Key micromechanics issues in integrated material design

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Abstract. Nowadays the acceleration of material discovery is essential more than ever to hold the fast evolving requirements of innovative products. This acceleration depends on our ability to set up a material design process for tailoring materials from targeted engineering performances. One of the important building block passages, in the material design journey, is the bridging of micro-scale to meso-scale through micromechanical models. Unfortunately, these models include a lot of uncertainties resulting from their inbuilt ad-hoc assumptions, which inevitably impacts the material design process performance. In the present paper, robust design methods are reviewed and subsequently applied to quantify uncertainty in micromechanical models and mitigate its impact on material design performances. This includes examining principles for evaluating the level degree of uncertainty on material design process, and their use in micromechanical models. Also, developing robust design approaches to alleviate uncertainty effects and improve the quality of the design performance. Ultimately, the limitations of these approaches are discussed and the research opportunities, to overcome the shortness of actual approaches in respect to micromechanical models, are clarified.

1. Introduction

Engineering materials and materials science have witnessed several evolution phases. Primarily, Materials have been discovered by chance then new materials have been developed with trial-and-error techniques, these techniques allowed materials to be treated as a black box subjected to repeated experiments [1]. Experimental results then were gathered in materials databases. Thus, engineering materials has been taught using the paradigm of selecting materials on the basis of tabulated databases of properties [1]. Consequently, the performance of many engineering products and systems is limited fundamentally by the properties of available constituent materials. Evidently, one can no longer limit the performance of systems to available materials. Thus, the focus shifted towards the design of materials with superior properties for particular applications. The goal is to tailor material microstructure for desired applications that satisfy performance requirements on the system level. Often, however, these performances are in conflict when choosing the microstructure. It is important to note, that these desired material properties and performance characteristics usually depend on phenomena that operate at different length and time scales. Material design is then built on a multi-scale journey from the smallest scale to the system level. One of the important multi-scale passages is the bridging of micro-scale to meso-scale through micromechanical models. The primary objective of this work is to discuss overall challenges in incorporating micro-mechanical models into materials design process.
2. **Leading challenges in integrating micromechanical models in material design process**

Micromechanical models play a crucial role in the achievement of materials design initiative. These models aim to predict accurately the response of a material under uniform load conditions from the properties of their constituents. Unfortunately, virtually all micromechanical models are embryonic from material design point view. It is important to emphasize that micro-mechanical models inevitably incorporate assumptions and approximations that impact the precision and accuracy of predictions. When added to the material design process, they bring their drawbacks and the uncertainty may be magnified when a model is utilized near the limits of its intended domain of applicability or when information propagates through a series of models [2]. Furthermore, microstructure itself has a random character, such as sizes and distributions of grains, phases, and so forth. These sources of uncertainty give rise to the need for considering sensitivity of properties and responses of interest to variation of microstructure at various scales, as well as propagation of model uncertainty through multiscale model chains. So one of the most important and challenging problems is the uncertainty in these models associated to various sources, including [3]: (i) insufficient knowledge about microstructure. (ii) natural variability and randomness in materials (phases introduced by processing conditions) that are not taken into account. (iii) Ad-hoc parameters used by these models to presumably describe the microstructure.

![Figure 1. Hierarchy of levels from atomic scale to system level in concurrent materials design.](image)

Uncertainty is prevalent in most facets of micro-mechanical models, the uncertainty of microstructure and model parameters impact significantly material design process. Consequently, a combined strategy of bottom–up and top–down modeling (figure 1) to target performance requirements will be very difficult [2,3]. In this respect, managing uncertainty and its propagation through a model is of paramount importance. The only way to gain this goal is by having a good understanding of microstructure (approximations and simplifications), in order to let the models be more realistic and transmit information without loss, by combining the approach with simulation tools, and finally by easing the decision making. To account of uncertainty, a practical approach includes many aspects [2,4], mathematical techniques for evaluating the level degree of uncertainties on material design journey, and design methods for performing and generating robust design, by seeking the robust solutions that are relatively insensitive to variation of microstructure and various other sources of uncertainty. In later sections of this paper all these methods will be investigated.

3. **Uncertainty quantification**

To properly quantifying uncertainty, it is necessary to categorize the types of uncertainty in a model.
The uncertainty quantification is the process of identifying different sources of uncertainty and developing corresponding mathematical representations, by estimating output uncertainty (probability distribution of system response) with variability in input parameters [2]. One must mention that quantification of aleatory uncertainty (inherent in the physical system and can only be quantified in a statistical sense) is relatively easier than quantification of epistemic uncertainty (arises from incomplete knowledge of a system) if measuring a system behavior is feasible [5, 6, 7, 8].

As presented in table 1, depending on the types of system model deterministic (there are no random errors in a system response) or non-deterministic and the type of input parameters are uncertain (without probability density functions due to lack of information) or may be presented as Probability distribution, uncertainty analysis methods have been classified as non-probabilistic and probabilistic methods. The probabilistic methods are further devised on statistical and non-statistical approaches. We can note from the table that the Monte Carlo simulation is the only method for quantifying non-deterministic system response variation with the probability distributions of input parameters. If the input variables are non-parametric, it is impossible to quantify uncertainty.

As aforementioned, the aleatory system uncertainty is quantifiable; however, epistemic uncertainty is virtually impossible to quantify [2]. Therefore, reducing uncertainty (instead of being quantified) is feasible when designer has large amounts of data and by increasing the knowledge or getting more information about system. Instead, researchers [9, 10, 11, 12] have focused on procedures to reduce uncertainty and validate a model’s accuracy. However, the restriction of these methods is that designers must have some true results. In some cases, we cannot obtain any better data than current data due to severe uncertainty in a system or restrictions of computational or experimental expenses, which is the case of multiscale materials design specially micromechanical model. Uncertainty analysis for nondeterministic simulation is indispensable for multiscale materials design since the simulation models for heterogeneous material behavior tend to be stochastic [4].

**Table 1.** Uncertainty analysis methods versus characteristics of a system [2].

| System model | Deterministic | Non-deterministic |
|--------------|---------------|-------------------|
| Input        | Uncertain     | Probability distribution |
| Available uncertainty analysis methods | Non-probabilistic methods: | Probabilistic methods: |
|              | Interval analysis | 1.Statistical methods |
|              | Fuzzy logic    | -Monte Carlo simulation |
|              |               | -Latin Hypercube sampling |
|              |               | 2.Non-statistical method |
|              |               | -First and second order moment methods |
|              |               | -Polynomial chaos expansion |
|              |               | -Stochastic response surface methods |
|              |               | N/A |
|              |               | Probabilistic methods |
|              |               | -Statistical methods: |
|              |               | Monte Carlo |

4. Uncertainty management

Uncertainty management process allows designing a system to be unresponsive to uncertainty without removing the underlying sources, by using robust design approaches. In other words, these approaches aim to alleviate uncertainty effects and improve the quality of a system performance [13], by making the system response insensitive to uncontrollable system input variations. This is also called parameter design. In robust design literature, design parameters are split into three categories: (i) control factors, parameters that a designer adjusts, (ii) noise factors, exogenous parameters that are not under a designer’s control, (iii) responses, are performance measures for the product or process. It is essential for designers to identify where the uncertainty sources are located in a system model in order to employ a relevant uncertainty management approach.
Robust design approaches are categorizing as: Type I robust design, originally proposed by Taguchi [14], focuses on designing a systems that fulfill the performance despite variations in noise factors which are parameters that designers cannot control in a system. Type II robust design [15] is used to design a system that fulfills the performance despite variations associated with parameters that a designer can control in a system. A method for Types I and II robust design has been proposed, namely the Robust Concept Exploration Method [16]. Briefly, it based on design of experiments for generating set points to achieve trade-off between performance measures and uncertainty components in the compromise decision support problem, for more detail of this method, see [17]. These types of robust design have been extended to include Type III [2], which considers sensitivity to uncertainty set in a model which is due to a combination of limited knowledge and data of nonparametric system noise or un-configured system noise. Type III robust design considers not only the objective function but also the two uncertainty bounds due to the non-parametric variability, un-configured variability, and model parameter uncertainty.

The final type of robust design is for multidisciplinary system which takes into account uncertainty and managing the uncertainty generated in the design process chain, this type of uncertainty arises from accumulated and propagated errors in decisions made by designers in subsequent series of uncertain subsystem models. To deal with this kind of uncertainty a method called The Inductive Design Exploration Method (IDEM) had been proposed by Choi et al [2,18], to identify adjustable ranges of design variable values under different types of uncertainty which is rise from natural variability, model uncertainty and uncertainty propagation in a design process chain. IDEM is schematically illustrated in figure 2. IDEM has two major objectives: (1) to explore top–down, requirements driven design, guiding bottom–up modeling and simulation, and (2) to manage uncertainty in model chains. It is based on three steps:

**Step 1:** It is necessary to define the design space exploration (x space in figure 2), the interdependent space (y space), and the performance space (z spaces). Discrete points are generated in each of these spaces (Discretizing).

**Step 2:** The discrete points which are generated are evaluated based on the mapping models (models f and g in figure 2) and the evaluated data sets which are composed of a discrete input point and output range are stored in a database. These two steps are called parallel discrete function evaluation in IDEM, process as follows:

- **Discretizing:** all possible combinations of discrete input of associated input variables are created
- **Grouping:** The discretized points created by the discretization process are grouped as input sets for mapping models.
- **Mapping:** The points in each group are evaluated in parallel by each mapping model and the evaluation results are stored with the input points.
- **Merging:** Sets of input points and corresponding outputs obtained in the mapping step are merged to form a set of evaluated original discrete points.

**Step 3:** Feasible regions in y and x spaces are successively identified using a metric called Hyper-Dimensional Error Margin Index (HD-EMI), for determining if a discrete point from an input space maps to a feasible design solution in the output space. It is the Inductive Discrete Constraints Evaluation (IDCE).
5. Critical evaluation

After presenting an overview of the actual methods and approaches of the design under uncertainty process, which comprise uncertainty quantification in engineering systems and uncertainty management methods, we critically evaluate the capabilities of those methods and approaches from material design perspective. Then we identify the research opportunities for facilitating the integration of micromechanical models in material design process.

As discussed, several methods have been performed to quantify and estimate the degree of aleatory uncertainty in a system, but the uncertainty analysis methods for non-deterministic system models have not been widely investigated in literature except for Monte Carlo method [2]. Monte Carlo method is the only method for quantifying a non-deterministic response variation with input parameters probability distributions; however, it is computationally too intensive to use into material design. In the case where the input variables are non-parametric, it is impossible to quantify uncertainty. Therefore, an uncertainty analysis method for non-deterministic simulation is indispensable. The epistemic uncertainty is reduced rather than quantified, but in the case of multiscale materials design especially micromechanical model, it is impossible to employ the actual approaches because of the limited knowledge about the material microstructure [2].

For managing uncertainty many robust design methods for designing a system to be insensitive to uncertainty were reviewed in the previous section. Type I robust design is not valid if noise factors cannot be quantified [19]. However the uncertainty in material design tends to be unparameterizable. Neither the types I and II robust design can design a system to be insensitive to uncertainty in system model such as the morphology variability in material, even if Type III robust design approach have been proposed, but It is nearly impossible to use this approach in materials design until any computationally inexpensive uncertainty analysis method have been performed [2].

The inductive design exploration method has been presented as potential approach for the multidisciplinary robust design methods; however, it’s still short, first because it cannot overcome the uncertainty in material models due to idealization associated with a lack of complete knowledge of a given phenomenon and its depiction. For example, there is uncertainty in the constitutive models which are used to represent behavior of individual phases. Second IDEM may be computationally intensive if the number of design variables is large or the simulation model is expensive [2], also if the design process is not sufficiently constrained, it may give large sets of feasible processing spaces in

**Figure 2.** A schematic procedure for IDEM [19].

IDEM has been extended to account for model parameter uncertainty [19]. Additional work needs to be performed to account for other representations of epistemic uncertainty.
the material design hierarchy and it becomes difficult to choose a single solution from these sets of solution [19].

The problem of uncertainty in material design process has been widely studied, but The main conclusion to be drawn is that none of the outlined approaches for mitigation uncertainty had satisfactory results to deal with this endemic uncertainty in constitutive models, which are used to represent behavior especially in micromechanical modeling, that why the improvement of the accuracy of this models and facilitate their incorporating in material design process is our primary proposes.

6. Conclusion

In this work, a number of issues related to integrating micromechanical models in material design process were identified. These issues were mainly associated to uncertainty quantification and uncertainty management in micromechanical models. This uncertainty is due mainly to idealization resulting from the lack of complete knowledge of microstructure and its description. The key methods and approaches for dealing with this uncertainty were reviewed and critically evaluated; first to identify their drawbacks and second to draw the research opportunities in this field. The main conclusion is that further work is needed to deal with uncertainty in micromechanical models for the ultimate goal to incorporate them in the material design process. The best way to do this, in our point of view, is by building a rational material design exigencies framework for developing efficient micromechanical models for the material design journey.

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