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Research domain(s), discipline(s)/sub-discipline(s)

Solid mechanics; materials science;

Title of Response

Data-driven tools to fill gaps in defining microstructure-property relationships

Abstract

New data-driven tools are needed that can construct a workflow for advancing candidate high performance structural alloys by microstructural design. This response details the needs for two classes of data-driven models. One type of data-driven model desired would help to accelerate the computational process for building authentic representative volume elements from 2D microstructure

datasets and the other kind aims to accelerate of screening candidate structural alloys for high strength and toughness in predefined, extreme service conditions.

Question 1 (maximum 400 words) – Data-Intensive Research Question(s) and Challenge(s). Describe current or emerging data-intensive/data-driven S&E research challenge(s), providing context in terms of recent research activities and standing questions in the field. NSF is particularly interested in cross-disciplinary challenges that will drive requirements for cross-disciplinary and disciplinary-agnostic data-related CI.

A grand challenge in the materials field is the advancement of new lightweight, structural alloys with radically superior structural performance in extreme conditions. Up and coming alloys are different from today's common structural metals, like steels and Al alloys, in that they are microstructurally complex at several length scales and deform easily by two distinct kinds of crystallographic deformation mechanisms: slip and twinning. It is well recognized that factors hindering wide incorporation of these newer, better alloys into structural applications include 1) trade-offs in strength, toughness, and formability, 2) their propensity to fail by a rare event, an instability that has a low probability of occurring at a given time and space, and 3) the lack of basic understanding of microstructure-property relationships. While both strength, toughness, and formability can be quantified in the laboratory, they require a large number of distinct tests (> 20 per alloy per pre-strain level per test conditions) and/or volumes of material (> cm3), hindering the accelerated design of new alloys. An important part of the solution towards new microstructure development are 3D computational materials models. These are large-scale calculations attempt to simulate these same mechanical tests starting with a 3D model of the material of interest. The initial state of the 3D material model aims to mirror as many microstructural features as the possible as the actual starting material, including the same granular microstructure and material components. In simulation, these features evolve at a microscopic level and the macroscopic response calculated, making them useful for microstructure-property relationships. To date, the numerical data from these simulations are proving valuable for determining how finer-scale stress concentrations (e.g., granular corners) can trigger small-scale instabilities (e.g., twins, slip bands), that can cascade to larger-scale instabilities (e.g., shear bands or cracks). These simulations are data-intensive. Each simulation outputs numerous types and forms of data. The microstructure model, referred to as representative volume element (RVE), contains on average half to a few million points. Each material point at each simulation time has an updated tensor stress, strain, and strain rate; a vector crystallographic orientation; and local material strength parameters (scalar values). Each simulation can represent a distinct microstructural realization of the same material or different deformation history. The more variable the microstructure, the more realizations that would be required to appraise the material.

Question 2 (maximum 600 words) – Data-Oriented CI Needed to Address the Research Question(s) and Challenge(s). Considering the end-to-end scientific data-to-discovery (workflow) challenges, describe any limitations or absence of existing data-related CI capabilities and services, and/or specific technical and capacity advancements needed in data-related and other CI (e.g., advanced computing, data services, software infrastructure, applications, networking, cybersecurity) that must be addressed to accomplish the research question(s) and challenge(s) identified in Question 1. If possible, please also consider the required end-to-end structural, functional and performance characteristics for such CI services and capabilities. For instance, how can they respond to high levels of data heterogeneity, data integration and interoperability? To what degree can/should they be cross-disciplinary and domain-agnostic? What is required to promote ease of data discovery, publishing and access and delivery?

At the initial stage, the aforementioned computational effort requires immense amounts of microstructural data to construct an initially authentic 3D RVE. The more complex the microstructure, such those exhibiting hierarchical, highly heterogeneous microstructures, characteristic of the more attractive high-performance alloys, the more data required. In addition, at the final stage, at the end of the simulation, large datasets of output are produced. Further, these calculations are computationally intensive; mandating that all the potentially useful data would need to be harvested on the first simulation run. To accelerate these two stages within the computational modeling effort, advancements in two types of data-driven models are indispensable. Regarding the first type, a computational data-driven tool is desired to take in calculated or measured statistical microstructure data and build the 3D RVEs needed for microstructural model calculations. Structural material behavior depends a lot on several microstructural features. The efficacy of the model consequently depends on adequate representation of the microstructure. Current computational methods do not allow for reliable predictions of macroscopic properties from 2D experimental information without making significant assumptions. At present, most modeling approaches obtain their initial RVEs by relating microstructural features to simplistic microstructure metrics obtained from 2D microstructure sections while a few, alternatively, use 3D experimental microstructure information. A new protocol could be developed for establishing a quantitative relationship between spatial statistics (n-point correlation functions) obtained from 2D microstructure sections and bulk properties with the aid of emerging machine learning approaches. Pertaining to the second one, while these microstructure sensitive calculations can be designed to quantify relationships between complex, hierarchical microstructures and macroscopic strength, running numerous these calculations will bear most of the computational cost in this end-to-end modeling process, which can hinder the efforts toward rapid screening of alloying compositions and processing conditions. To overcome this computational burden and substantially boost the effectiveness of workflows, a data-driven training set or surrogate model could be built. Such a training set would employ an a priori designed set of RVEs that enclose microstructure space of candidate alloys, based on performance measures of interest (e.g., figures of merit) that can be calculated by the 3D material simulations. A trained surrogate model in the form of an analytical function would allow for rapid calculations (in seconds rather than days) for target figures of merit.

Question 3 (maximum 300 words) – Other considerations. Please discuss any other relevant aspects, such as organization, processes, learning and workforce development, access and sustainability, that need to be addressed; or any other issues more generally that NSF should consider.

Another need concerns workforce development, starting with training undergraduate, graduate, and postdoctoral students. Materials-focused students at all these levels are undoubtedly enthusiastic about the exciting prospects of data-driven science and eager to apply them to materials problems. It appears, however, that unique training skills are needed so that they can become equally proficient in several scientific and technological fields, including computational science and engineering, data science, information science, materials science and engineering, solid mechanics, and statistics and probability. Strategies and devices need to be created to connect engineers and scientists who may not meet otherwise, to provide opportunities to work together, overcome professional cultural and terminology differences, encourage information exchange.

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