Acta Materialia 223 (2022) 117471

Contents lists available at ScienceDirect

Acta Materialia

journal homepage: www.elsevier.com/locate/actamat

# On the importance of microstructure information in materials design: PSP vs PP

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ARTICLE INFO

*Article history:*
Received 18 September 2021
Revised 17 October 2021
Accepted 5 November 2021
Available online 6 November 2021

*Keywords:*
Closed-loop Bayesian optimization
Microstructure design
Structure-property relationship
Computational thermodynamics
Micromechanical modeling

ABSTRACT

The focus of goal-oriented materials design is to find the necessary chemistry/processing conditions to achieve the desired properties. In this setting, a material's microstructure is either only used to carry out multiscale simulations to establish an invertible quantitative process-structure-property (PSP) relationship, or to rationalize *a posteriori* the underlying microstructural features responsible for the properties achieved. The materials design process itself, however, tends to be *microstructure-agnostic*: the microstructure only mediates the process-property (PP) connection and is—with some exceptions such as architected materials—seldom used for the optimization itself. While the existence of PSP relationships is the central paradigm of materials science, it would seem that for materials design, one only needs to focus on PP relationships. In this work, we attempt to resolve the issue whether 'PSP' is a superior paradigm for materials design in cases where the microstructure itself cannot be (directly) manipulated to optimize materials' properties. To this end, we formulate a novel *microstructure-aware* closed-loop multi-fidelity Bayesian optimization framework for materials design and rigorously demonstrate the importance of the microstructure information in the design process. The problem considered here involves finding the right combination of chemistry and processing parameters that maximizes a targeted mechanical property of a model dual-phase steel. Our results clearly show that an explicit incorporation of microstructure knowledge in the materials design framework significantly enhances the materials optimization process. We thus prove, in a computational setting, and for a particular representative problem where microstructure intervenes to influence properties of interest, that 'PSP' is superior to 'PP' when it comes to materials design.



## 1. Introduction

Further advancement of numerous important technologies [1–3] depends on the discovery and development of enabling materials [4,5]. Historically, materials development has advanced through a mix of Edisonian approaches and serendipity. Yet, the need to increase the rate at which materials are developed demands a much more focused and goal-oriented exploration of the material design space through experimental, computational, and/or data-driven methods [6–9]. The central paradigm of goal-oriented materials design [6] is to understand and then exploit processing/chemistry - microstructure - property (PSP) relationships (Fig. 1). Within this paradigm, a material is treated as a complex hierarchical system ultimately described by linkages along the PSP chain [6–8,10–13]. In theory, then, materials design occurs when such PSP relationships are inverted to map desired properties to the required chemistry and processing protocols through *optimal* microstructures [4,8,9,14–18]. Despite the *theoretical* importance of microstructural information to materials design, it is worth examining to what extent such information truly accelerates the materials development process, *in practice* [9].

In a computational setting, virtual PSP chains are built to establish quantitative relationships connecting inputs (i.e., chemistries and/or process protocols) to outputs (i.e. properties). While microstructures mediate these connections, microstructural features are not directly manipulated to achieve the desired properties. We note that in a virtual material design setting, one could potentially focus the optimization scheme on the microstructure itself. However, this 'microstructure-centric' approach to materials design

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https://doi.org/10.1016/j.actamat.2021.117471
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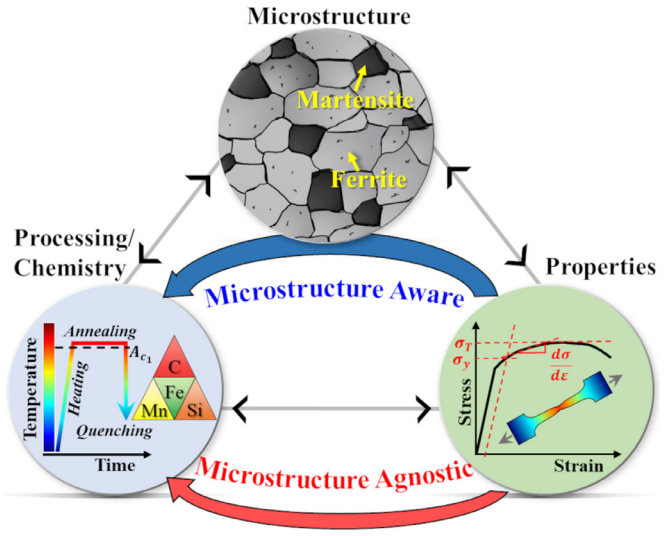


**Fig. 1.** Processing/Chemistry-Microstructure-Property (PSP) paradigm in materials science. In the traditional, *microstructure-agnostic*, approach the microstructure information is not directly exploited for material design, as shown. While in the proposed *microstructure-aware* approach the microstructure information is directly exploited for material design, and it is shown that this *microstructure-aware* approach helps us arrive at processing/chemistry conditions that yield optimum properties more efficiently than the traditional *microstructure-agnostic* approach.

runs the risk of identifying optimal, yet infeasible (or unattainable) microstructures. In an experimental setting, the degree to which microstructure knowledge is exploited to carry out the design (or optimization) of a material is even more questionable. After all, one could argue that one can treat the material's microstructure as a 'black box,' amenable for optimization by evaluating how changes in its inputs (i.e. chemistry and/or processing) affect its outputs, *without necessarily having to characterize/know the state of the microstructure* at every stage of the materials optimization process. While the notion of *microstructure-awareness* has been a central paradigm in materials optimization, in practice both virtual and real efforts to optimize a material's performance tend to be *microstructure-agnostic*—see Fig. 1.

*Microstructure-agnostic* material design is the norm rather than the exception, even in recent state-of-the-art successful materials design examples [19–21]. For example, the authors in ref. [19], experimentally designed a refractory high-entropy alloy with enhanced ductility by optimizing the material's chemistry. Here, microstructure characterization was only used to gain understanding and rationalize the impact of processing/chemistry on the mechanical properties of the alloy *a posteriori* but was not explicitly used to guide the step-by-step exploration of the material design space. Similarly, the authors in ref. [20], experimentally designed a high-strength, low-cost nanostructured beta-titanium alloy consisting of homogeneous distribution of micron- and nano-scale $\alpha$-phase precipitates within the $\beta$-phase matrix. In this work, as in the previous example, analysis of the microstructure, after finding an optimal property, was used to uncover the ultimate cause for the superior mechanical properties. Yet again, microstructural information was not explicitly used to guide the search for materials with optimal mechanical response. Another example of such efforts includes the work by authors in ref. [21], who were able to identify alloys defeating the strength-ductility trade-off by forming a dual-phase microstructure through 'phase metastability engineering.' In this case, the alloy design principle was based on a hypothesized enhancing mechanism verified, *a posteriori*, via experimental characterization.

While the examples just described certainly expanded our knowledge of the materials performance space by careful and ground-breaking analysis of the connections between processing/chemistry and resulting properties (i.e., analysis of the direct PP relationships) mediated by the material microstructure, the latter was not used as a direct input in the materials design process. Rather, an analysis of the material microstructure state was carried out to explain the attained properties. Thus, even though our aspiration as material scientists is to unravel the principles that govern material properties and performance, from a practical engineering standpoint, explicit knowledge of the microstructure does not appear to be a necessary condition for a successful materials design campaign.

Given the centrality of PSP relationships to materials science as a field, it is worth investigating whether microstructural information can help us arrive at processing/chemistry conditions that yield optimum properties *more efficiently than otherwise*. If the answer ends up being negative, then, from an admittedly pragmatic point of view, the argument for building explicit PSP relationships as a necessary condition towards accelerated materials design is not very strong. The microstructure state of the system, thus, can be simply replaced by a 'black box' without affecting the outcome of the design process i.e., identification of the region in the material design space (processing/chemistry parameters) that yields optimal properties. Knowledge of the microstructure then would only serve to rationalize observations and augment our knowledge of the material under investigation, rather than to assist in the decision-making process as one navigates the material design space. On the other hand, showing that microstructure information can be explicitly exploited to accelerate the materials design process through *each step of the materials optimization cycle* provides a stronger footing to the notion of PSP relationships as the fundamental, exploitable, encoding of materials information relevant to materials design.

In this work, we attempt to show how to formulate and solve a *microstructure-aware* materials design problem while answering the *fundamental question* whether microstructure information is essential to materials design. In essence, we attempt to address whether explicit inversion of PSP relationships is truly necessary to optimize a given material, that is, whether PSP, rather than PP (i.e., direct processing/chemistry - property) relationships need to be learned and exploited in a specific closed-loop materials discovery task. From a scientific perspective, understanding how microstructure information can be explicitly incorporated in materials design can contribute to better understanding of PSP relationships, while from a pragmatic standpoint, the answer to this question can help develop better frameworks for materials design, including newly proposed closed-loop autonomous materials research (AMR) platforms [22,23]. As we will see below, our investigation provides tantalizing clues as to the outcome of the *PSP vs PP* comparison, in the context of materials design.

## 2. Overview of the present work

Herein, we carry out a rigorous analysis to probe the importance (if any) of the microstructure information in the materials design process. The specific problem considered here involves finding the right combination of material chemistry and processing conditions that maximizes a target mechanical property of a model dual-phase steel. We first solve this problem by following a traditional *microstructure-agnostic* (Fig. 1) approach where the material design space includes the material's chemistry and processing routes while the microstructure information is only used to carry out multiscale (or multi-level) simulations to establish forward quantitative PSP relationships. Next, we set up the same material design problem by following a novel *microstructure-aware*

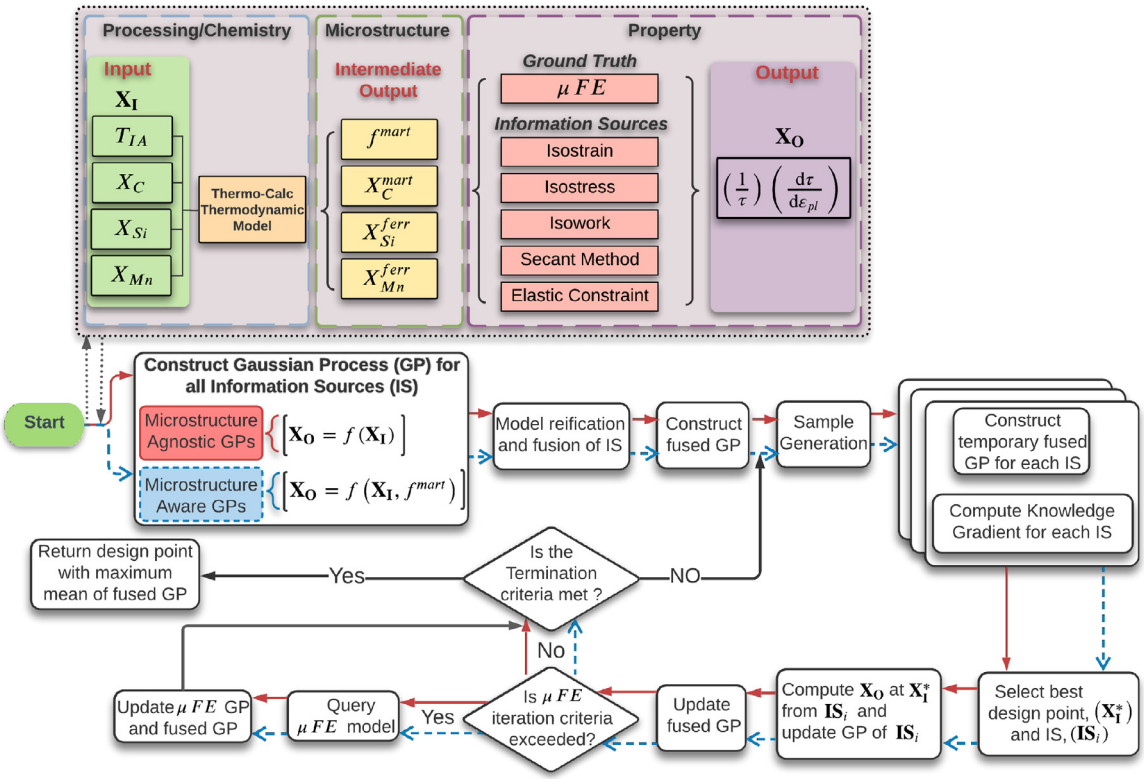


**Fig. 2.** Schematic representation of the *microstructure-agnostic* and *microstructure-aware* closed-loop multi-information source Bayesian Optimization (BO) approach to designing a model dual-phase (ferrite-martensite) steel. Here, $\mathbf{X_I}$ corresponds to the input variables with $T_{IA}$ being the intercritical annealing temperature, $X_C$, $X_{Si}$ and $X_{Mn}$ correspond to the molar fraction of carbon, silicon and manganese in the alloy, while the output, $\mathbf{X_O}$, is the stress-normalized strain hardening rate $((1/\tau)(d\tau/d\varepsilon_{pl}))$, with $\tau$ and $\varepsilon_{pl}$ being the flow stress and the plastic strain, respectively). Also, $f^{mart}$ is the volume fraction and $X_C^{mart}$ is the Carbon content of the martensite phase; while $X_{Si}^{ferr}$ and $X_{Mn}^{ferr}$ are the Silicon and Manganese content, respectively, of the ferrite phase.

(Fig. 1) approach where the material design space not only includes the material's chemistry and processing routes, but also information about the microstructure state of the material being optimized.

Note that apart from the explicit incorporation of the microstructure information in the material design space in the latter approach, the two approaches are essentially identical, with the same inputs and the same quantitative PSP relationships. In order to establish the *microstructure-aware* materials design protocol, it is first necessary to decide how to incorporate microstructure information within the design framework. This is not a trivial task for a couple of reasons. First, microstructure is essentially causally related to the chemistry and processing routes, i.e., it is a dependent variable(s). Second, explicit incorporation of microstructure information in the material design space increases the dimensionality of the problem and the complexity of the optimization task.

## 3. Methods

Our model material design problem involves finding the right combination of the parameters in the input (design) space, $\mathbf{X_I}$, that maximizes the output (objective), $\mathbf{X_O}$, Fig. 2. In this problem, the input space includes the processing condition (intercritical annealing temperature, $T_{IA}$) and the material chemistry (the amount of alloying elements, carbon, $X_C$, silicon, $X_{Si}$, and manganese, $X_{Mn}$); while the output is a targeted mechanical property (stress-normalized strain hardening rate, $(1/\tau)(d\tau/d\varepsilon_{pl})$, with $\tau$ and $\varepsilon_{pl}$ being the flow stress and the plastic strain, respectively) of a model (ferritic-martensitic) dual-phase steel. The $(1/\tau)(d\tau/d\varepsilon_{pl})$ is an important mechanical performance indicator, as higher values are associated with increased ductility and formability [24,25]. The feasible input space for this design problem is considered bounded, i.e., we consider a material system with carbon within 0.05 to 1 wt%, silicon within 0.1 to 2 wt% and manganese within 0.15 to 3 wt%, and intercritical annealing heat treatment within a temperature range of 650 °C to 850 °C as processing parameters.

Next, we employ computational thermodynamics using a commercial code Thermo-Calc™ as in refs. [18,26] to compute the microstructure (characterized by the volume fraction, $f^{mart}$, of the martensite phase) and chemical composition (characterized by the carbon content of the martensite phase, $X_C^{mart}$, and silicon, $X_{Si}^{ferr}$, and manganese, $X_{Mn}^{ferr}$, contents of the ferrite phase) of the resultant phases as a function of $\mathbf{X_I}$, Fig. 2. The details of the microstructure and chemical composition are then used to predict the mechanical behavior of the dual-phase steel using five low-fidelity micromechanical models. These are considered low-cost 'information sources' within our multi-information source fusion BO framework [27,28]. In addition, a high fidelity 3D microstructure-based finite element model ($\mu FE$) is used as the 'ground truth' (Fig. 2). The first three low-fidelity models, *isotrain* [29], *isostress* [30] and *isowork* [31] assume that different mechanical quantities (strain, stress and work of deformation, respectively) are equipartioned among the different constituent phases of the microstructure. The other two low-fidelity models, i.e. the *secant method* and the *elastic constraint* models, are more complex micromechanical models ref. [32]. The *secant method* is based on Hill's weakening constraint power in a plastically-deforming matrix. The *elastic constraint* model, on the other hand, is based on Kröner's analysis of the matrix-inclusion problem under elastic constraints [32]. The 'ground truth' ($\mu FE$ model), on the other hand, utilizes a full-field finite element analysis of a 3D representative volume element

(RVE) of the material microstructure [18,33–35] constructed from information about the phase fraction of the constituent phases for a given chemistry-heat treatment combination. A typical finite element mesh of the RVE employs 27,000 C3D8 brick elements from the ABAQUS/standard element library [36], and is subjected to a monotonically increasing uniaxial tensile deformation under fully periodic boundary conditions. Readers are referred to refs. [18,33] for a more detailed description of the $\mu FE$ model.

The constituent phases, ferrite and martensite, are modeled in the $\mu FE$ simulation as isotropic elastic-plastic materials with Young's modulus of 200$GPa$ and Poisson's ratio of 0.3, and constitutive relations (relating flow stress, $\tau$, equivalent plastic strain, $\varepsilon_{pl}$, and the chemical composition, $X_i^P$, in weight fraction) as,

$$\tau = \tau_0^F + C_{Si}(X_{Si}^{ferr})^{1/2} + C_{Mn}(X_{Mn}^{ferr})^{1/2} + K^F(\varepsilon^{pl})^{n^F} \tag{1}$$

and

$$\tau = \tau_0^M + C_c(X_C^{mart})^{1/3} + K^M(\varepsilon^{pl})^{n^M} \tag{2}$$

for the ferrite and martensite phases, respectively, with $\tau_0^F = 200\text{MPa}$, $C_{Si} = 732\text{MPa}$, $C_{Mn} = 213\text{MPa}$, $K^F = 2200\text{MPa}$, $n^F = 0.5$, $\tau_0^M = 400\text{MPa}$, $C_c = 10^5\text{MPa}$, $K^M = 450\text{MPa}$ and $n^M = 0.06$. The choice of the (representative) constitutive parameters in Eqs. (1) and (2) are based on the prior observations that the strength of the martensite phase is predominantly related to its carbon content, and it does not exhibit significant work-hardening; while the ferrite phase is softer compared to the martensite phase and exhibits significant work-hardening and its strength depends on its silicon and manganese contents [37–39]. The five (low-fidelity reduced-order) micromechanical models use the constitutive relations as per Eqs. (1) and (2).

As shown schematically in Fig. 2, the established PSP relationship for the model dual-phase material can now be exploited using our recently developed closed-loop multi-information source fusion (multi-fidelity) BO framework [18] to solve the goal-oriented material design problem by either following the traditional *microstructure-agnostic* or a novel *microstructure-aware* approach. Here, we briefly describe our closed-loop multi-fidelity BO framework with a focus on highlighting the differences between the proposed *microstructure-aware* approach and the traditional *microstructure-agnostic* approach. A more complete description of the closed-loop multi-fidelity BO framework can be found in ref. [18]. In the *microstructure-agnostic* approach, the decision-making process does not involve knowledge of the material's microstructure and the optimization problem is simply posed as

$$\mathbf{x}^* = \arg\max_{\mathbf{x}\in\mathbf{X_I}} \mathbf{X_O}(\mathbf{x}) \tag{3}$$

where $\mathbf{x}^*$ is the optimal design vector within the feasible input space, $\mathbf{X_I} = [T_{IA}, X_C, X_{Si}, X_{Mn}]$. In the proposed *microstructure-aware* approach, on the other hand, the material design space not only includes the material's chemistry and processing conditions, but also the microstructure information; and the decision-making process explicitly involves the knowledge of the material microstructure and the optimization problem is posed as

$$\mathbf{x}^* = \arg\max_{\mathbf{x}\in\mathbf{X_I}} \mathbf{X_O}\left(\mathbf{x}, f^{mart}(\mathbf{x})\right) \tag{4}$$

with $f^{mart}$ being dependent on the input vector, $\mathbf{x}$.

The closed-loop multi-fidelity BO framework for both approaches first involves the construction of surrogate models for the 'information sources' and 'ground truth' based on the current knowledge of the design space. Herein, we utilize a Gaussian process (GP) model with a squared exponential kernel as surrogate for the 'information sources' and 'ground truth'—in practice, there is a wide range of potential kernels that can be used, depending on our degree of knowledge of the function being modeled. GP models tend to be used as surrogates of black box functions due to their useful mathematical properties such as their ability to easily predict the mean and variance of the quantity of interest, as well as the way in which correlations between points in the design space can be modeled through the covariance or kernel function [40]. The behavior of a GP surrogate model is controlled by the hyperparameters of the kernel, and it is necessary to tune their values based on the current knowledge of the input-output connection. The optimum values of the hyperparameters in this work are estimated by finding the maximum of the log marginal likelihood. Note that the Gaussian process model for the *microstructure-agnostic* approach correlates the input $\mathbf{X_I}$ to output $\mathbf{X_O}$; while for the *microstructure-aware* approach the input $\mathbf{X_I}$ is *augmented with an extra dimension* corresponding to the volume fraction of the martensite phase, $f^{mart}$, to explicitly incorporate the microstructure information in the materials design process.

Since all the 'information sources' i.e., the low fidelity reduced-order micromechanical models attempt to describe the relationship between the material's microstructural descriptors and the corresponding mechanical behavior, one can expect that they would be correlated with each other and with the 'ground truth' i.e., the $\mu FE$ model. By exploiting these correlations through the 'reification' process [28,41–43] we generate a fused Gaussian process model. This model encodes our most up-to-date knowledge of the correlation between the design space and the objective value. In a multi-fidelity iterative design optimization problem, one needs to answer two questions at every iteration: (i) which point in the design/input space to query, and (ii) which 'information source' to use to query the selected point. To determine this, we generate potential sample design points using Latin hypercube sampling in the input design space and evaluate them from each of the Gaussian process models of 'information sources' and then construct a temporary fused Gaussian process model for each 'information source.' Next, among these potential design points, we seek to identify the design point and 'information source' to query such that it will result in maximum improvement in our knowledge of the maximum objective value.

In this work, we use the Knowledge Gradient (KG) [44] as the metric that quantifies the expected change in our knowledge of the maximum value of the quantity of interest when evaluating a potential design point with a given 'information source'. We then compute the Knowledge Gradient for the set of potential design points on the temporary fused Gaussian process model of each 'information source.' The best design point-'information source' pair, $\mathbf{X_I^*} - \mathbf{IS_i}$,is the one that maximizes the KG and is thus selected for the next query within the BO loop. Following this, we evaluate the response of the selected 'information source,' $\mathbf{IS_i}$, by computing the input-output correlation at the selected design point, $\mathbf{X_I^*}$. After this evaluation, the GP emulating the selected $\mathbf{IS_i}$ and the fused GP are updated. Now, based on either a total budget or a fixed number of queries, the 'ground truth' model ($\mu FE$ model) may also be queried to update our knowledge of the objective value. Here, we query the 'ground truth' at every ten design iterations. Using this evaluation of the 'ground truth' model, we update the Gaussian process model of the 'ground truth' as well as the fused Gaussian process model. This entire process is repeated until we reach the end of the optimization which in this case is a preset number of design iterations. Finally, at the end of the optimization, the best design point that maximizes our objective function is reported.

## 4. Results

The material design problem of finding the right combination of parameters in the input space, $\mathbf{X_I} = [T_{IA}, X_C, X_{Si}, X_{Mn}]$, that maximizes the output, $\mathbf{X_O} = [1/\tau\left(d\tau/d\varepsilon_{pl}\right)]$, of a model dual-phase steel is solved using our closed-loop multi-fidelity BO framework following both the traditional *microstructure-agnostic* and the novel

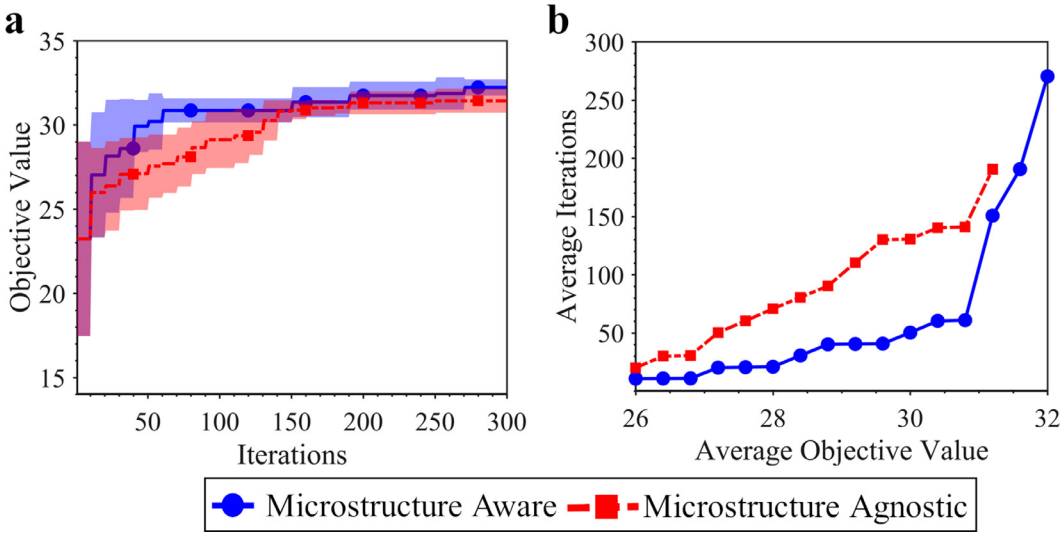


**Fig. 3.** A comparison of the performance of the traditional *microstructure-agnostic* and the novel *microstructure-aware* material design approaches. (a) Comparing the maximum objective value found as a function of the number of design iterations for five realizations of the design process. (b) Comparing the average number of design iterations required to reach an average maximum objective value over five realizations of the design process.

*microstructure-aware* approaches, as shown schematically in Fig. 2. The first step to set up our design framework requires construction of Gaussian process models using the initial knowledge of the $\mathbf{X_I} - \mathbf{X_O}$ correlation. To this end, we evaluate $\mathbf{X_I} - \mathbf{X_O}$ correlation at ninety sets of randomly selected parameters in the input space using computational thermodynamics and each of the low fidelity micromechanical models referred to as 'information sources.' Meanwhile, the $\mathbf{X_I} - \mathbf{X_O}$ correlation is evaluated at only five sets of randomly selected parameters in the input space using computational thermodynamics and the high fidelity $\mu FE$ model referred to as 'ground truth.' To avoid any bias in the design process due to the initial sets of randomly selected parameters in the input space, in particularly that of the five sets evaluated using the 'ground truth' model, we carried out five realizations of the design process. A realization here basically refers to different sets of initially known five 'ground truth' $\mathbf{X_I}$ - $\mathbf{X_O}$ correlations.

The overall performance of the two materials design approaches are compared in Fig. 3. The plot in Fig. 3(a), compares the maximum objective value (i.e., the stress-normalized strain hardening rate) achieved as a function of the number of design iterations for five realizations of the design process; while the plot in Fig. 3(b) compares the average number of design iterations required to reach an average maximum objective value over five realizations of the design process. In Fig. 3(a), the lines correspond to the average values and the shaded regions represent the variance over the five realizations of the design process. As can be seen in Fig. 3(a), at any design iteration, the maximum objective value achieved using the *microstructure-aware* approach is greater than that using the *microstructure-agnostic* approach. An alternate representation of the same in Fig. 3(b) also shows that, on average, far fewer design iterations are needed to obtain the same average objective value using the *microstructure-aware* approach compared to the *microstructure-agnostic* approach. Furthermore, even though after a large number (greater than 150) of design iterations the predictions of the *microstructure-agnostic* approach tends to catch up with those of the *microstructure-aware* approach, the maximum objective value achieved by the *microstructure-agnostic* approach at the end of the optimization (i.e., after 300 design iterations) is lower than the value achieved by the *microstructure-aware* approach. Thus, the results presented here clearly demonstrates that an explicit incorporation of the knowledge of the material microstructure in the design framework **not only accelerates the materials design process but also results in comparatively better design solutions**.

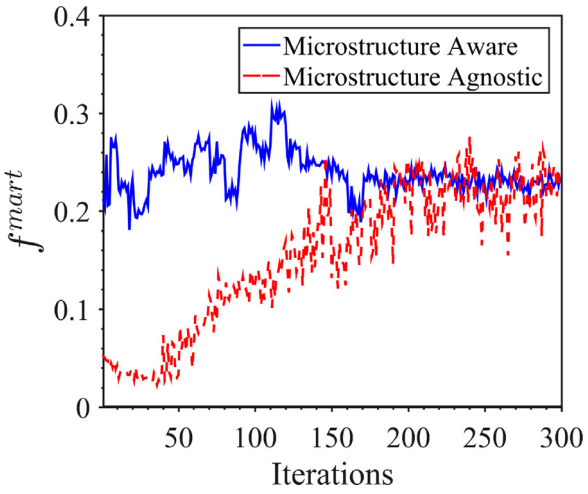


**Fig. 4.** A comparison of the average value of the optimum microstructure parameter (characterized by the volume fraction of the martensite phase, $f^{mart}$) predicted by the traditional *microstructure-agnostic* and the novel *microstructure-aware* material design approaches at each design iteration over five realizations of the design process.

Since the mechanical properties of a material are inherently controlled by the microstructure, we now analyze how the two design approaches explore and converge in the material microstructure space during the design process. A comparison of the average value of the microstructural parameter, i.e. volume fraction of the martensite phase, $f^{mart}$, that corresponds to the average maximum objective value at each design iteration over five realizations of the design process as predicted by the *microstructure-agnostic* and *microstructure-aware* design approaches are shown in Fig. 4. As can be seen in the figure, even though both design approaches start the design process with the same knowledge of the $\mathbf{X_I} - \mathbf{X_O}$ correlation, the value of $f^{mart}$ predicted by the two approaches during early stages of the design process are very different. The *microstructure-agnostic* approach initially predicts a very small value of $f^{mart}$ which then evolves as the design process/iteration continues and finally tends to saturate af-

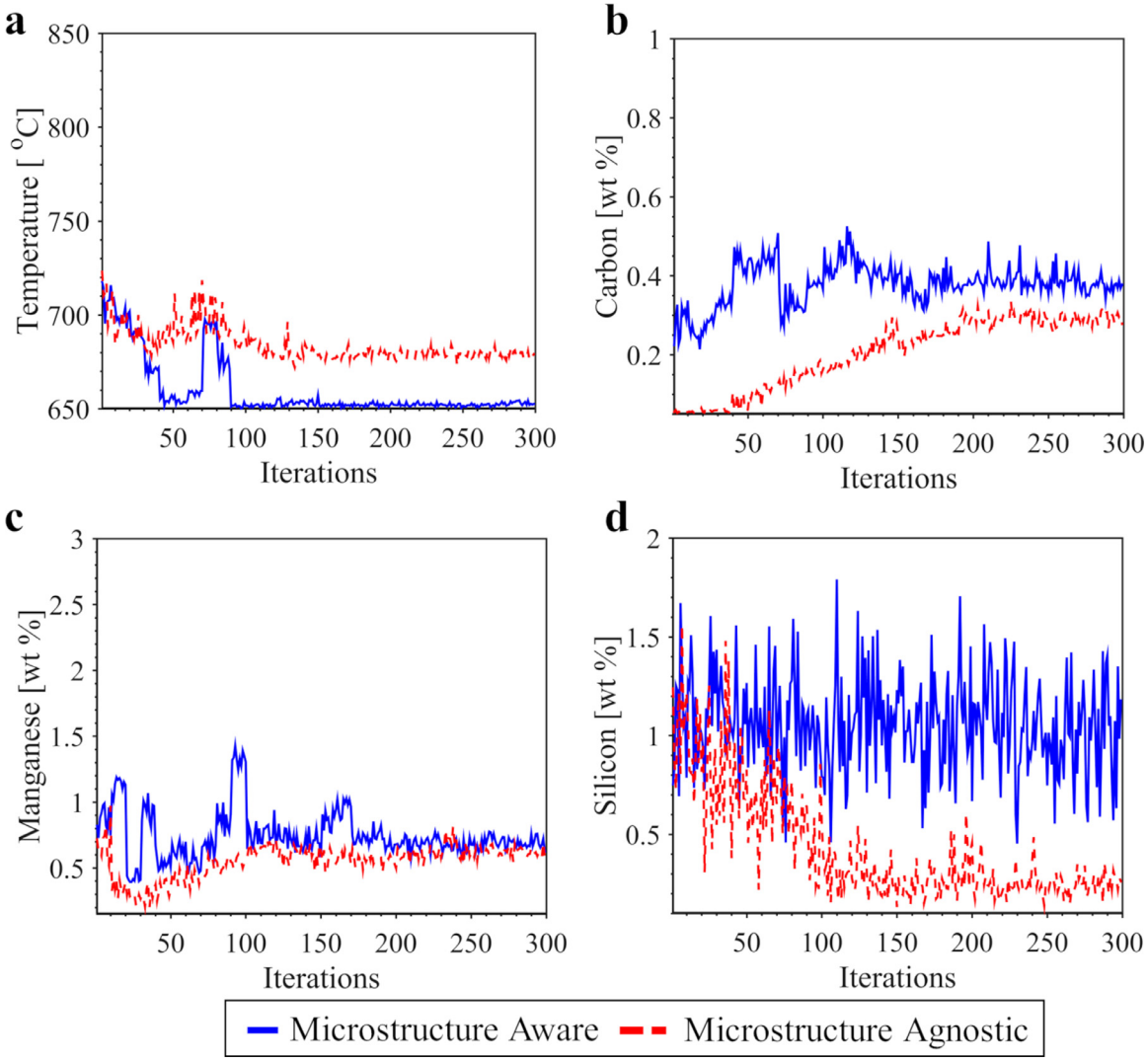


**Fig. 5.** A comparison of the optimum processing/chemistry parameters identified by the traditional *microstructure-agnostic* and the novel *microstructure-aware* material design approaches. (a)-(d) Comparing the average optimal values of the processing parameter, intercritical annealing temperature, and the amount of alloying elements, carbon, manganese and silicon that correspond to the average maximum objective value at each design iteration over five realizations of the design process.

ter a large number (greater than 150) of design iterations. On the contrary, the *microstructure-aware* approach predicts a value of $f^{mart}$ that is close to the saturation value of $f^{mart}$ predicted by the *microstructure-agnostic* approach since the beginning of the design process. This early knowledge of the feasible material's microstructure space that corresponds to the maximum objective value enables the *microstructure-aware* approach to be more efficient than the traditional *microstructure-agnostic* approach.

Next, we compare the average values of the design (i.e., input) variables, intercritical annealing temperature, and the amount of alloying elements, carbon, manganese, and silicon that correspond to the average maximum objective value at each design iteration over five realizations of the design process as identified by the *microstructure-agnostic* and *microstructure-aware* design approaches in Fig. 5. In this particular problem, we note that irrespective of the design approach, the framework is expected to converge into a region rather than a unique point. This is because the objective value i.e., normalized strain hardening rate can be achieved by more than one combination of the processing condition and chemical composition [18]—this is due to the one-to-many mapping between materials properties and microstructures/chemistries [45]. As can be seen in Fig. 5, although the two design approaches are trying to maximize the same objective, they follow different routes and also, on average, converge to different parameter sets in the design space. For example, both *microstructure-aware* and *microstructure-agnostic* approaches identify a similar intercritical annealing temperature in the early stages of the design process, but the *microstructure-aware* approach explores more in this design space in search of the optimum solution and finally converges to a lower value compared to the *microstructure-agnostic* approach. On the contrary, the two approaches identify a very different optimal carbon content in the early stages of the design process and the *microstructure-agnostic* approach explores more in this design space in search of the optimum solution but finally converges to a value close to what is identified by the *microstructure-aware* approach. Both approaches, however, on average follow a similar route and also finally converge to a rather similar value of the amount of manganese. While both approaches identify similar amounts of silicon content in the early stages of the design process, the *microstructure-agnostic* approach explores more in this design space and finally converges to a lower value compared to the *microstructure-agnostic* approach.

Our closed-loop multi-fidelity BO framework employs multiple 'information sources' to estimate the objective as described

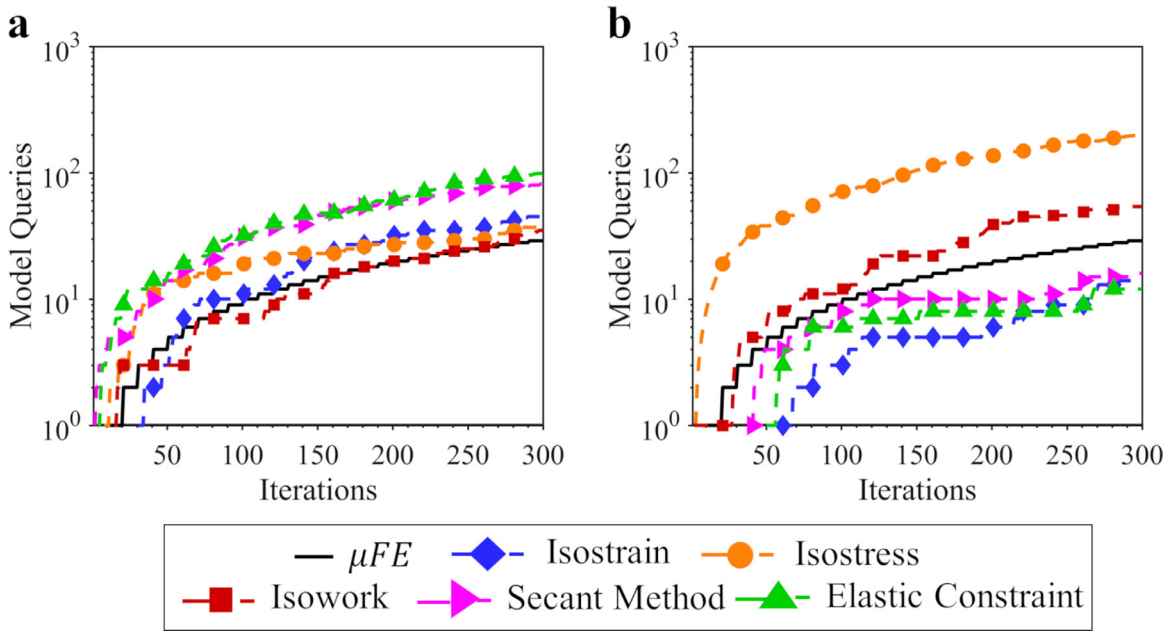


**Fig. 6.** Exploitation of 'information sources' (*isostrain, isostress, isowork, secant method* and *elastic constraint* reduced-order models) and the 'ground truth' ($\mu FE$) model at each design iteration by the (a) novel *microstructure-aware* and the (b) traditional *microstructure-agnostic* material design approaches. The results are shown for one realization of the design process.

in Fig. 2. Thus, we now analyze the impact of the *microstructure-aware* and *microstructure-agnostic* design approaches on the selection of different 'information sources' during the design process. Note that none of the five low-fidelity reduced-order micromechanical models are capable of reproducing the response predicted using the high-fidelity 'ground truth' $\mu FE$ model over the entire microstructure space [35]. Also recall that the criteria to query the 'ground truth' model is set here to every ten design iterations for both design approaches. The results presented in Fig. 6 show the progression of queries made to different 'information sources' as a function of the design iterations for one realization of the design process. As shown in Fig. 6(a), the *microstructure-aware* approach extensively queries the design space using the more sophisticated *secant method* and *elastic constraint* models while the *microstructure-agnostic* approach favors querying the design space using the simple *isostress* model during the early stages of the design process. At later stages of the design process, both approaches begin querying the design space through all available 'information sources.' This may be due to the fact that they have exhausted the potential value of the 'information sources' initially detected as most useful to the design task.

The results presented thus far clearly demonstrate that the two design approaches not only take very different routes in the design space but also utilize different 'information sources' to query the design space in search of the same objective. The results also demonstrate that the *microstructure-aware* approach converges rapidly in the microstructure space and provides a better design solution compared to the *microstructure-agnostic* approach.

To understand what enables the superior performance of the *microstructure-aware* approach compared to the *microstructure-agnostic* approach we compare the predictions of the initial (at the very first design iteration) fused Gaussian Process models built using the two approaches with that of the predictions of exhaustively querying the chain of computational thermodynamics and the 'ground truth' model in Fig. 7, for one realization of the design process. As shown in Fig. 7(a) and (b), despite the fact that the same five sets of $\mathbf{X_I} - \mathbf{X_O}$ correlations are used to build the initial fused Gaussian process models for both the approaches, the predictions of the initial fused Gaussian process model for the *microstructure-aware* approach correlates extremely well with the 'ground truth' compared to the predictions of the initial fused Gaussian process model for the *microstructure-agnostic* approach. The parity plots in Fig. 7(c) and (d) also highlight the quantitatively better correlation between the predictions of the initial fused Gaussian process model for the *microstructure-aware* approach and the 'ground truth' compared to that of the *microstructure-agnostic* approach. In conclusion, an explicit incorporation of the knowledge of the material microstructure in the design framework significantly enhances the initial knowledge of the microstructure-property correlations that in turn leads to more efficient and effective design process.

## 5. Discussion

As material scientists and engineers, we aspire to unravel the underlying PSP relationships of materials. In practice, however, microstructure information is not used as a direct input in a materials design process, and only an analysis of the same is carried out *a posteriori* to rationalize the attained properties. This raises a fundamental question, *"can the intermediate microstructure information aid in the materials design process?"* To answer this question, we have carried out a rigorous analysis to probe the importance of the microstructure information in the materials design process. The latter involves finding the right combinations of material chemistry and processing condition that maximizes a targeted mechanical property of a model dual-phase steel using a closed-loop multi-fidelity BO framework. We first solve this material design problem by following the traditional *microstructure-agnostic* approach where the material design space includes the material chemistry and processing condition, while the microstructure information is only used to carry out multi-level simulations to establish PSP relationships. Next, we solve the same material design problem by following a novel *microstructure-aware* approach where the material design space not only includes the material chemistry and processing condition but also the microstructure information. Our results clearly show that an explicit incorporation

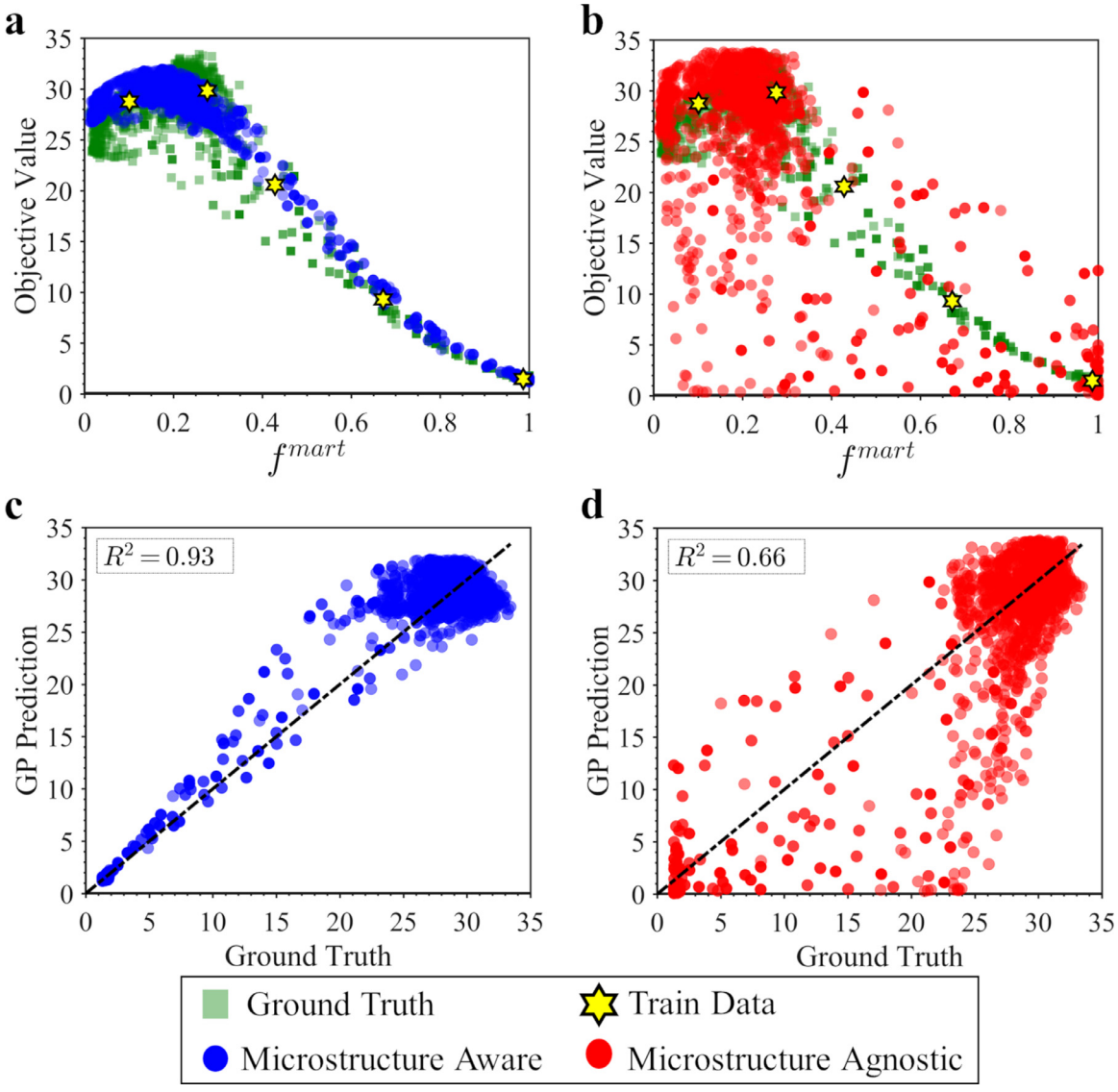


**Fig. 7.** A comparison of the predicted variation of the objective value as a function of the material microstructure characterized by the volume fraction of the martensite phase, $f^{mart}$, obtained by exhaustively querying the chain of computational thermodynamics and 'ground truth' ($\mu FE$) model and by querying the initial (at the very first design iteration) fused Gaussian Process model for the (a) *microstructure-aware* and (b) *microstructure-agnostic* approaches. Parity plots of the objective value obtained by exhaustively querying the chain of computational thermodynamics and 'ground truth' and by querying the fused Gaussian Process model for the (c) *microstructure-aware* and (d) *microstructure-agnostic* approaches. The results are shown for one realization of the design process, and the five initially known 'ground truth' information are marked with stars in (a) and (b).

of the microstructure knowledge in the decision-making process not only accelerates the materials design process, but also results in comparatively better design solutions. A detailed analysis of the materials design process following the *microstructure-agnostic* and *microstructure-aware* approaches show that the two design approaches not only take very different route in the design space but also utilize different set of 'information sources' to query the design space in search of the same objective. The superior performance of the *microstructure-aware* design approach is rooted in the fact that an explicit incorporation of the knowledge of the material microstructure in the design framework significantly enhances our initial knowledge of the microstructure - property correlation that in turn leads to a more efficient and effective design process.

Since it is the difference in the initial knowledge of the microstructure - property correlation that leads to the superior performance of the *microstructure-aware* design approach compared to the *microstructure-agnostic* design approach, it is warranted to compare their performance for a range of known initial design space (input) - objective (output) correlations used to initiate the design process. To this end, we compared the performance of the two design approaches by setting up the design framework using only 1, 10 or 25 randomly selected sets of initially known 'ground truth' input - output correlations. Additionally, to avoid any bias in the design process due to the initial sets of randomly selected input - output correlations, we carried out five realizations of the design process for each sets of initially known input - output correlations. The results of this exercise are given in the Supplementary Figs. S1-S15. Our results clearly show that irrespective of the number of initially known input - output correlations used to initiate the design process, the performance of the *microstructure-aware* design approach is always better than the *microstructure-agnostic* design approach. Furthermore, our results also show that the relative performance of the *microstructure-aware* design approach is even better than the *microstructure-agnostic* design approach when a smaller number of initially known input - output correlations are used to initiate the design process.

Moreover, an explicit incorporation of microstructure information in the *microstructure-aware* materials design approach more accurately represents the trajectory of PP relationships as the microstructure state evolves. This is not necessarily true for a *microstructure-agnostic* materials design approach. Since the microstructure has a strong dependence on chemistry and processing history, simple parametrization that ignores the former are bound to be subjected to considerable uncertainty. Furthermore, from the perspective of irreversible thermodynamics, omission of microstructure evolution renders intrinsic dissipation as a hidden parameter and is completely sidestepped by *microstructure-agnostic* approaches. Such approaches may thus run the risk of establishing PP relationships that are inconsistent with the second law of thermodynamics. Thus, contrary to the *pragmatic* argument of focusing only on the 'black box' PP relationships, this work suggests that explicit consideration of (even very approximate) PSP relationships is a *necessary and sufficient* condition for materials design. Our results show that the way microstructure information improves the materials design process is by acting as a 'through point' that mediates PP relationships, effectively filtering out intrinsically inconsistent regions in the processing space. Microstructure-aware materials design frameworks thus may be considered to belong to the general class of physics-constrained or physics-informed machine learning approaches capable of overcoming many of the shortcomings of data-only methods [46].

Note that incorporating the microstructure information in the material design space increases the dimensionality of the problem. In general, adding dimensions to a design space makes the BO more inefficient [47]. Yet, our results counterintuitively show a positive impact on the decision-making process by *increasing the dimensionality of the design space*. The positive impact of increasing the dimensionality of a given problem has been explored and exploited in a variety of scientific and engineering problems.

For example, the so-called 'kernel trick' of machine learning [48], which replaces inner products with kernel functions to enable nonlinear learning, effectively raises the dimensionality of a machine learner from low dimension to high and even infinite dimensions [49]. This is very common when using support vector machines for classification. In model order reduction, recent methods for lifting maps [50,51] introduce auxiliary variables to a system model to provide more mathematical structure. For example, the introduction of auxiliary variables through lifting maps can lead to polynomial systems of differential-algebraic equations or in other cases, system dynamics with quadratic structure. The resulting well-behaved mathematical structure of the problem caused by the increase in dimensionality leads to far more efficient solution strategies enabling larger problems to be tackled computationally [52].

The identification of new, relevant dimensions in a given problem can also have a profound impact on an entire field of study. For example, the celebrated Buckingham $\pi$ theorem [53] from the study of dimensional analysis [54] states on physical grounds that physics-based equations may be rewritten in terms of dimensionless parameters providing there is some physical connection among the variables in the equation. This identification of a latent governing parameter or set of parameters has had a profound impact on the field of fluid mechanics, where parameters such as the Reynolds number, the Mach number, and the Froude number have been discovered. These parameters are all derived from the original variables of a given problem, and therefore, even though they increase the dimensionality of the problem, their use leads to a dramatic increase in the physical understanding of the phenomena at play.

The proposed *microstructure-aware* closed-loop multi-fidelity BO framework for materials design is demonstrated here to be extremely efficient and effective in realizing goal-oriented material design using a combination of models and simulation techniques. Importantly, this design framework can also be put into practice even for an entirely experimental materials design campaign by using ever-growing high-throughput material processing and characterization techniques. It is also important to note that since each 'information source' is represented in our design framework as a stochastic model (i.e., Gaussian process), there is no fundamental limitation on using a combination of experimental, modeling and/or simulation based 'information sources,' *as long as they are all represented as Gaussian processes or other stochastic models*.

Our proposed framework can also be further enhanced by utilizing more sophisticated thermodynamics/kinetics-based modeling schemes (e.g., phase-field simulations [55]) to not only predict the phase volume fraction and composition but also the size and morphology of the constituent phases, and by incorporating them explicitly in the decision-making process. Another future direction to enhance the performance of the proposed materials design framework will be to incorporate adaptive active subspace method to efficiently handle the large dimensionality of the design space [56,57] by taking advantage of the fact that in materials design problems the objective function in general is more sensitive to some design variables compared to others.

## 6. Concluding remarks

In this work, we have presented a *microstructure-aware* closed-loop multi-information source fusion (multi-fidelity) Bayesian Optimization framework for goal-oriented materials design. The specific material design problem considered here involved finding the right combination of materials chemistry and processing condition that maximizes a targeted mechanical property of a model dual-phase steel. We solved this material design problem by using both a traditional *microstructure-agnostic* approach where the microstructure information is only used to establish PSP relationships and the proposed *microstructure-aware* approach where the microstructure information is also used in decision-making as we navigate through the material design space. Our analysis clearly shows that incorporating microstructure knowledge into the materials design process (for a problem where microstructure intervenes to influence properties of interest) results in better, faster solutions to the same problem. This improved performance can be ascribed to the fact that microstructure information helps 'shape' our initial understanding of microstructure - property correlations.

This is a remarkable finding since, *a priori* it would not make much sense that a derived quantity would have such a positive effect. Yet, there are many examples in science and engineering when lifting the dimensionality of a problem makes it more solvable. These additional dimensions (for instance, microstructural information in this particular case) are derived from the original parameters of the problem, and therefore, even though they increase the dimensionality of the problem, they lead to a dramatic increase in the physical understanding of the phenomena at play.

We close by briefly discussing the implications of this work on the design of new platforms for autonomous materials discovery/design. Our finding that microstructure information indeed can help accelerate the materials discovery process in a concrete way provides a theoretical support to the importance of adding one or many microstructure characterization steps within a materials discovery workflow. Moreover, it provides some ideas on what other interesting problems such platforms could tackle. For example, it would be very interesting to develop systems capable of actively discovering objective-relevant microstructural features. Such an adaptive AI-enhanced characterization framework would then become more efficient over time, by focusing only on the microstructure information most relevant to the problem at hand. In our admittedly 'toy-like' problem, for example, the volume fraction

of the martensite phase makes obvious sense as the microstructure feature most correlated with the plastic response of the composite microstructure. When considering fracture, on the other hand, the topology, connectivity or other higher-order microstructural features may be more important. In the future, we intend to explore these ideas further, using both *in silico* and *in vivo* platforms for materials discovery and design.

## Declaration of Competing 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.

## Acknowledgment

The authors acknowledge the financial support provided by the U.S. National Science Foundation through grant number NSF-CMMI-1663130, *DEMS: Multi-Information Source Value of Information-Based Design of Multiphase Structural Materials*, and the high performance research computing resources provided by Texas A&M University. DA and RA also acknowledge grant number NSF-DGE-1545403. RA also acknowledges the grant numbers NSF-IIS-1849085 and NSF-IIS-1835690.

## Supplementary material

Supplementary material associated with this article can be found, in the online version, at 10.1016/j.actamat.2021.117471.

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