"Materials Genome Initiative for Accelerated Materials Discovery and Advanced Manufacturing" by M. Sunkara et al., University of Louisville

Rationale

The discovery and development of advanced energy materials and their large-scale, low-cost manufacturing and deployment is and will be a critical research need for the foreseeable future for economic growth of any region. Unfortunately, the current strategy used for discovery to development uses a linear methodology of discovery-manufacturing-verification which takes over twenty years or more for translation to market. The White House and several federal agencies have outlined a materials genome initiative specifically to accelerate the discovery and development of new advanced materials and to reduce the time required for their deployment to market (*Holdren, J. P. Materials Genome Initiative Strategic Plan. Initiative, 2014*). It is predicted that if one combines materials genome type algorithms to materials/manufacturing development continuum methodology, the time scales for discovery to deployment of both materials and advanced manufacturing will reduce by half to less than 10 years. Because of such a high significance, **materials genomics has become a top priority for several federal agencies and is certainly part of NSF's top ten big ideas.**

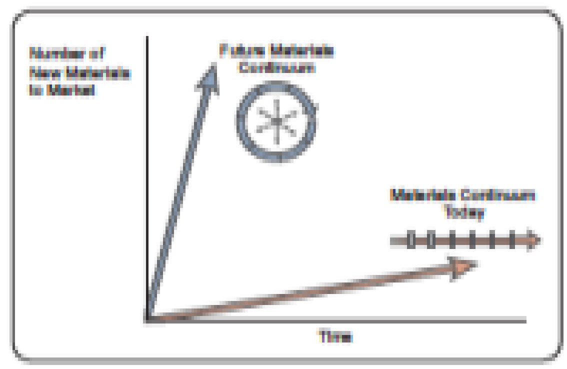

Figure 1. Acceleration of manufacturing to practice with a new materials continuum strategy (adapted from Holdren et al., 2014).

Concept

The new materials/manufacturing discovery to deployment continuum methodology will involve a strategy outlined in the Figure 2. The new materials genome type continuum strategy will involve the following: combinatorial experimental tools, rapid device screening facilities, computational intelligence methods to analyze experimental data, and low cost and scalable manufacturing. Specifically, they include (a) combinatorial experimental tools for preparing and characterizing materials for structure-property-process-functionality data sets; (b) infrastructure necessary for an experimental data repository with data flowing directly from lab note books and the web-based analysis tools; and (c) discovery and manufacturing roadmaps for specific challenges.

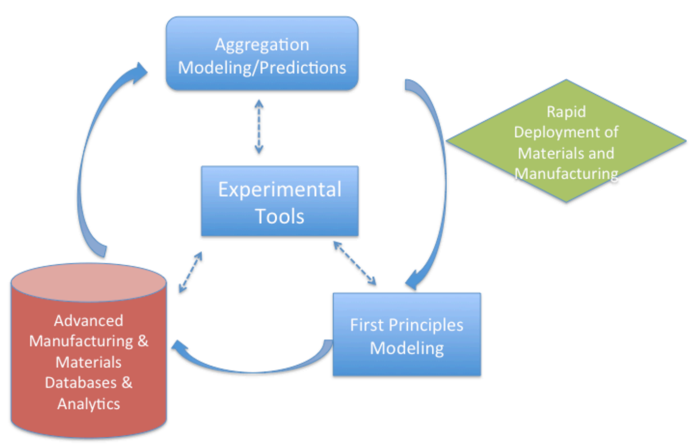

Figure 2. Proposed materials genome based discovery to manufacturing continuum strategy for rapid deployment of new materials in to manufacturing.

Despite rapid advances in computing power and theory, the first principles-based techniques for predicting properties of materials are time consuming. In many cases, the search process itself requires some direction. One approach has been to utilize a combinatorial, high throughput sample creation from different elements as a means of screening materials. *This project seeks to develop a fundamentally transformative strategy by using an informatics-guided computational and experimental approach for proposing and testing new materials and processes.* The team extracts design rules to systematically identify critical structure-property-process relationships in a quantitative fashion to determine the exact role of specific combinations of materials/solvents/process descriptors that govern a given property/functionality of interest. Statistical inference methods are used and developed to identify and experimentally validate new materials and processes with new properties. This information is then linked to a targeted first principles modeling step to provide a physical interpretation of mechanisms controlling properties and functionality. Unlike biological systems, the data sets for advanced materials are sparsely available, necessitating the development of new tools. The project involves several faculty and staff from multiple disciplines to develop tools and techniques for creating data sets; establishing the much needed data repository and deep data analytics techniques necessary for discovering materials/processes for three challenges. The techniques and tools developed under this project will be available to researchers worldwide and easily be used for other research topics and challenges.

***Materials Discovery Challenge*:** The challenge of discovering new compound chemistries in a manner that is both driven by a mechanistic understanding of structure-property relationships and exploring all possible stoichiometric combinations is at first glance a daunting task. Despite advances in theory and computation, we still do not have sufficiently robust physical models that can span enough chemistry to explain how atoms interact. To understand the complexity of the problem, consider the 76 useful stable elements in the periodic table. There are 2,850 binary, 70,300 ternary, 1,282,975 quaternary and > 10^9 heptanary combinations of these 76 elements! Moreover, the combinations can have various ratios of the constituent elements and come wide variety of forms. It would be almost impossible to model all permutations of atomic scale interactions, let alone experimentally synthesize different chemistries. This, in essence, defines the challenge that materials scientists face in <u>systematically</u> designing new material chemistries. Even advances in high performance computing have not been sufficient to come up with an *a priori* method for developing reliable atomistic models for chemically complex solids.

***Accelerated Manufacturing Process Discovery Challenge*:** The materials discovery methodology typically overlooks the processing history and hence once the materials are discovered and validated through theory and experiment, there is a need for infrastructure to validate them for use in manufacturing-scale processes, and assess their applicability through techno-economic analysis. New materials discovered computationally or in the laboratory often run into roadblocks during scale up synthesis or processing, and a significant amount of fundamental optimization of the manufacturing processes is required. For example, existence of closely bordered phase structures can lead to decomposition during processing destroying the efficacy of the manufactured product. Phase transitions and solubility can impede roll-to-roll processes where higher temperatures are often used to accelerate film drying. Finally, many materials will often be subjected to severe conditions over extended periods (UV and heat over 30 years) and manufacturing processes must also be developed to insure robustness of devices, which includes interfaces that may be compromised during manufacturing.