemented in prior work for microstructure classification [38,45,46], extraction of structure-property linkages [14], and decision support in phase-field simulations [37].

In prior work [14], the reduced order representation of microstructure and machine learning approaches were utilized mainly to build computationally efficient metamodels for structure-property linkages. The viability of the reduced order representation for microstructures simulated by phase-field models was also demonstrated [37]. In this paper, we explore and demonstrate for the first time, the viability of applying this new framework to establishing process-structure linkages from microstructures simulated by phase-field models. Since it is generally much more difficult to extract process-structure linkages when compared to the effort involved in extracting the structure-property linkages, this work represents a significant advance in the field. Specifically, we demonstrate that it is possible to undertake this task in a templated workflow (see Fig. 1) comprising three main components: (i)

are derived with the Lagrange multiplier $\lambda=\frac{1}{N}\sum_{\alpha=1}^{N}\text{rhs1}_\alpha+\text{rhs2}_\alpha$ to ensure the constraint $\sum_{\alpha=1}^{N}\phi_\alpha=1$.

The interface kinetics is described by the parameter τ, coupling the different time scales in the simulation. The form of the interface is modeled by the gradient energy density a as well as the potential energy ω, and its thickness is related to ε. The driving forces for the phase transitions in Eq. (1) are comprised in the differences of the Grand potentials. These potentials ψ_β are interpolated with h_β [49].

The evolution of the temperature T during the directional solidification process, is calculated analytically according to the simplified condition

$$\frac{\partial T}{\partial t}=\frac{\partial}{\partial t}(T_0+G(z-vt))=-Gv\,, \tag{2}$$

where T_0 is the base temperature, G is the gradient, z is the spatial position in the growth direction, v is the velocity, and t is the time.

The evolution of the chemical potentials $\boldsymbol{\mu}$ is derived from the energy functional