Project Summary

"Approved for Public Release"

Current approaches to exploring materials and manufacturing (or processing) design spaces in pursuit of new/improved engineered structural materials continue to rely heavily on extensive experimentation, which typically demand inordinate investments in both time and effort. Although tremendous progress has been made in the development and validation of a wide range of simulation toolsets capturing the multiscale phenomena controlling the material properties and performance characteristics of interest to advanced technologies, their systematic insertion into the materials innovation efforts has encountered several hurdles. The most common of these are related to (i) the lack of a generalized (applicable to a wide variety of materials classes and phenomena) mathematical framework that allows objective extraction and synergistic integration of the high value materials knowledge (defined from the perspective of producing reliable process-structure-property (PSP) linkages) from all available datasets (including a variety of multiscale experiments and simulations), while accounting for the inherent uncertainty associated with each dataset, (ii) the lack of formal approaches that identify objectively where to invest the next effort (could be a new experiment or a new simulation) for maximizing the likelihood of success (i.e., meeting or exceeding the designer-specified combinations of materials properties) at any step of the innovation effort, and (iii) the lack of experimental techniques that are specifically designed to provide the quality and quantity of information needed to calibrate the large number of material parameters present in most multiscale materials models.

The proposed effort aims to address the gaps identified above through the pioneering development of (i) a new mathematical framework that allows a systematic and consistent parametrization of the extremely large spaces in the representations of the material hierarchical structure (spanning multiple length/structure scales) and governing physics across a broad range of materials classes and phenomena, (ii) a new design formalism that evaluates all available next steps in a given materials innovation effort (i.e., various multiscale experiments and simulations) and rank-orders them based on their likelihood to produce the desired knowledge (expressed as PSP linkages), and (iii) novel higher-throughput experimental assays that are specifically designed to produce the critically needed fundamental materials data for calibrating the numerous parameters typically present in multiscale materials models.

The scientific foundations (i.e., frameworks, formalisms, assays) developed in this effort will completely revolutionize current practices in materials innovation efforts and lead to an unprecedented rate of aggregation and curation of the critical materials knowledge and workflows needed to propel advanced technologies. The development of this new framework will be guided by case studies involving inelastic deformations and damage in ceramic-matrix composites, and large plastic strains in metal alloys. The case studies will be selected to demonstrate the general applicability of the developed framework to a variety of materials classes and multiscale phenomena specific to the applications of interest to various Department of Defense (DoD) research groups. An equally important goal of the proposed effort will be the recruitment and training of a new cadre of undergraduate, graduate and postdoctoral students with unique cross-disciplinary skillsets in materials, mechanics, statistical sciences, and data sciences, and their introduction to DoD laboratories through summer internships and placements after graduation. Strong emphasis will be placed on US citizenship and enhancing diversity in the recruitment of the researchers for the proposed effort.