Plasticity-Related Microstructure-Property Relations for Materials Design

David L. McDowell\textsuperscript{a}, Hae-Jin Choi\textsuperscript{b}, Jitesh Panchal\textsuperscript{c}, Ryan Austin\textsuperscript{d}, Janet Allen\textsuperscript{e} and Farrokh Mistree\textsuperscript{f}

GWW School of Mechanical Engineering, Georgia Institute of Technology, Atlanta, GA 30332-0405 USA

\textsuperscript{a}david.mcdowell@me.gatech.edu, \textsuperscript{b}haejin.choi@me.gatech.edu, \textsuperscript{c}jitesh.panchal@me.gatech.edu, \textsuperscript{d}gtg580s@mail.gatech.edu, \textsuperscript{e}janet.allen@me.gatech.edu, and \textsuperscript{f}farrokh.mistree@me.gatech.edu

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Abstract. Design has traditionally involved selecting a suitable material for a given application. A materials design revolution is underway in which the classical materials selection approach is replaced by design of material microstructure or mesostructure to achieve certain performance requirements such as density, strength, ductility, conductivity, and so on. Often these multiple performance requirements are in conflict in terms of their demands on microstructure.

Computational plasticity models play a key role in evaluating structure-property relations necessary to support simulation-based design of heterogeneous, multifunctional metals and alloys. We consider issues related to systems design of several classes of heterogeneous material systems that is robust against various sources of uncertainty. Randomness of microstructure is one such source, as is model idealization error and uncertainty of model parameters.

An example is given for design of a four-phase reactive powder metal-metal oxide mixture for initiation of exothermic reactions under shock wave loading. Material attributes (e.g. volume fraction of phases) are designed to be robust against uncertainty due to random variation of microstructure. We close with some challenges to modeling of plasticity in support of design of deformation and damage-resistant microstructures.

Introduction

Traditionally, materials are selected from a materials database in which properties of materials are tabulated. However, the paradigm is now evolving into designing materials concurrently with products/components to meet specific performance requirements. By definition, a multifunctional material is one for which performance dictates multiple property requirements that are often conflicting, for example both strength and ductility. In view of the complexity of modeling material process history and nonequilibrium changes of microstructure during inelastic deformation, emerging capabilities in computational materials science and constitutive modeling must be combined with systems engineering methods to realize this goal. McDowell [1,2] recently discussed challenges to microstructure design of materials in relation to elastic-plastic deformation and damage evolution. This paper describes a methodology developed in the intervening years to address, in part, these challenges.

Olson [3] has provided a philosophical underpinning of the goal-oriented approach to materials design. The conventional approach in mechanics modeling of hierarchical processes and systems is a “bottom-up”, cause-and-effect, deductive methodology of modeling the material’s process path, nanostructure and microstructure, resulting properties, and then relating properties to performance, as shown in Fig. 1. In contrast, we seek “top-down”, goals/means, inductive methods to design the process route and resulting microstructure and mesostructure of a material if our goal is to tailor a material to a set of specified performance requirements.

We see that certain mappings (models, codes, and heuristics) are necessary to support materials design according to Olson’s hierarchy in Fig. 1:
Process-structure (PS) relations: Establish manufacturing constraints, cost factors, thermodynamic feasibility, and kinetic feasibility (feasibility of rates of process, necessary driving forces, and long term stability of metastable microstructures)

Structure-property (SP) relations: Relate composition, phase and morphology information, expressed using distribution functions or digital representations amenable to computation, to response functions that relate to properties of relevance to the design. This is most often an intrinsically hierarchical modeling exercise.

Property-performance (PP) relations: Relate feasible properties to response functions that are relevant to imposed performance requirements, either through detailed point-by-point computational models or by construction of approximate response surface or surrogate models, depending on the degree of computational intensity.

Figure 2 shows how this hierarchy is broken down into mappings of vertical type (PS, SP, PP) and lateral type, the latter involving a reduction of order of the material representation to affect a reduction of the degrees of freedom. Vertical mappings of SP type are sometimes referred to as homogenization relations that associate a certain microstructure idealization with a set of desired property and response attributes.

Of course, this goal of top-down materials design has many challenges:

- The role of extreme value distributions (not just mean field averages) of certain microstructure features that control properties such as fracture and fatigue must be addressed.
- The nonlinear, path dependent behavior of metals and alloys limits extent of parametric study and parallelization of continuum analyses. Moreover, it engenders dependence upon initial conditions and limits pursuit of inverse problems in a strict sense.
- A wide range of local solutions can be realized for specified objective functions in terms of property or performance requirements, leading to non-uniqueness and perhaps large families of possible solutions.
- Representation of microstructure representation presents challenges in terms of how much information to store and in what format. Moreover, the goal of materials design is to explore microstructures that do not exist, using computational simulations to estimate properties. One cannot neglect the fact that process capabilities constrain achievable microstructures,
and that thermodynamics and kinetics (history) considerations limit the range of accessible or feasible microstructures. Hand-in-hand with selection of material representation is the issue of computational tractability.

- Major sources of uncertainty in processing, microstructure, modeling, etc. must be taken into account, as they can dominate the configuration of the design process and range of acceptable solutions. Uncertainty in assigning local properties of phases is significant. In fact, this consideration often demands robust design approaches against such uncertainty rather than some sort of multi-objective optimization.

- Material models (PS, SP) and design results must be validated, using principles of internal consistency, statistical realizability, and validation of material response at various length scales by direct or indirect measurement [4]. Certain microstructure features are quite amenable to high resolution characterization over substantial fields of view, such as grain size and orientation information. Others are not, such as fine scale precipitates.

### Multiscale Modeling and Materials Design

There are at least two compelling reasons to understand and model plasticity over a range of length scales [1]:

1. to design material microstructures to tailor plastic deformation-related properties, and
2. to develop consistent, unified theories of the formation and evolution of defects during plastic flow at various length scales (cf. [5]).

The hierarchy of mappings in Fig. 2 is closely related to a hierarchy of material length (and time) scales that are of utility in materials design, shown in Fig. 3. Numerous methods for multiscale modeling have been developed, including concurrent multiscale models, domain decomposition for discrete to continuous transitions, two scale homogenization, statistical mechanics of evolutionary systems, “Handshaking” methods for informing reduced DOF models based on results of higher DOF models, variational principle of virtual velocities (PVV), based on the working rate of microstructural rearrangements (dislocation glide, diffusive rearrangements, relative grain boundary motions, etc.) (cf. [6]), and a number of other emerging multiscale homogenization approaches.

There are, of course, practical limitations to concurrent multiscale modeling in addition to computational issues, such as assignment of initial conditions for all microstructure features and evolving, embedded finer scale attributes (e.g., dislocation densities for various populations, crack distributions, etc.). With regard to materials design objectives, concurrent multiscale modeling schemes or homogenization concepts may not be necessary in many cases, because the goal is not to accurately predict properties but to understand sensitivity to microstructure and to capture essential dominant mechanisms and their transitions as a function of forcing functions and responses applicable to the given design scenario. Although seamless ‘bottom-up’ modeling is scientifically appealing, it is often too idealized and chained with a compilation of approximations that may compromise viability for materials design. For purposes of materials design, we seek to employ models in the range for which they are most appropriate and accurate, and use decision-based (e.g., utility theory) protocols for informing models/decisions based on these analyses. The necessity of seamless scale transitions must be determined by the degree of coupling in the system and the utility of information gained by modeling that coupling in great detail. In general, a hierarchy of models at
various scales may be employed, with different purposes, at different length and time scales, to inform decisions.

**Uncertainty in Materials Design**

One must deal with various sources of uncertainty in designing materials, since it is inherently an exercise of stochastic character, including [7]:

**Natural Uncertainty (system variability)**
- Parameterizable: Errors induced by processing, operating conditions, etc. (noise and control factors)
- Unparameterizable: random microstructure

**Model Parameter Uncertainty (parameter uncertainty)**
- Incomplete knowledge of model parameters due to insufficient or inaccurate data

**Model Structural Uncertainty (model uncertainty)**
- Uncertain structure of a model due to insufficient knowledge (approximations and simplifications) about a system.

**Propagated Uncertainty in a Process Chain (process uncertainty)**
- Propagation of natural and model uncertainty through a chain of models.

To address these sources of uncertainty in designing materials, there are several possible routes. One is to improve models and characterization of material structure. Another practical approach is to quantify the uncertainty to the extent possible and then design to seek solutions that are less sensitive to variation of microstructure and various sources of uncertainty. To this end, we introduce the compromise Decision Support Problem (cDSP) methodology [8], in which multiple design objectives are set as targets, with deviations from these goals minimized subject to user preferences to select from among a family of solutions, subject to a set of constraints (cf. [9,10]). Effectively, we employ this decision-based strategy for linking information from one sort of simulation or heuristic to advise inputs to another model within a hierarchical structure, as shown in Fig. 4. Materials design typically involves multiple objectives mapping into several property domains; for example, gas turbine engine blades involve thermal, chemical, mechanical and thermomechanical properties. The notion of optimization, typically applied to a single objective, is sensible only for limited sensitivity to variation of microstructure and various sources of uncertainty. To a demanding set of considerations! For multiple design objectives, robustness establishes preference among candidate solutions; we seek solutions with less sensitivity to variation of noise and control parameters. In addition, we seek designs that are robust against variability associated with process route and initial microstructure, forcing functions, cost factors, design goals, etc. Moreover, we introduce new methods to deal with uncertainty due to microstructure variability and models [11] as well as chained sequences of models in a multi-level (multiscale) context [12]. The designer effectively receives decision support from the cDSP and must make choices within the flexibility of the design process.

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<th>Given</th>
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<td>m, number of system goals</td>
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<td>g(x), constraint functions</td>
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<td>g(x)=0 \ i=1,...,p</td>
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<td>g(x)&lt;0 \ i=p+1,...,p+q</td>
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<td>Bounds:</td>
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<td>X_i^{min} \leq X_i \leq X_i^{max}</td>
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Figure 4. Compromise Decision Support Problem (cDSP) formulation for multi-objective design, with deviations from multiple goals minimized within constraints.
New Types of Robust Design for Materials Design

Robust design, proposed by Taguchi [13] is a method for improving the quality of a product by minimizing the effect of uncertainty on product performance. From Taguchi’s perspective, design performance should be on-target with low variability. This philosophy leads to designs that are very different from traditionally preferred optimum solutions. ‘Optimal’ solutions offer performance that may be on-target nominally but often deteriorates significantly when conditions or assumptions change. Herbert Simon proposed a philosophy similar to Taguchi when he introduced the notion of “satisficing” and contrasted it with optimizing: “The decision that is optimal in the simplified model will seldom be optimal in the real world. The decision maker has a choice between an optimal decision from an imaginary simplified world, or decisions that are ‘good enough’, that satisfice, for a world approximating the complex real one more closely.” [14]

Our philosophy in designing materials is grounded in the philosophies of Simon and Taguchi. Because material systems are complex and prone to many of the sources of uncertainty discussed in the previous section, we seek materials design solutions that are satisficing and robust. There are several categories of robust design, associated with different types of uncertainty. Type I robust design, originally proposed by Taguchi, centers on achieving insensitivity in performance with regard to noise factors—parameters that designers cannot control in a system. Relevant examples of noise factors are variation of ambient temperature, morphology changes, etc. Type II robust design, proposed by Chen and coauthors, relates to insensitivity of a design to variability or uncertainty associated with design variables—parameters that a designer can control in a system. A method for Types I and II robust design, namely, the Robust Concept Exploration Method [8,9] has been proposed. The Robust Concept Exploration Method (RCEM) is a domain-independent approach for generating robust, multidisciplinary design solutions. Robust solutions to multi-functional design problems are preferable trade-offs between expected performance and sensitivity of performance due to deviations in design or uncontrollable variables. These solutions may not be absolute optima within the design space.

The types of robust design have been extended to include Type III. Type III robust design considers sensitivity to uncertainty embedded within a model (i.e., model parameter/structure uncertainty). Model parameter/structure uncertainty is typically different from the uncertainty associated with noise and control factors, because it could exist in the parameters or structure of constraints, meta-models, engineering equations, and associated simulation or analysis models. The approach for Type III robust design is focused on incorporating the Error Margin Indices [11] within the RCEM (RCEM-EMI), and it is based on simultaneous incorporation of Type I, II, and III robust design techniques. Type III robust design is typically required to manage (a)
inherent variability that is difficult or impossible to parameterize, such as stochastic microstructure, (b) limited data, and (c) limited knowledge in new domains such as a new class of microstructures, as shown in Fig. 5.

Figure 6 clarifies the application of Types I-III robust design, showing that while application of traditional Types I-II robust design methods seek solutions that are insensitive to variations in control or noise parameters, Type III robust design additionally seeks solutions that have minimum distance between upper and lower uncertainty bounds on the response function(s) of interest associated with material randomness and model structure/parameter uncertainty. These bounds are determined from the statistics obtained from application of models over a parametric range of feasible microstructures and process conditions relevant to the simulations necessary to support design decisions (cf. [11]). This combination of “flat regions” of the objective function and tight bounds of variability associated with uncertainty of the functional relationship between control/noise and response is a new concept introduced to address realistic considerations in materials design.

In view of the hierarchy of length scales corresponding to microstructure and mechanisms that affect PS and SP relations, another essential ingredient of robust design is designing a system that is insensitive to the propagated uncertainty in the design process. The basic idea of our approach for finding solutions that are robust against the propagated uncertainty in an multi-level model chain is passing down the feasible solution range in an inverse manner, from given final performance range to design space, instead of a bottom-up manner, passing mean and variance (or deviation) of a output to the next model. This approach allows for a designer to find not just a single robust solution, but also ranged sets of robust solutions among which a designer expresses preference for a solution.
Figure 7 illustrates our concept for selecting the most effective robust solution in multi-level robust design, applicable to multiscale modeling and simulation. If we assume that we have two candidate solutions, Designs 1 and 2, of which final performances are identical, then which design should we select among the two? Since the projected range of Design 2 in the intermediate space of Y is farther from the constraint boundary than Design 1, we believe that Design 2 is better than Design 1; Design 2 is more reliable with regard to potential errors (unquantified uncertainty) in the mapping functions, $f$. Current robust design method cannot address this issue since the method only focus on the final performance range. With this approach, we believe, the better solution may be obtained considering model uncertainty that is hard to quantify as well as quantified propagated uncertainty.

Materials Design as a Process

The foregoing framework of multi-objective decision support for designing materials can be readily extended to incorporate the design of the material (composition, morphology, etc.) as part of a larger overall systems design process. Results of models at multiple length scales and time scales can be analyzed as necessary to provide decision support for selection of hierarchical morphology and process path to deliver a required set of multifunctional, often conflicting properties. Moreover, the same framework can embody the hierarchy of process-structure-properties-performance set forth by Olson [3], shown in Fig. 1. The inductive goals/means engineering approach is relevant to design, and contrasts with the usual approach taken in application of the scientific method, which focuses on deductive cause-and-effect (bottom-up). Figure 8 shows a flow diagram of the design process, with design requirements as inputs and robust sets of design specifications as output. We can map Olson’s inductive goals/means concept of materials design directly to the systems-based approach adopted in the present work, as indicated in Fig. 8. Effectively, process-structure-property relations inform the designer and map directly into the design process that facilitates transformation of overall design requirements into a set of robust specifications for the material system of interest.

Example: Reaction Initiation with Dynamic Plasticity in an Energetic Material

Multiphase energetic materials (thermite mixtures) are mixtures of micron scale (or finer) metal and metal oxide (sometimes intermetallic) powders with a binder and limited porosity. Hence, these are complex, three or four phase mixtures. Shock compression of these materials can result in the initiation of exothermal chemical reaction that may or may not propagate in self-sustained manner at scales well above the mean particle size. Shock compression of spatially-resolved particle systems must be modeled to understand the effects of dynamic plastic deformation, particle interactions and pore collapse at the mesoscale on the reaction initiation behavior to design the mixture for specified reaction initiation conditions (shock strength). The simulations involve propagating shock waves through aluminum-iron oxide thermite systems (Al+Fe$_2$O$_3$) composed of micron-size particles suspended in a polymer binder [16]. As shown in Fig. 9, a fully thermomechanically coupled
Eulerian code RAVEN [17] is used to model the progression of a shock wave induced by imposed high particle velocity on a statistic volume element (SVE) of microstructure. The simulated (reconstructed) microstructures are based on particle size distributions, volume fractions, and levels of porosity measured experimentally for as-processed materials. The measured nearest neighbor distribution of the Al particles (largest particles in Fig. 9, approximately 1-2 microns in diameter) is met through simulated annealing, followed by constrained Poisson point placement of the Fe₂O₃ particles and pores. The epoxy binder then constitutes the remainder. Post-processing enables determination of the shock velocity in the mixture (Hugoniot behavior), the pressure profile through the SVE as a function of wavefront position, and the detailed temperature rise throughout the SVE. Appropriate rate- and temperature-dependent constitutive equations are used for the constituents (Klepazcko model [18] for 1100 Al, Hasan-Boyce model [19] for Epon 828, and an athermal model for elastic-plastic behavior of Fe₂O₃).

The probability of shock-induced reaction initiation is then evaluated from the temperature field at hot spots using the Merzhanov instability criterion for thermal explosion [20], which essentially considers whether or not heat generated at hot spots by the reaction can be transferred by conduction to the surrounding material at a rate high enough to quench the reaction. Because the SVE is not large enough relative to the particle size and spacing, it cannot serve as a representative volume element (RVE) for the desired response (number density of sites for reaction initiation) and it is necessary to build up the statistics for number density of sites from a set of instantiations or realizations of SVEs for the same microstructure subjected to the same shock loading condition. It is noted that the RVE size is not based simply on spatial statistics of geometric features, as is commonly implied, but must come from analyses of responses; certain responses, such as localized plasticity, or in this case reaction initiation, depend on extrema of microstructure features and therefore require much larger (too large for computational practicality) volumes of material to be analyzed. From these simulations, statistics are compiled and the mean response (f̄) and 99% prediction interval for upper (f₁) and lower (f₂) uncertainty bound functions represented using an iterative re-weighted generalized linear model, with variance function estimation by maximizing the Pseudolikelihood estimator. In this case, variance is due largely to microstructure stochasticity. For given Al and Fe₂O₃ particle size distributions, for example, Fig. 10 shows the number density of reaction initiation sites as a function of mean void size and volume fraction. This facilitates either optimization (based on mean) or Types I-III robust design outlined earlier of a mixture with specified reaction initiation requirements.

To facilitate higher length scale calculations, it is necessary to use the discrete particle simulations to inform extended irreversible thermodynamics continuum internal state variable models with additional flux terms to model delay of macroscopic reaction propagation at component length scales [21]. Multi-level robust design concepts, as shown in Fig. 7, come into play in facilitating such hierarchical relations.
The challenge is to extend these robust design concepts to tailor microstructures that deliver required performance requirements with consideration of multi-physics in problems involving, for example:

- Phase morphologies of alloy systems for multifunctionality
- Fracture resistant microstructures without a priori specification of fracture paths
- Evolution of microstructure (e.g. plasticity, phase transformation, diffusion, etc.)
- Texture and grain boundary networks for fracture and fatigue resistance
- Precipitate distributions and morphologies for fatigue resistance
- Microstructures with resistance to or preference for shear banding
- Formable materials with transformation- or twinning-induced plasticity
- Processing with targeted porosity control
- Surface treatments, heat treatments, inclusions, and residual stresses

**Closure**

A systems-based approach has been developed for designing material microstructures to meet multiple performance/property requirements. The approach embodies robust design rather than single objective optimization owing to the prevalence of uncertainty in process route, stochasticity of microstructure, and nonequilibrium, path dependent nature of inelastic deformation and associated constitutive models. Challenges for design of practical alloy systems and inelastic deformation and damage mechanisms are outlined. We suggest a hierarchical materials design framework in which mechanistic models are exercised to inform designers regarding decisions that contribute to the goal of robust design. The approach is characterized by a confluence of engineering science and mechanics, materials science/physics, and systems engineering. Potential benefits include more efficient, concurrent design of material and components to meet specified performance requirements, the capability to prioritize models and computational methods in terms of degree of utility in design, prioritizing mechanics and materials science/chemistry/physics phenomena to be modeled, and conducting feasibility studies to establish probable return on investment of new material systems.
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