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An inverse design framework for prescribing precipitation heat treatments from a target microstructure

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ABSTRACT

The computer-aided materials design process is highly iterative in nature and as such requires flexible tools that have the ability to link processing, properties, and performance not only in the usual forward direction but also in the inverse direction more associated with a goal-oriented/design framework of Integrated Computational Materials Engineering (ICME). While many computational techniques exist that relate properties to performance in both forward/inverse directions, tools that prescribe a process when given a desired microstructure have not been developed in detail. This research fills that gap by coupling physics-based precipitation models with "mesh adaptive direct search" optimization techniques as a strategy to develop (inverse) microstructure-processing relations. This framework is demonstrated by prescribing heat treatments in Ni-rich NiTi shape memory alloys that will result in a desired size distribution of Ni_4Ti_3 precipitates. This prescriptive technique provides a rigorous strategy for the identification of materials processing schedules—provided the forward models connecting processing and microstructure are available—that yield specific microstructural features and that can significantly reduce the experimental search space that needs to be explored, accelerating the materials development process.

1. Introduction

The Materials Genome Initiative (MGI) [1] has guided research in materials science by emphasizing the need to integrate materials design into the overall product/technology development process. The key to successful materials design integration is the development of a top-down design approach in the context of the process–properties–performance hierarchy (PPP) shown in Fig. 1. The dashed arrow in this top-down design represents the prescription of processing steps based on a desired microstructure, while approaches such as materials optimization via microstructure-sensitive design (for example) [2] address the connectivity between properties/performance and microstructure.

In traditional materials design and development, the processing steps to achieve specific microstructural features—yielding in turn desired property/performance metrics—are typically arrived at through extensive iterative processing–characterization cycles. Due to the complexity of the relationships between processing and microstructure, the determination of processing schedules relies extensively on prior work conducted on similar systems, results from prior iterations in the materials development cycle and/or intuition of the materials developer. This framework is powerful as can be attested by the vast number of technologies that have been enabled by the discovery/development of new materials over the past centuries. Despite its success, such an approach may be cost-prohibitive and extremely time consuming, leading to product design scenarios in which the (sub-optimal) material functionality/performance is the limiting design factor in the entire product/technology development cycle.

Over the past years, significant efforts have been made toward the development of effective computational, experimental, and/or hybrid approaches to accelerate the materials development process. On the computational side, much work has focused on the forward problem of finding the response/behavior of specific microstructures. While the inverse problem connecting property/performance to (optimal) microstructures has been recently tackled [2–4], much less effort has been put into the inverse problem connecting desired/optimal, microstructural features to specific processing schedules. Here we note that the overall inverse problem (see Fig. 1) must be solved (either through simulation, experiments or hybrid approaches) if one is to change the materials development paradigm.

This paper details a computational materials science framework (Fig. 2) that can prescribe the processing steps required to achieve application-specific microstructural features. Specifically, we propose and demonstrate a strategy for the prescription of heat treatment schedules to achieve specific precipitate population distributions where the

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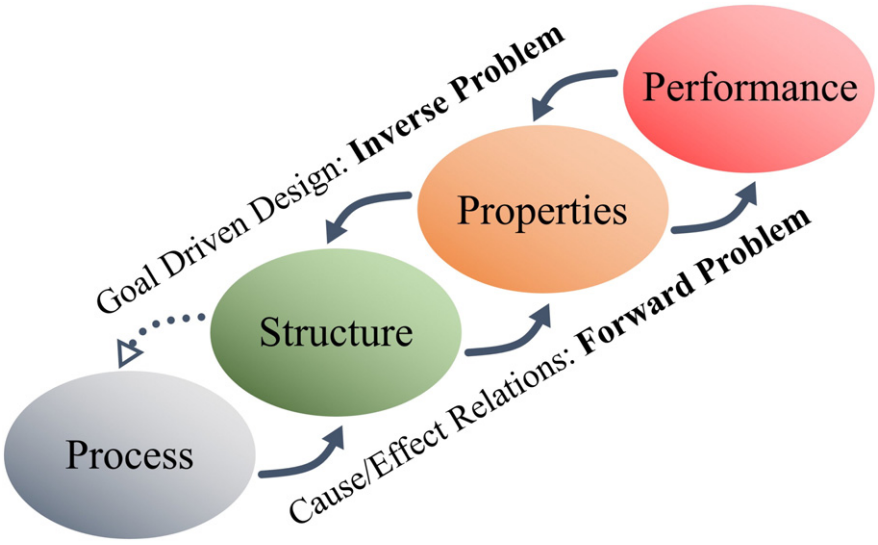

Fig. 1. The forward and inverse problems in materials science development.

connection between heat treatment and precipitate distribution is made through physics-based nucleation/growth models.

The proposed approach reduces the cost and time necessary to develop a new material by replacing the iterative *physical experiments* with the iterative *computational modeling* and *optimization*. There are many similarities between the computation and experimental approaches to materials development other than just their iterative nature: prior research and material scientist intuition are encapsulated in the prescriptive framework through the material model and microstructure comparison metric(s) while results from prior iterations are considered within the optimization tool.

Before discussing the framework, an example material system with cost-prohibitive process-limited applications needs be selected to showcase its capabilities. The costs associated with experimental identification of the relationships between heat treatment parameters and microstructure in NiTi Shape Memory Alloys (SMAs) are so high that the usual approach to their deployment is limited to the design of the actuation mechanism around off-the-shelf alloys with predetermined transformation behavior. This, however, does not need to be the case.

SMAs exhibit the so-called shape memory effect (SME) and superelasticity (SE) as a result of reversible thermoelastic martensitic transformations [5,6]. The behavior in *Ni-rich* NiTi SMAs is highly dependent on the process (heat treatment) history of the material due to strong sensitivity of transformation behavior to the matrix composition [7,8], which in turn can be modified through the formation of secondary precipitate phases. While there are several phases that may coexist in (meta)stable equilibrium with the B2 matrix [9], the precipitation of the metastable Ni_4Ti_3 phase is of interest due to its drastic influence on the material's transformation temperatures [10–13], phase constitution [8,14,15], and cyclic stability [16].

In this paper, the focus is the description of the theory and implementation of the three components that comprise this framework (fitness metric, material model, and optimization technique). The results and discussion section is devoted to examples of heat treatments prescribed by this framework. Finally, the concluding remarks contain a very brief summary of the framework and point to potential applications of this framework (or variants of it) for future research.

2. Fitness metric

Mathematically, the search for the heat treatment schedule that yields optimal microstructures is an optimization problem. As such, the first major piece of such a prescriptive framework is the development of a fitness metric that can quantify the difference between a target microstructure and the microstructure resulting from any candidate

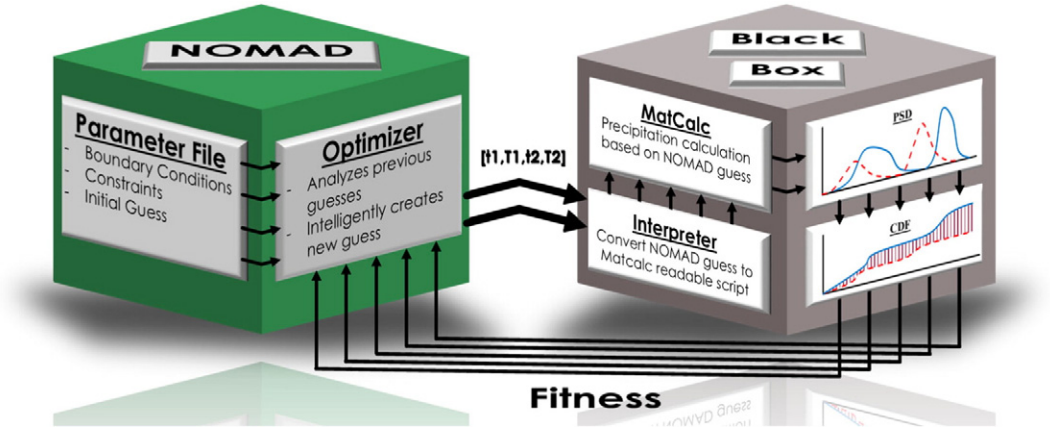

Fig. 2. Flowchart depicting the flow of information in the prescriptive heat treatment framework.