

# NUMERICAL MODELING OF MICROSTRUCTURAL EVOLUTION IN THREE-PHASE POLYCRYSTALLINE MATERIALS

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## الخلاصة:

إن معظم السبائك الهندسية تستخدم على شكل متعددة البلورات، وهذا يعني أنها عبارة عن عدد كبير من الحبيبات الصغيرة، وهذا التركيب من الحبيبات الصغيرة ليس ثابتاً بل يتطور مع الزمن، وفهم التركيب المجهرى لهذه المواد وتطورها مع الزمن يساعدان على التحكم في الأداء والعمر الزمني للسبائك الهندسية، وطريقة المحاكاة المستندة على نموذج مونت كارلو بوتس لتطور التركيب المجهرى لنظام ذي حالتين امتدت لدراسة تطور التركيب المجهرى لنظام ذي ثلاث حالات. وفي هذه الدراسة تم تطوير الأنموذج ووصفه، والتحقق منه بمقارنة نتائج المحاكاة للنظام ذي الثلاث حالات بنتائج المحاكاة للنظام ذي الحالتين. وقد أشارت النتائج بأن الحبيبات الصغيرة تنمو تحت سيطرة الانتشار على طول حدود الحبيبات، وتتبع علاقة النمو التالية  $d \sim t^{1/n}$  حيث  $n=1/4$ .

## ABSTRACT

Most engineering alloys are used in polycrystalline form. This means that they are made of a large number of grains. The structure formed by the grains is not steady but evolves with time. Understanding the material's microstructure and its evolution helps to control the performance and lifetime of engineering materials. The simulation method based on the Monte Carlo–Potts model of microstructural evolution in a two-phase system has been extended to study microstructural evolution in a three-phase system. The model has been developed and characterized in this study. The model is verified by comparing simulation results of grain growth in the three-phase system to the simulation results in a two-phase system. It is found that grain growth is controlled by diffusion along grain boundaries and follows the power-growth relationship,  $d \sim t^{1/n}$  with  $1/n=1/4$ .

**Key words:** material science, numerical modeling, engineered processes and materials

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## NUMERICAL MODELING OF MICROSTRUCTURAL EVOLUTION IN THREE-PHASE POLYCRYSTALLINE MATERIALS

### 1. INTRODUCTION

Practically all metals, ceramics, and rocks are polycrystalline materials. They consist of a mixture of tiny grains which are attached together by interatomic forces. The structure formed by the grains is unstable and evolves with time when the material is heated and/or deformed. Ceramists, metallurgists, and geophysicists have long recognized that the microstructure of a polycrystalline material directly affects its mechanical properties and substantial efforts have been devoted to understanding how the microstructure of polycrystalline materials evolves with time. Grain growth is a process in which the average grain size of a single-phase polycrystalline material increases with time, driven by the reduction in the total grain boundary energy. The value of the grain growth exponent,  $n$ , is 2 for pure metals and ceramics [1–3]. On the other hand, Ostwald ripening is defined as the process during which large second-phase particles grow while small particles reduce in size and disappear. The grain growth exponent for Ostwald ripening of particles in polycrystalline materials is  $n = 3$  if grain growth is controlled by volume diffusion [4, 5],  $n = 4$  in case of grain boundary diffusion controlled grain growth, and  $n = 5$  for diffusion on dislocations [6].

Grain growth in the major phase may happen simultaneously with Ostwald ripening, especially, in two-phase polycrystalline materials. If the second-phase particles were stable, grain growth in the major phase would stop as soon as the grain size reaches some maximum value which is proportional to the second-phase grain size [12]. If the second-phase particles undergo Ostwald ripening, the grains of the major phase can grow too. Hillert [13] and Gladman [14] proposed that after an adequately extended time, grain growth in two-phase systems in which both phases grow is controlled by Ostwald ripening of the dispersed particles and is coupled due to Zener pinning. There is experimental proof of such coupled growth [7, 8, 15–20]. These materials, such as ceramics and metallic alloys, have important engineering applications. Particular examples are two-phase zirconia–alumina ( $ZrO_2$ – $Al_2O_3$ ) in ceramics [7] and two-phase titanium alloys in metallic systems [8, 9]. One of the methods to reduce the brittleness of intermetallic compounds is to introduce multi-phases, including ductile disordered phases [10]. Microstructure control was used to improve the ambient temperature ductility of the E21/B2/Co three-phase alloys [11].

Different numerical models have been developed to simulate the microstructural evolution of materials. These simulation methods can be classified into four groups. The first one is made up of Voronoi [21] and modified Voronoi [22, 23] methods. The second includes curvature-driven grain growth [24–26] simulations, followed by continuum thermodynamics models such as finite difference solutions of the Cahn–Hilliard equation, phase field models [27], and the diffusion equation [28–30]. The last consists of cellular automata [31] models. All four simulation methods depend on recognizing the phenomenological features of the system. In comparison, the thermodynamic and kinetic characteristics are inherent to the Monte Carlo–Potts model. There is no need to include the material behavior such as velocity of grain growth boundary or the function of free energy into the model.

The microstructural evolution of two-dimensional three-phase polycrystals is considered in this study. There are three reasons for choosing two-dimensional (2-D) systems [32]. The first reason is that 2-D system gives a logical simple starting point to test the concept of grain growth in three-phase polycrystals. The second one is that grain boundary curvature in 2-D has a single component,  $\kappa$ ; in addition, grain topology and grain growth rate depend on  $\kappa$ . However, the curvature in three-dimensions (3-D) has two orthogonal components, also, grain topology depends on the Gaussian curvature of a boundary while growth rate depends on the geometric curvature. For curvature driven grain growth, some rules of grain topology and growth rate can be derived in 2-D which have no recognized consequence in 3-D. Lastly, when grain growth is spatially uniform, stereological relationships require that a 2-D system resemble a cross section of the corresponding 3-D system. Physically, a 2-D polycrystal may be viewed as a polycrystalline thin film in which the grain size is larger than the film thickness.

The Potts–Monte Carlo model was developed more than four decades ago as an extension to the ferromagnetic Ising model for magnetic domain evolution [33]. The Ising model [34] represents a magnetized material as a collection of spins, where only two states are possible, namely up or down. Although this model has been developed a long time ago, not until much later, has it found a variety of applications [35]. Potts later generalized the Ising model and allowed for  $Q$  states for each particle in the system, hence the term " $Q$ -state model". It is the Potts model that has been used most extensively to simulate mesoscopic behavior of materials such recrystallization and grain growth [36]. In particular, it was very successful in describing grain growth in polycrystals. The reason for this is a similarity between the ferromagnetic Potts structures and grain structures; both being characterized by an array of cells having the same spin or crystal lattice orientation. These cells are separated by boundaries which evolve in such a way as to minimize total interfacial energy.

The algorithm of modeling of microstructural evolution in polycrystals has been developed for both one- and two-phase systems [32, 37–42]. The purpose of this paper is to develop a Monte Carlo–Potts model to describe grain growth in three-phase solid systems. The three-phase results reduce to the published two-phase results in the limit of zero-volume fraction of the third phase. This establishes the plausibility of the model to simulate grain growth in three-phase system. The simulation results are compared to simulation results of grain growth in two-phase system in order to verify the model.

## 2. THE SIMULATION MODEL

Monte Carlo–Potts model is developed to study the microstructural evolution of three-phase polycrystals. The three-phase polycrystalline material is treated as two-dimensional square array of sites. Each site is assigned a spin,  $q_i$ , between 1 and  $Q$ . The spin,  $q_i$ , corresponds to the orientation of the grain in which it is embedded. Lattice sites that are adjacent to sites having different grain orientations are regarded as being separated by a grain boundary, whereas a site surrounded by sites with the same orientation is in the grain interior. The grain boundaries may divide two grains of unlike spins (homophase boundaries) or two grains of dissimilar phases (heterophase boundaries). The sites that correspond to the first phase (phase *A*) are given odd positive numbers,  $2q_i+1$ . The sites correspond to the second phase (phase *B*) are given even positive numbers,  $2q_i$ . The sites correspond to the third phase (phase *C*) are given negative numbers. Although in reality, the range of spins is continuous, the results do not depend on the number of spins provided  $Q$  exceeds a value of about 50 [38, 42–44]. The independence of  $n$  on  $Q$  suggests that it is possible to simulate a real infinite degenerate system with a finite- $Q$  Potts model. The change in  $n$  is attributed to an artificial grain coalescence process which dominates when  $Q$  is small. Coalescence occurs when grains of the same orientation touch to form one grain. At low values of  $Q$ , grain growth is controlled by coalescence, resulting in a high value of  $n$ . At larger values of  $Q$ , the probability for a grain to have like-neighbor grains of like orientation is lower and the occurrence of coalescence is lower. We found that the value of  $Q = 100$  is sufficiently large to eliminate the effect of coalescence. This value is used in all our simulations.

The total system energy depends only on the spin exchange energy which can be written as follows,

$$E = \frac{1}{2} \sum_{i=1}^N \sum_{j=1}^8 [1 - \delta(q_i, q_j)] \quad (1)$$

where  $N$  is the total number of sites,  $\delta$  is the Kronecker delta function and  $q_i$  is the spin of  $i^{\text{th}}$  site. The only energy considered in the simulation is the interfacial energy. There are six types of interfacial energies: three homophase boundaries for two grains of unlike spins (*AA*, *BB*, and *CC*), and three heterophase boundaries for two grains of dissimilar phases (*AB*, *BC*, and *AC*). It is assumed that all grain boundaries are isotropic and have the same value; therefore, for any pair of sites, different spins result in an interfacial energy of unity and same spins result in an interfacial energy of zero.

The microstructural evolution occurs as a result of two processes: grain boundary migration and long-range diffusion. Therefore, the evolution of the structure is modeled by two different grain growth algorithms: a spin flip rule and a spin exchange rule. The spin flip rule within one phase is used to simulate grain growth controlled by grain boundary migration. This rule is applied by picking a site and a new orientation at random from the set of allowable values. The new orientation is chosen from all possible spins, from 1 to  $2Q+1$  or from 2 to  $2Q$  or from  $-1$  to  $-Q$ . If the spin of the selected site is even or odd or negative, then the allowable new spin is even or odd or negative respectively. The spin is not allowed to change to even or negative spin if the chosen spin is odd that would mean growth of one phase at the expense of the other. The change in total system energy  $\Delta E$  for reorienting the site is computed using Equation (1). Next, the probability for the spin flip is calculated with the help of the transition probability,

$$P = \begin{cases} 1, & \Delta E \leq 0 \\ 0, & \Delta E > 0. \end{cases} \quad (2)$$

The second process is long-range diffusion which transfers material from one phase to another through the grains of the other phases. This requires spin exchange between the phases. Numerically, the algorithm of a spin exchange rule is used. In this rule a site and its neighbor are selected randomly. If the two sites belong to different phases, they are allowed to exchange their spin. This can create an isolated spin of *B* phase and *C* phase. The spin of *B* phase can randomly walk through the *A* phase until it reaches another or the same (depending on random walking results) grain of *B* phase. The same is follows for the spin of *C* phase. The total change in energy for the spin exchange is determined by calculating the energy of the old and new configuration using Equation (1). The probability function for spin exchange must have a non-zero probability for the events with positive energy difference. Otherwise, there would be no exchanges. Therefore, instead of using the simplified probability function (Equation 2) it is necessary to use the full Metropolis algorithm,

$$P = \begin{cases} 1, & \Delta E \leq 0 \\ e^{-\frac{\Delta E}{k_B T}}, & \Delta E \geq 0, \end{cases} \quad (3)$$

where  $k_B$  is the Boltzmann constant and  $T$  is the temperature. If the energy change is negative or zero the move is accepted. If the energy change is positive, a random number  $R$  between 0 and 1 is generated such that if  $R \leq P$  the change will be accepted.

One Monte Carlo time step (MCS) is typically defined so that each one of the  $N$  sites is tested for one orientation switch. The number of Monte Carlo steps is assumed to be proportional to the real time. The structure of three-phase polycrystalline materials is initialized using a  $400 \times 400$  square lattice. The initial microstructure used in this study is generated by randomly seeding solid A-, solid B-, and solid C-spin sites with the desired volume fraction of A, B, and C. The physical properties of the phases can be quite different. For example, different species can be the bottle neck in the diffusion processes controlling the coarsening rates. The interfacial energies are also known to depend on the misorientation angle. However, these are poorly constrained so that the controlling parameters of the three phases are chosen to be identical, and all grain boundaries are assumed to have the same interfacial energy. In particular, this means that the case of a volume fraction of  $x_B\%$  of the second phase is corresponding to one with a volume fraction of  $x_C\%$  of the third phase and to one with a volume fraction of  $(100 - x_B - x_C)\%$  of the first phase and vice versa. Several values of the volume fractions of the three phases are considered.

### 3. SIMULATION RESULTS

#### 3.1. Two-Phase Grain Growth

During grain growth, grain boundary migration is driven by decrease in the total interfacial energy. The boundary moves with velocity  $v \sim \dot{d}$  which is proportional to the driving pressure,  $\dot{d} = MP$  where  $M$  is the Mobility and  $P$  is the driving pressure, taken here to be the product of boundary energy,  $\gamma$ , and curvature,  $\kappa$ ,  $P = \gamma\kappa$ . Assuming that the average curvature of all grains is inversely proportional to the mean grain size,  $d$ , then, the driving pressure for grain growth will be inversely proportional to the grain size, we obtain

$$\dot{d} = \frac{2\alpha\gamma M}{d} \quad (4)$$

where  $\alpha$  is a geometric constant of the order of unity. Integrating Equation (4) produces

$$d^2 = d_0^2 + Kt \quad (5)$$

where  $K = 4\alpha\gamma M$ .

In the limit when  $d \gg d_0$ , then

$$d = kt^{\frac{1}{2}} \quad (6)$$

This equation can be rewritten in a more general form [44]

$$d = kt^{\frac{1}{n}} \quad (7)$$

where  $n$  is the grain growth exponent.

Two-phase grain growth simulation is reproduced to verify the code. Figure 1 displays the average grain size,  $d$ , as a function of time,  $t$ , on a logarithmic scale. The standard deviation obtained after running each case 10 times is relatively small and is not shown. The slope of a straight line fit through  $\log d$  versus  $\log t$  plot by least square fit is one over the grain growth exponent. The grain growth exponent is a simple metric that is used to compare steady-state growth rates of simulations. To estimate the asymptotic grain growth exponent, we draw the inverse of grain growth exponent,  $1/n$ , versus time as shown in Figure 2. The value of  $1/n$  was calculated in a time window which was moving along the time axis. The logarithmic width,  $t_2/t_1$  of the time window was about 5. These calculations show that  $1/n$  is close to the theoretical value  $1/4$  expected for grain-boundary diffusion controlled grain growth. The value of the inverse of the grain-growth exponent for two-phase systems is found to be about  $1/4$  in previous numerical results for two-dimensional systems [37, 38].

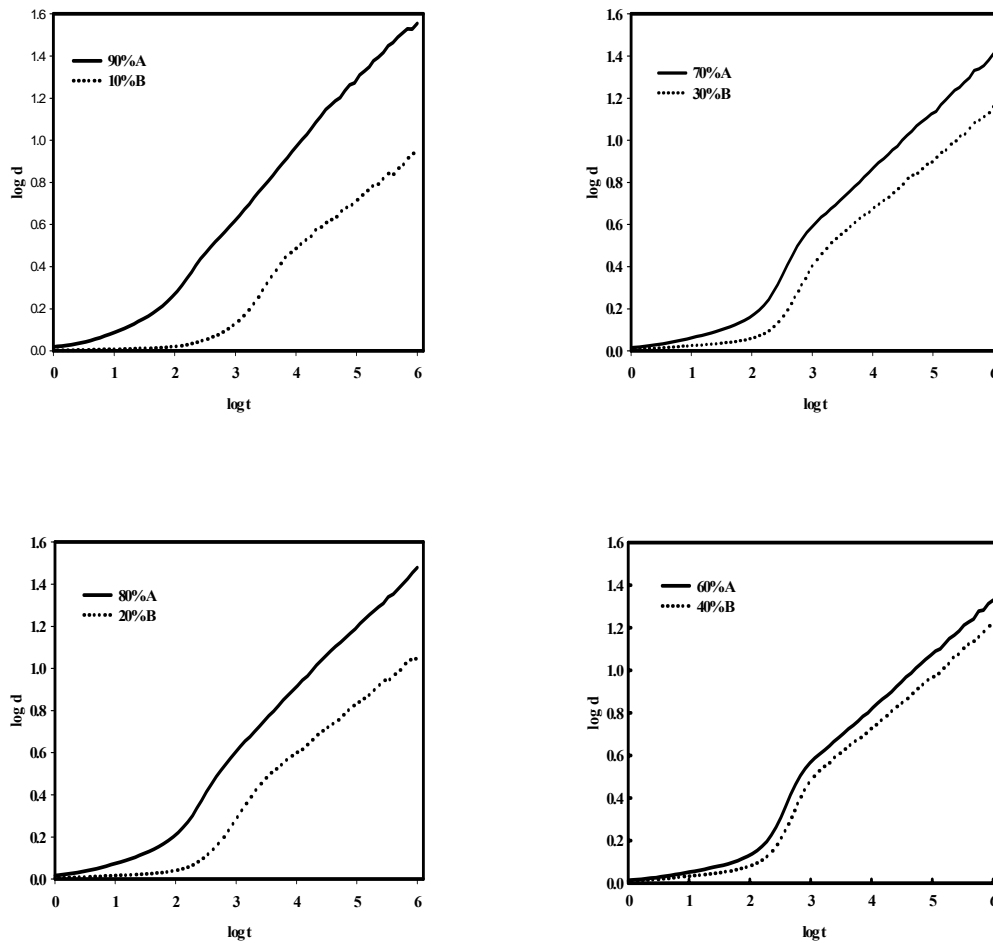


Figure 1. Time dependence of the average grain diameters for two phases (A and B).  
The volume fraction of each phase is specified

### 3.2. Three-Phase Grain Growth

Figure 3 illustrates the microstructural evolution of three-phase systems for different fractions of each phase. The volume fraction of phase A has the values 60, 60, and 20%. The volume fraction of phase B has the values 20, 30, and 40%. The volume fraction of phase C has the values 20, 10, and 40%. All phase grains are coarsened while remaining equiaxed and regular. In 60% A-phase, 20% B-phase, and 20% C-phase simulation, the A phase formed a continuous matrix around isolated B-phase and C-phase grains. In these simulations, the grain boundary energy of A phase, B phase, and C phase are equal. Therefore, the thermodynamic equilibrium angles at trijunctions formed by two A grains and a B grain (AAB) are similar to those formed by one A grain and two B grains (ABB). This is valid for the thermodynamic equilibrium angles at trijunctions formed by any combination of three grains for the three phases. At any trijunction, the equilibrium angle will be  $120^\circ$ . As a result, an isolated grain surrounded by other phase grains will have convex boundaries if the number of grain edges is equal to or less than 6. In 60% A-phase, 30% B-phase and 10% C-phase simulation, the A phase and B phase formed a continuous matrix around isolated C-phase grains. In 20% A-phase, 40% B-phase and 40% C-phase simulation, the B phase and C phase formed a continuous matrix around isolated A-phase grains. Percolation analysis is another tool for understanding the properties of microstructures in which a key concept is the percolation threshold [45].

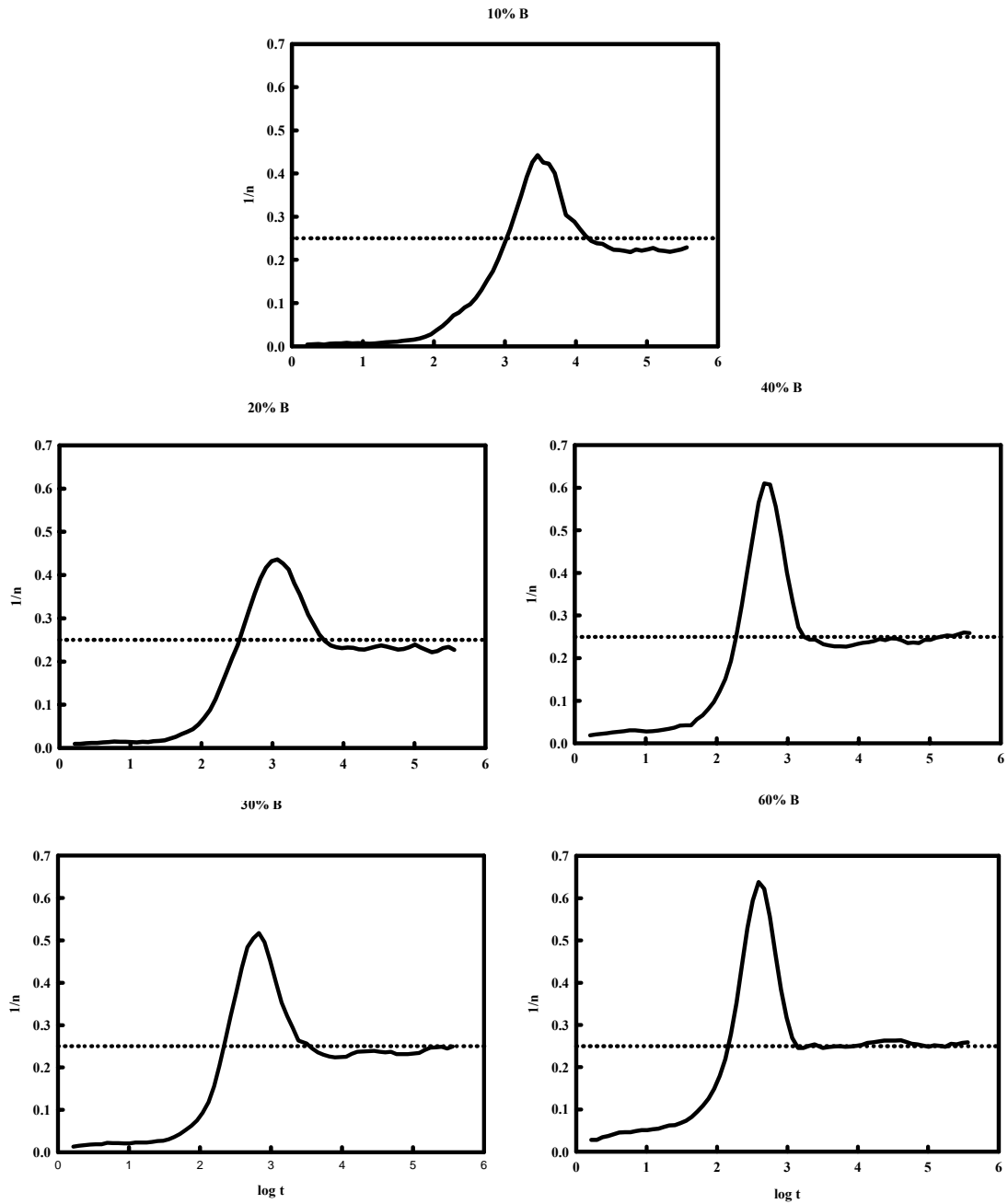
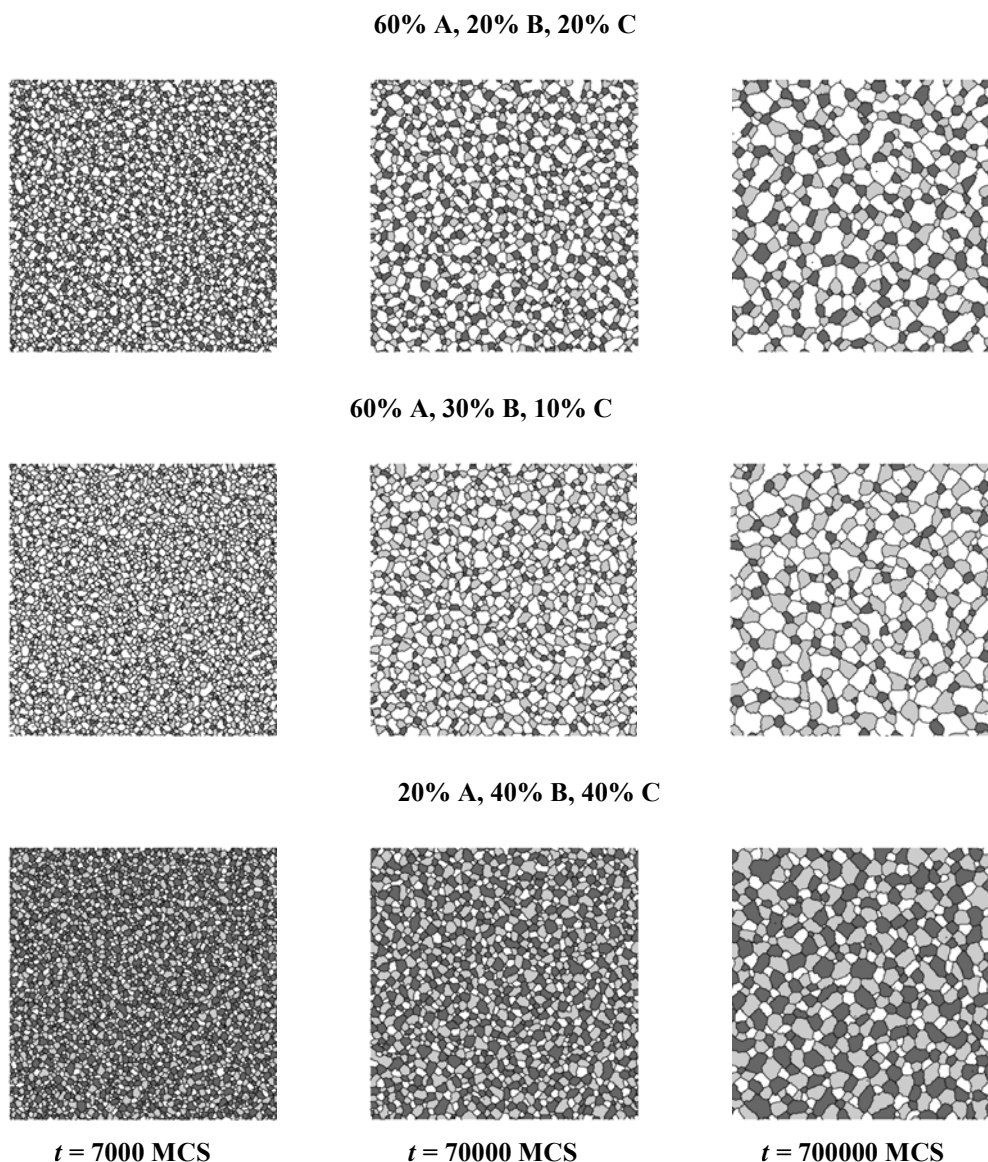


Figure 2. Inverse of grain growth exponent,  $1/n$ , as a function of time for different volume fractions of the B phase. The dotted horizontal lines show the theoretical value  $1/n = 1/4$



*Figure 3. Microstructural evolution of three-phase system with different volume fractions for each phase. The white grains are phase A, The light gray grains are phase B, and the dark gray grains are phase C. Each row corresponds to one run. The boundary conditions are periodic in both vertical and horizontal directions. The square box used in our simulations can be thought of as a part of an infinite array of identical square boxes*

Figure 4 gives the variation of the grain size with time. The standard deviation obtained after running each case 10 times is relatively small and is not shown. All runs utilize Equation (1) with Metropolis probability (Equations (3) and Equation (4)) on a 160 000 site simulation with periodic boundary conditions. As can be observed from Figure 4, at the beginning of evolution, the system passes through a transitional regime which is due to initial conditions and grain boundary migration in one-phase regions. The regime which is independent of the initial conditions is the asymptotic regime. The presence of a finite initial grain size,  $d_0$ , in the grain growth Equation (5), guarantees that the slope of the  $\log d$  versus  $\log t$  plot increases at long time. All of the simulations have approximately the same  $d_0$ . In fitting the available simulation data in two dimensions to determine the grain growth exponent, we found that the results were sensitive to the time regime examined. To estimate the asymptotic grain growth exponent, we draw the inverse of grain growth exponent,  $1/n$ , versus time as shown in Figure 5. The value of  $1/n$  was calculated in a time window which was moving along the time axis. The logarithmic width,  $t_2/t_1$  of the time window was about 5. These calculations show that  $1/n$  is close to the theoretical value  $1/4$  expected for grain-boundary diffusion controlled grain growth. The cases with the lowest volume fractions (10% and 20%) do not seem to fully reach the asymptotic regime.

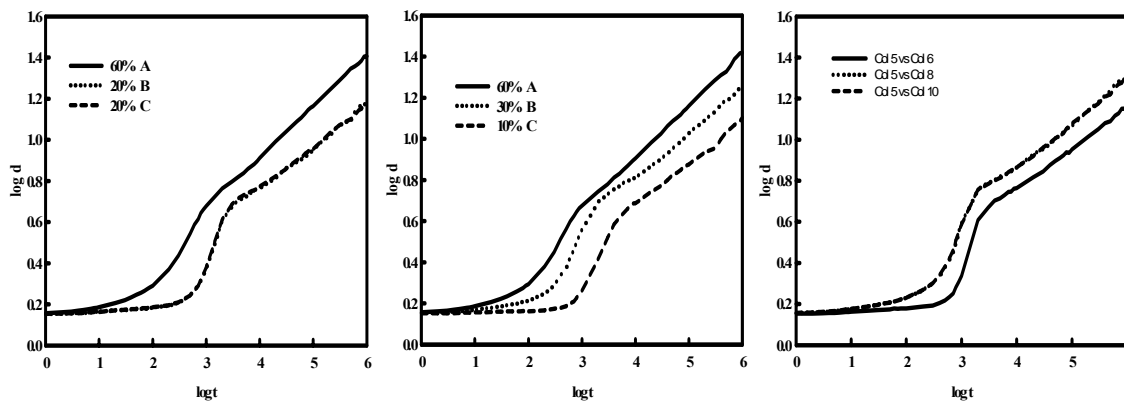


Figure 4. Time dependence of the average grain diameters for three phases (A, B, and C). The volume fraction of each phase is specified

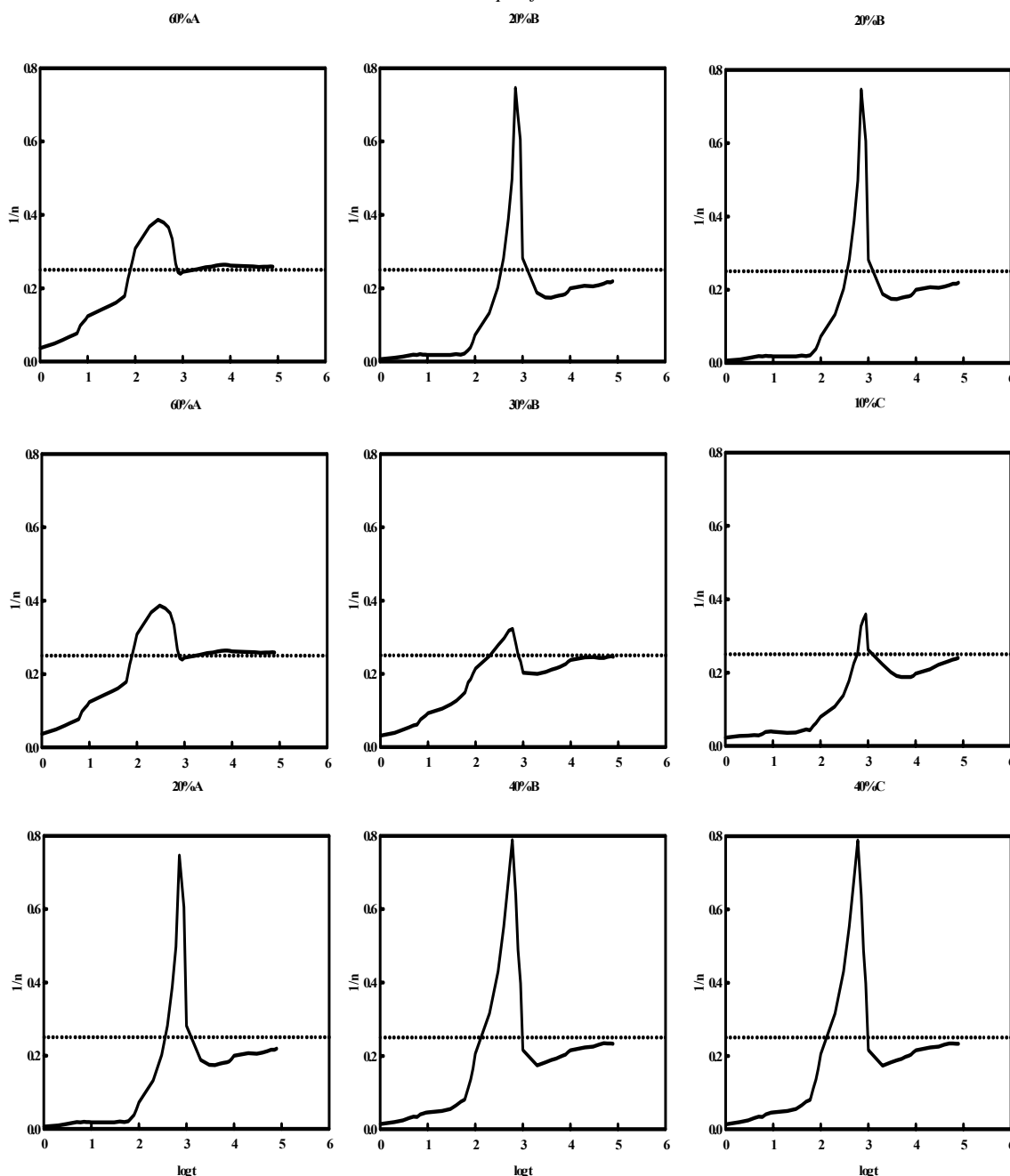


Figure 5. The slope of the curves in Figure 4 as a function of time for different volume fractions of the B phase and the C phase. The horizontal dotted lines show the theoretical value  $1/n = 1/4$



Many theoretical models of coarsening second phase inhibiting grain growth have different physical or geometrical bases. Under certain conditions, however, the relationship between the matrix grain size and the second phase parameters has been proposed to be,

$$\frac{d}{r} = \frac{c}{f^\beta} \tag{8}$$

where  $d$  is the matrix grain size,  $r$  is the second phase grain size, and  $c$  and  $\beta$  are constants. It was considered that  $\beta = 1$  by the early Zener model [11]. Computer simulations obtained  $\beta < 1$ , e.g.  $\beta = 1/2 \sim 1/3$  [20, 40, 46, 47].

Hellman and Hillert [47] showed that  $d/r$  is proportional to  $1/f^{1/3}$  for a 3-D system when most of the particles are located at grain corners and boundaries. On the other hand, Srolovitz *et al.* [48] showed that  $d/r$  is proportional to  $1/f^{1/2}$  for a 2-D system by assuming all particles distributed at grain boundaries. The mean grain size of A phase ( $d_A$ ) is plotted against the mean grain size of B phase ( $d_B$ ) and the mean grain size of C phase ( $d_C$ ) for different volume fractions ( $f_v$ ) in Figure 6.

It is shown from Figure 6 that the ratio of A-phase/B-phase grain size ( $d_A/d_B$ ) is constant at a given volume fraction of B-phase. Similarly, the ratio of A-phase/C-phase grain size ( $d_A/d_C$ ) is constant at a given volume fraction of C phase. It is clear that a good linear relationship exists between  $d_A$  and  $d_B$  at all B-phase volume fractions. Also, a good linear relationship exists between  $d_A$  and  $d_C$  at all C-phase volume fractions.

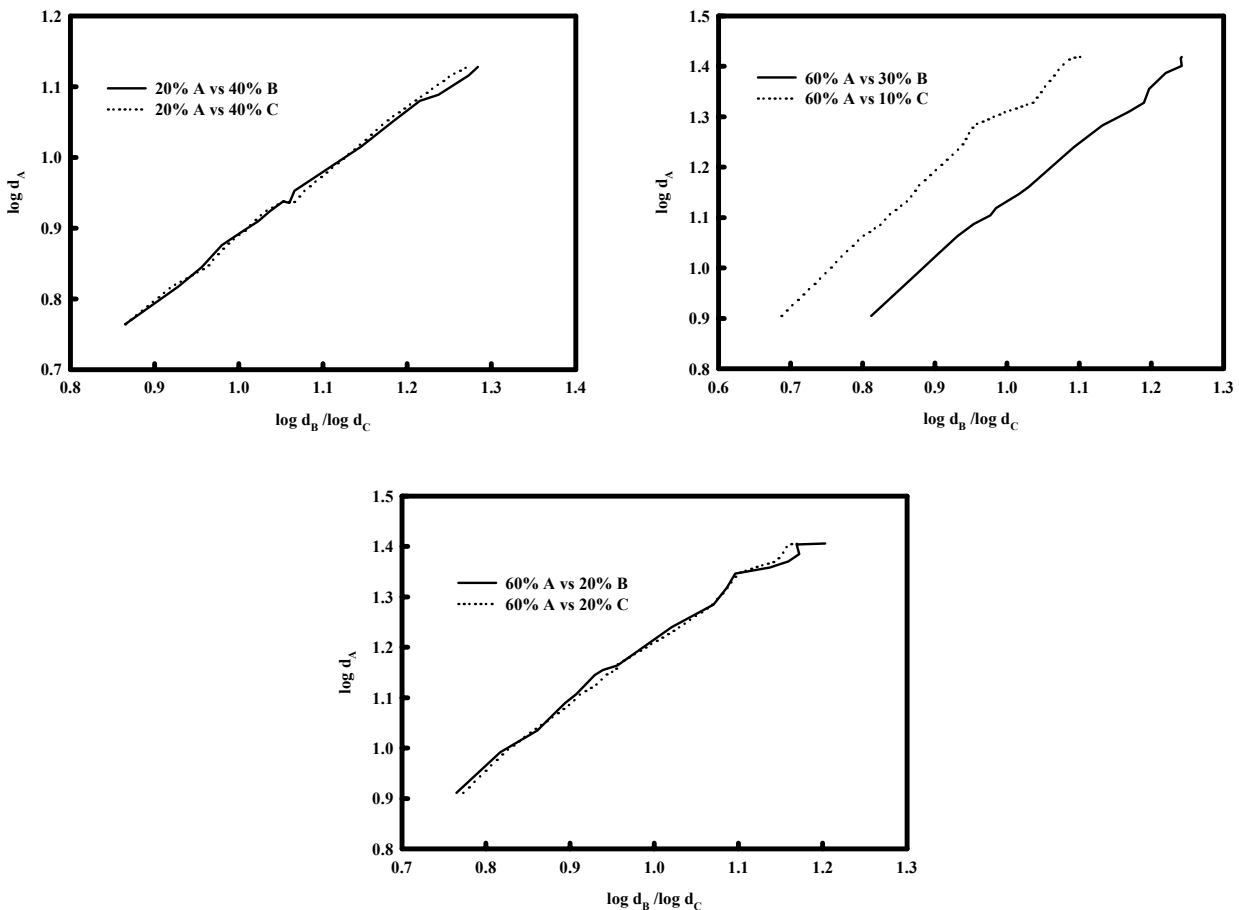


Figure 6. The dependence of mean grain size of A phase on the mean grain size of B phase and C phase as a function of B- and C-phase volume fraction. The volume fraction for each phase is specified

#### 4. CONCLUSION

The kinetics of grain growth in three-phase system has been investigated through computer simulations. The simulation results show that the kinetics and microstructural evolutions are in qualitative agreement with previous numerical simulations for grain growth in two-phase systems. It is found that the coupled grain growth and coarsening in three-phase systems is controlled by long-range diffusion and follow the power-growth relationship,  $d \sim t^{1/n}$  with  $n = 4$ , which is independent of initial conditions and volume fractions of each phase. It is found that a good linear relationship exists between  $d_A$  and  $d_B$  at all  $B$ -phase volume fractions. Also, a good linear relationship exists between  $d_A$  and  $d_C$  at all  $C$ -phase volume fractions. These results are consistent with the hypothesis that grain growth in three-phase systems in which both phases grow is controlled by Ostwald ripening of the dispersed particles and is coupled due to Zener pinning.

Future numerical models need to include the effects which are present on small time scales but disappear on large time scales such as elastic stress. This would help to fully use the information provided by the laboratory experiments. It is also important to extend the simulations to three dimensions. Although grain growth exponents are unlikely to change, some processes such as Zener pinning, are not accurately described by two-dimensional models [49].

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