Monte Carlo Simulations of Nano-Powders from Mechanical Milling

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ABSTRACT

In this study, we performed Monte Carlo simulations to model the nano-structure of the powder undergoing mechanical-milling processes as a function of milling time, milling intensity and milling frequency. Under the framework of the kinetic Ising model, the Monte Carlo simulation was performed on a square lattice. Based on the equipartition of energy theorem, the kinetic energy being obtained during the milling process gives rise to both mechanical-shearing work and the thermal energy which increases the diffusivity of atoms in the powder. The process of these actions determines the size of the powder. During the simulation, the size of the biggest powder at a particular milling time was recorded to investigate how parameters of the mechanical milling affect the powder size. From our results, it is found that the mechanical milling reduces the size of the powder, but the diffusivity caused by thermal energy (at low-enough temperatures) grows the powder up as the time passes by. When both the milling and diffusing were taken in action, the powder size was found to reduce sharply at the early milling stage and then slightly fluctuated around its mean size. Based on this phenomenon, it is clear that the powder size is controllable if a right set of milling parameters is chosen. As a result, the study can be concluded to successfully model the mechanical-milling method to obtain powders at nano-scale.

Key words: Nanostructure, Mechanical milling, Monte Carlo, Ising model, Kawasaki algorithm

INTRODUCTION

Being simple but functional, the mechanical milling is a sophisticated technique to synthesize powders in a non-equilibrium (dynamic) phase. Particularly, the mechanical activation can mix the immiscible elements even the considered system is currently in its thermodynamically-unstable state. This is from the fact that, during the milling process, the non-equilibrium phase is maintained as the effect of fracture, cold-welding and deformation of powders which allows the non-equilibrium phase to become dynamically-stable. As a result, some powders can be synthesized by the mechanical activation even at room temperature which offers another pathway to ceramics processing, besides the conventional solid-state reaction of mixed oxides. Furthermore, the mechanical activation can refine the powder into nano-scale structure to suit various applications (Jiang et al., 1997; Jiang et al., 1999; Tan, et al., 2004; Yadav, et al., 2004). This offers the possibility of synthesizing nano-composite ceramics by adjusting the temperature, milling time and the milling intensity. Consequently, the mechanical milling is of a great interest since nano-composite materials can strengthen the material hardness (Hellmig and Ferkel, 1999), and enhances the activity of