Modeling of Nano-Structure via a Spinodal Decomposition: An Extended Range of Monte Carlo Investigation

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ABSTRACT

In the study, we proposed a Monte Carlo package to investigate the spinodal decomposition which is a pathway to obtain nano-structure phase of materials. The modeled system consists of two different species of the Ising spins where the order parameter is conserved. The interaction range among atoms, being assumed to take an inverse square law behavior, was extended to the third nearest-neighbor range, i.e., two times the lattice spacing. A separate simulation on only the first nearest-neighbor range was also taken for a comparison. The growth of the mixing and de-mixing of the Ising spins was observed in terms of the nucleation growth of similar atoms via the correlation length. From our results, the nano-stripe pattern of spinodal decomposition was evident. The power law relation between the spinodal domain size and the simulation time was found for both the first and the third nearest-neighbor interaction range. However, the exponent to the growth rate of the third nearest-neighbor interaction system is slightly smaller than that of the first nearest-neighbor interaction system, suggesting a slower growth in time. This proposes that the growth exponent is sensitive to the interaction range, and an appropriate interaction range must be used to model spinodal decomposition in real materials.

Key words: Nanostructure, Spinodal decomposition, Monte Carlo, Ising model, Kawasaki algorithm

INTRODUCTION

Recent advances in the physical science and engineering have been focused on expanding the limits of our understanding of material behaviour to ever-shrinking-length scales, using a complimentary array of atomic-scale modeling techniques and sub-nanometer scale characterization methods. These efforts have resulted in numerous successes, most notably including the advent of nano-materials which impacts numerous facets of our society. Within the broad spectrum of nano-materials, a wide range of technological capabilities exist which draw upon the unique characteristics of the behaviour of materials at the nanoscale. These include novel chemical and biological sensors (Tu and Chen, 2002), nanoscale microprocessors (Plouchart, 2003), photonic crystals (Leung et al., 2003), nano-electromechanical systems (NEMS) (Tang, 2001), and many others. One of the most critical aspects of designing nano-scale devices is the ability to manipulate or assemble materials at the nanoscale. Numerous approaches have been attempted with various degrees of success. Even in single-phase systems, it is difficult to preserve a nano-crystalline structure because of the strong driving forces for grain growth which lowers the energy of the system by reducing surface or grain-boundary energy. Therefore to synthesize bulk nano-crystalline metals or ceramics, it is often necessary to use non-equilibrium process conditions to preserve the nano-crystalline