Chapter 4
Computational Design of Microstructure: An Overview

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ABSTRACT

During the last couple of decades, treatment of microstructure in materials science has been shifted from the diagnostic to design paradigm. Design of microstructure is inherently complex problems due to non linear spatial and temporal interaction of composition and parameters leading to the target properties. In most of the cases, different properties are reciprocally correlated i.e., improvement of one lead to the degradation of other. Also, the design of microstructure is a multiscale problem, as the knowledge of phenomena at range of scales from electronic to mesoscale is required for precise composition-microstructure-property determination. In the view of above, present chapter provides the introduction to computationally driven microstructure engineering in the framework of constitutive length scale in microstructure design. The important issues pertaining to design such as phase stability and interfaces has been explained. Additionally, the bird-eye view of various computational techniques in order of length scale has been introduced, with an aim to present the picture of combination of various techniques for solving microstructural design problems under various scenarios.

1. INTRODUCTION

The microstructure can be described as the length scale based ensemble of the representative units, which evolve the solid state material structures through the multi-scale spatiotemporal interaction under the specific energetic pathway. The hierarchical nature of the microstructure originates from the length scale of the constituent phases and defects originated through the path of evolution. At the smallest scale, electronic interaction among the constituent elements decides the nature of coordination among the ele-

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ments. In such length scale, thermodynamically stable one dimensional defect such as vacancy also play the crucial role. In the next level of integration, the coordinating atoms may aggregate themselves in the form of amorphous, quasi-crystalline and non-crystalline or crystalline order. The defect structure in this scale comprises dislocation, stacking faults, grain boundaries etc. The distinct structure on such defects originates through the interactions occurring at lower scale, e.g., stacking fault width.

In the manufacturing framework, microstructures inherit not only the footprints of the process and compositional variables but also the blue-print of the properties. Keeping this in view Figure 1 enumerates the integrated multiscale approach of microstructure based design of materials (Anand, Dey, Kok, Chakraborty, & Chattopadhyay, 2014). Contrary to the conventional imprecise approach of describing the microstructure in terms of the empirical composition-process-property framework, diagnostic framework relies on the deterministic design method, while employing range of experimental and simulation techniques (Anand, Datta, & Chattopadhyay, 2013).

2. COMPUTATIONALLY DRIVEN MICROSTRUCTURE ENGINEERING

The multi-scale nature of the microstructure evolution and the corresponding range of relaxation times result into the dynamic nature of materials structure with the "spatiotemporal hierarchy". This dynamic nature leads to the complexity in the materials design causing the limited predictability (Olson, 1997). In such complex situation, Cohen's "reciprocity principle" is an effective tool to improve the predictability. In this approach, structure-property correlation is considered as the two-way phenomena, as perception of microstructure is also guided by the specific properties to be considered (Cohen, 1976). The structure-property framework can be expanded to include the processing and performance, as shown in Figure 2,

Figure 1. Framework of microstructure based design (Chattopadhyay, 2014)