Physica A 392 (2013) 4121–4126

Contents lists available at SciVerse ScienceDirect

Physica A

journal homepage: www.elsevier.com/locate/physa

Investigation of nucleation and grain growth in 2-dimensional systems by using generalized Monte Carlo simulations

Hakan Cetinel [a,*], Ozhan Kayacan [b], Demet Ozaydin [a]

[a] Department of Mechanical Engineering, Faculty of Engineering, Celal Bayar University, 45140 Muradiye, Manisa, Turkey
[b] Department of Physics, Faculty of Arts and Sciences, Celal Bayar University, 45140 Muradiye, Manisa, Turkey

HIGHLIGHTS

- Nucleation and grain growth were studied by using 2-dimensional generalized Monte Carlo simulations and experiments.
- Generalized Monte Carlo simulations were performed in studying of nucleation and grain growth phenomena.
- It is shown that the results of simulations and experiments match well.

ARTICLE INFO

Article history:
Received 12 April 2012
Received in revised form 28 March 2013
Available online 2 May 2013

Keywords:
Tsallis thermostatistics
Phase transformation
Kinetics
Computer simulation

ABSTRACT

In this study, nucleation and grain growth was studied by using 2-dimensional generalized Monte Carlo simulations and experiments. As an attempt to improve the JMAK model, we proposed a new differential equation to be able to model nucleation and growth phenomena using nonextensive thermostatistics. One of the reasons that we would like to perform generalized Monte Carlo simulations in studying of nucleation and grain growth phenomena is that the generalized Monte Carlo algorithm was shown to be more effective than the standard Monte Carlo algorithm and also than the standard Molecular Dynamic algorithm in locating the minimum energy configuration. Therefore, for a given temperature, the fact that a configuration of the system with lower energy could be obtained by using the generalized Monte Carlo simulation means that a different textural configuration of grain growth could be also expected. In this respect, it is possible to say that the nonextensive statistics might be an appropriate tool in studying of nucleation and growth phenomena.

1. Introduction

Recrystallization is one of the most important subjects in metallurgy. The variation of microstructure with time can be regarded as a nucleation and a growth process. In this direction, Kolmogorov [1], Johnson and Mehl [2] and Avrami [3–5] first treated the kinetics of a phase transformation characterized by constant rates of nucleation and radial growth. This model is known as the JMAK model in the literature and assumes the growth rate to be constant in all directions. The JMAK model has been applied to both non-isothermal and isothermal situations. According to the JMAK model, for isothermal transformation the variation of transformed fraction volume with time is given by

$$V_\alpha(t) = 1 - \exp\left(-I\frac{\pi}{3}k^3t^4\right). \tag{1.1}$$

* Corresponding author. Tel.: +90 236 2012361; fax: +90 236 2412143.
E-mail address: hcetinel@cbu.edu.tr (H. Cetinel).

0378-4371/$ – see front matter © 2013 Elsevier B.V. All rights reserved.
http://dx.doi.org/10.1016/j.physa.2013.04.040

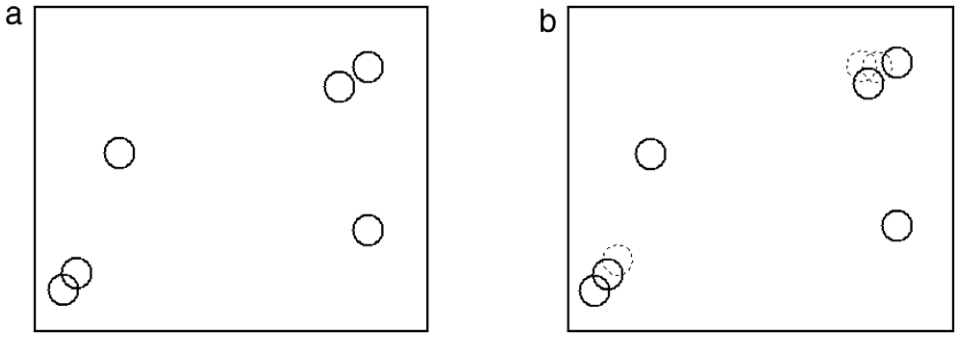

Fig. 1. Two-dimensional distributions of grains according to JMAK theory. Broken circles represent overlaps of grains.

Here $V_\alpha(t)$ stands for the transformed volume fraction, I is called nucleation rate and represents the number of nuclei per unit volume per second, k is the radial growth rate and t is the time since the start of transformation. It is well-known that when the growth rate is small, the JMAK model gives good approximation. On the other hand, if growth rate starts to assume high values sufficiently, then the JMAK model fails and an alternative approach is needed. Some limitations of the JMAK model were reported and discussed in detail in the literature [6–8]. The JMAK model assumes that the nucleation occurs with a constant nucleation rate in both transformed and untransformed materials and this process requires infinite time for completion. On the other hand the corresponding geometrical process of coverage is finite [6–8]. It was reported in these studies that one of the problems may come from the effect of overlapping. In the JMAK model, a grain can also grow to another grain, as illustrated in Fig. 1. This leads to a serious problem in that the transformed fraction is overestimated. Therefore the deviations of the predicted value of the JMAK equation from the true value is of crucial importance. It is worth noting that these insufficiencies can be overcome by defining a new kinetic differential equation within nonextensive formalism.

As an alternative model, instead of the JMAK model, we proposed a new differential equation [9,10]

$$\frac{dV(t)}{dV_{ex}} = (1 - V(t))^q \tag{1.2}$$

where q is called entropic index and comes from the Tsallis entropy [10]

$$S_q = k\frac{1 - \sum_{i=1}^{W} p_i^q}{q-1}, \quad q \in R \tag{1.3}$$

in which k is a constant, p_i is the probability of the system in the ith microstate, W is the total number of configurations. Eq. (1.3) is the generalization of Boltzmann–Gibbs entropy and in the limit $q = 1$, we recover the classical Boltzmann–Gibbs entropy, $S_1 = k\log(W)$.

In this study, we have performed Monte Carlo simulations of the Potts model using nonextensive statistics, to handle the kinetics of phase transformation and to improve the predictions of the JMAK equation. The paper is organized as follows: first the details of experimental setup and then nonextensive formalism are introduced. Next the implemented rules of Monte Carlo simulations are summarized and finally the obtained results are interpreted within nonextensive formalism.

2. Experimental setup

Standard electrolytic electric wires having 99.93% Cu composition were chosen as the material. They were prepared as specimens cutting to Ø5 mm × 10 mm dimensions in order to treat by heat. They were annealed at 450 °C for 60, 90, 120 and 180 min, and then cooled to room temperature in air. Firstly, Specimens were molded into polyester matrix. Molded samples were grinded with 180, 220, 400, 600, 800, 100 and 1200 grid roughness levels and then polished with 1 and 0.3 μm diamond paste in order to examine the microstructures. Then, specimen surfaces were etched with etching solution containing 120 ml pure water, 30 ml hydrochloric acid and 10 g Fe (III) chloride in order to make clear the grains. Microstructure of the etched surfaces was examined by NIKON SMZ1000 light microscope and Clemex camera and image analyzer software set. Image of the microstructure with clear grain boundaries were transported to computer in order to examine by using image analyzer software. Finally, average grain size (μm^2) and number of grains were determined.

3. Nonextensive formalism

Tsallis thermostatistics has been widely used to investigate the various physical phenomena [11,12]. The fundamental property of Tsallis entropy, Eq. (1.3), is that it exhibits nonextensive character. If a physical system consists of two