Abstract

The microstructure of advanced materials is of fundamental importance to their performance and reliability in engineering applications. In this proposal, we describe a basic research program that will significantly and materially advance the state-of-the-art in *predictive computational materials quantification* by creating a novel open source framework for the modeling of materials characterization modalities that are essential for 3D materials quantification, a high priority and pervasive research area for DoD. The new framework will focus on the 3D microstructures of structural materials, but will also be applicable to other materials classes, such as electronic and functional materials as well as nano materials. The new microstructure quantification framework will consist of physics-based forward models for diffraction as well as image and spectroscopy-based modalities in combination with a unified mathematical model for the description of the microstructure. The framework will be a game changer for the materials community because it will allow researchers to predict the outcome of characterization experiments for a given microstructure. Furthermore, the framework will provide the ability to validate both the microstructure models and the forward models that describe the experimental modalities, so that the accuracy and uncertainty of the measurements can be quantified based on solid physical principles. The materials community, both at DoD laboratories and in academia, will be provided with a new open source tool that can be used to "close the loop," i.e., to ascertain that a model obtained from the data is the best possible and most accurate model. On the educational side, the proposed program will lead to the creation of a new master of science degree program at Carnegie Mellon University. The new MS program in Integrated Computational Materials Science and Engineering will contribute highly qualified personnel to the defense and national security workforce.