Chapter 1
Computational Materials Design:
Different Concepts and Aspects

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ABSTRACT

The chapter primarily deals with brief description of different methods of materials modeling which utilizes the scientific theories in different length scales. It also gives an account of the available tools for situations where data driven models are required. Utilization of imprecise knowledge of a materials system for developing mathematical models is also discussed. A brief account of the use of optimization techniques for designing materials is discussed here.

INTRODUCTION

For the last few decades the concept of computational materials design is growing fast due to the advent of high power computational facilities. So many computational concepts, particularly the concepts using the fundamental science of materials systems, could not have been utilized, if strong computer back ups are not provided. As in case of all other computational engineering design procedures, materials design also depends on three aspects, modeling, simulation and optimization. The domain of materials modeling is huge, and it can be divided into three parts. The first and dominant part of materials modeling is the concept of modeling where the fundamental physics and chemistry of the system is utilized in different length scales. The fundamental principles of physics and chemistry, governing the states and properties of condensed matter also paves the way for materials theory for quantitative modeling of structural and

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functional properties of materials. This consequently provides the path of designing and predicting novel materials and devices with enriched performance. It is an important and fundamental aspect of material science that is becoming more important day by day due to its predictive power at different length and time scale. The length scale varies from atomic to the macroscopic level. This includes electronic structure and properties of materials determined by ab initio and/or semi-empirical methods, atomic level properties of materials, microstructural level phenomena, continuum-level modelling relating to material behavior. It is a scientific approach to technological problems which uses and combines various tools from both fundamental science and materials engineering and bridges length and time scales across many orders of magnitudes by wise selection of quantum mechanical, atomistic, continuum and statistical mechanical approximations. The mathematical and computational tools developed and used are not only accurate, quantitative and predictive as well as robust and reliable. So, modeling is applicable and beneficial to all the established as well as new newly emerging fields of material research which saves huge laboratory resources, and energy by predicting the best possible path to get the best fit product and at the same time gives concrete theoretical background to it (Janssens, Raabe, Kozeschnik, Miodownik, & Nestler, 2007).

When the science behind the behavior of a material system is not fully explored, but several observations are available, then materials scientists and engineers depend on the statistical techniques like regression analysis to develop models correlating the parameters. Several data-driven techniques similar to statistical concepts, like artificial neural network, genetic programming, support vector machines, capable to map highly complex and non-linear relations, are developed by computer scientists. We can think of a domain of modeling in between the physical and empirical modeling concept, for such situation where the knowledge about a system is available, but in imprecise form. In such cases the fuzzy logic can be used to develop models utilizing the system knowledge in such form. This concept is also getting used in materials modeling.

Virtual experimentation using the mathematical models, known as simulation, is advantageous for materials design. Using simulation technique an in-depth idea about the role of different parameters in a materials system could be explored. It can also help to find combination of parameters for a material to achieve its required performance. But the best way to find such solution, in the composition and/or processing parameters for any material, is to go for optimization. The property of a material to be optimized needs an objective function, which is nothing but a correlation between the property and the input parameters like composition and processing parameters. Any model developed through any of the above methods can be utilized as this objective function. Two different approaches of optimization are most common, and they are the classical derivative based optimization approach and the newer non-derivative based evolutionary approach. In this chapter we shall try to introduce some of the common modeling and optimization techniques in brief.

MATERIALS MODELING IN DIFFERENT LENGTH SCALES

As discussed above, the scientific theory behind a material system could be utilized to form mathematical models, which can be utilized for design and development of new materials, as shown in Figure 1. Such modeling could be done using different length scales, starting from atomic or even sub-atomic level to level of microstructure. Depending on length scale there are a number of theories engaged in modelling of materials such as Density Functional Theory (DFT), Molecular Dynamics (MD), Phase Filed Theory and Finite Element method, etc. (Figure 2).