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Simulation of Two-Dimensional Polycrystalline Material by using Monte Carlo Approach

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ABSTRACT

Microstructure evaluation is one of the key element to determine the properties and performance of a material which has been great eternal towards humanity and industrial applications. The present research work aims to study the grain growth kinetics influenced by various second phase particles and also homogeneity of the grains using Potts model under the Monte Carlo simulation method. A 2D square lattice with optimum matrix size (N), Q-States (Q), and MCS was employed. The mean grain size (Rmean) and maximum grain size R(max) was determined for various surface fractions, implying average grain growth and microstructure consistency. The results are found to be in complete harmony with the proven theoretical and simulated values. The average size of the grains under the influence of particles was found to obey the square root dependence.

KEYWORDS

Potts Model, Grain Growth Kinetics, Second Phase Particles, Grains Homogeneity, 2D Simulation.

INTRODUCTION

Grain size is an essential factor to consider when defining a material property, especially when combining different materials. It is one of the most significant difficulties in crystal structure control [1]. This type of research usually entails a thorough examination and evaluation of morphological data, which was expected, accomplished utilizing massively parallel computing capacity [2]. The most well-known and commonly utilized computer simulations and grain growth simulation theory were presented in this paper, using the Monte Carlo method. The Monte Carlo methods conceptual foundation and the physical aspects of grain refining have an intriguing relationship. Both are strongly reliant on statistics and chance, so the technique adequately depicts the trend [3, 4]. A novel Monte Carlo technique is used to examine the kinetics of two-dimensional grain growth. The model used maps the microstructure to a secure lattice [5]. A number between 1 and Q is given to each layer site possibility. The original orientation distribution was picked at random. The system gradually degrades the amount of unlike crystallographic orientation closest-neighbor pairs [4].

The initial orientation is chosen at random. The method restricts the number of closest pairs of crystallographic orientation to a minimum lattice [6]. It is possible to examine the kinetics of grain boundary motion by counting the number of orientation shifts assigned to each lattice. The model also reproduces the morphology of grains and the kinetics of grain growth and recrystallization [7, 8]. The Monte Carlo method is a predictive unit simulation technique used in computational mechanisms. It analyzes the growth and associated theories [9]. Despite estimating group features of microstructure creation through model outcomes, computer simulations have provided snapshots of the microstructure over time [10]. The local and group characteristics of the microstructure can be calculated on these snapshots with the empirical variant of the microstructural analyzes [11]. The Monte Carlo simulation is among the most effective techniques of microstructure evolution in object science, of the few simulation software technologies developed over the years. The launch of the Simulation Model can be followed back to the early nineteenth century during the construction of models for the study of ferromagnetism applications in the realm of physics.

The Ising [12] formed a magnetic object as a set of rotations with only two possible states, namely up and down,

improved on this model by allowing each particle in the system to handle Q states rather than just two [13]. This method was refined to study neutron diffusion in fissile substances [14, 15]. Local and ensemble features of the microstructure can be decided using this simulation technique in metallography. Over the years, several computer simulation strategies have been tested [5] and proposed the Monte Carlo method as one of the most effective methods for simulating microstructure development in polycrystals. This method was initially designed to research neutron diffusion in highly enriched materials [16]. Still, it was extended to grain growth investigations because the underlying mechanism was unpredictable [17]. In this research work, the standard potts model under the Monte Carlo simulation method is used to investigate the stimulated normal grain growth and grain growth under static particles lying within the grains and on the grain boundaries in polycrystalline materials. The grain growth exponent was determined under the influence of inert particles. The homogeneity and distribution of the grains are studied by using topology and also standard distribution curve.

MATERIALS AND METHODS

Q-States Potts-Model Simulation By Metropolis Algorithm

The generic materials are used for the present study. The nature of mobility of the grain boundaries in the material selected exactly resembled the grain boundaries from simulation approach. The grain growth simulation study was carried out using Monte Carlo methodology with the help of the metropolis algorithm mentioned below [18]:'N' represents the output of lattice sites. Lattice sites are denoted by a random scale from 1 to Q, indicating the crystal's crystallographic position. Select Q-state value other than 1 to apply the % of second phase particle f in the matrix. A random site is picked from the N2 elements in the matrix and compared to all of its closest neighbor elements, which are eight in the instance of the square lattice. The Metropolis Algorithm and Glauber dynamics are used in Monte Carlo methods to study the grain growth kinetics by simulation.

- Choose the size of the lattice and the percentage surface fraction that is randomly placed in the matrix.
- A square matrix of size 'N' generated with N2 lattice sites is represented by a series of random values ranging from 1 to Q, where Q denotes the number of grain orientations.
- Select the second Phase particles inert in the matrix and choose the value of Q other than 1: Q. f=0 if monophonic.
- The Hamiltonian for the 3x3 matrix is now constructed using the following formula:

$$\text{Hamiltonian (E1)} = -J\sum_{i}^{n} \partial si\, \partial sj - 1 \quad (1)$$

i = occupying the place element (2, 2) and j = any other aspect compared with Then,

$\partial ij = 0$ if $i \neq j$

$\partial ij = 1$ if $i = j$

Where ∂ij i=j, the interfacial grain boundary energy between the two grains is known as the Kronecker delta, and J = the metal's surface energy.

- The grain growth of the selected element was replaced with a new element at random, and the Hamiltonian (E2) is computed for the new element. The intended impact is determined,

$$\Delta E = E2 - E1 \quad (2)$$

If $\Delta E \leq 0$, the modification has been accepted, else if $\Delta E > 0$, compute Probability,

$$P = e^{(-\Delta E/kT)} \quad (3)$$

Where k = Boltzmann constant, and T = temperature, If $(r < P)$ where r is uniformly distributed from a random number between 0 and 1, the change is still allowed; otherwise, it is rejected.Steps 3 to 5 are repeated after cycle 'N^2' multiple times, resulting in one Monte Carlo Step (MCS), the simulation's time measurement.

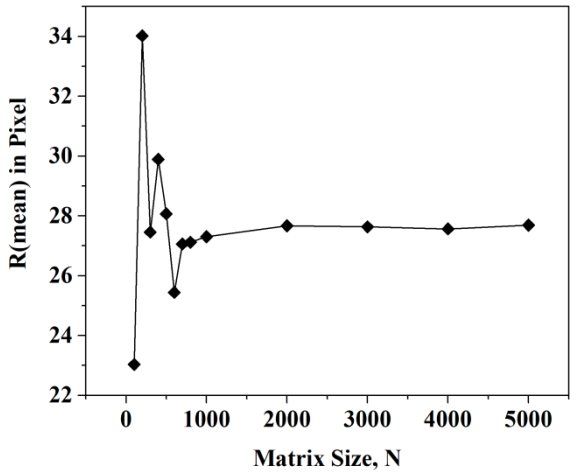
This system would be used to perform a large-scale computation of crystal lattice migration. The program needs

as much computing power as is practicable. Therefore, the design needs to be as compact as possible to maintain the capability of the PSU (power supply). Everything tests were conducted on a specially configured 16GB RAM system, Dell OptiPlex 7070 with 9th Gen Intel Core TM i7 9700 (8-Core, 12MB Cache, Intel Turbo Boost Technology, up to 4.7GHz) and JAVA (Version 14.02 of Java Development Kit), Eclipse (Photon). In the Java programming language, compelling, scalable, and ultra-fast code has been written. However, close attention has been paid to time-saving memory management. The simulations have gone through over a million Monte Carlo steps that take about 60 seconds to run 1,000 Monte Carlo steps on a 2000×2000 matrix size containing 10^9 Metropolis algorithm iterations

RESULTS AND DISCUSSION

Normal Grain Growth

The regular grain growth simulations are run with a matrix size of 2000×2000; beyond this matrix size, the mean grain size R (mean) almost remains constant. It means there is no sufficient change in the grain boundary interfacial energy (Hamiltonian Energy), as shown in figure 1. Initially, the grain growth rate increases with an increase in q-states, as it reaches q-state 64, the grain growth exponent drops significantly as the q-state reaches 64 the Q-States, as shown in figure 2. Finally, we chose the optimum value of matrix size and Q-states to calculate the optimality of simulation conditions, which impacts the simulation.



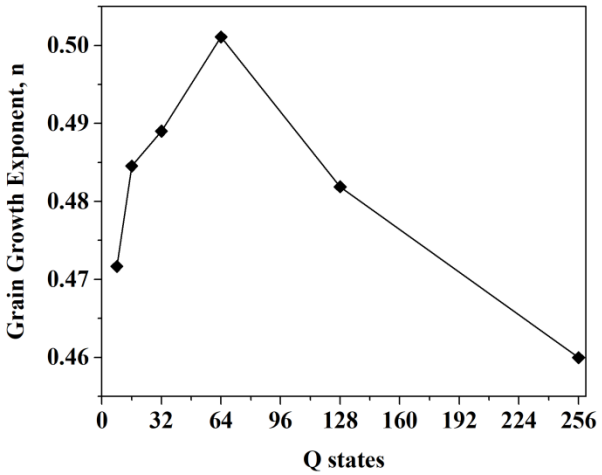


Figure 1. Mean grain size R (mean) vs. N and **Figure 2.** Grain Growth Exponent (n) vs. the Q States

Grain growth takes place with the aid of a grain boundary movement when there is a massive reduction in their interfacial free energy of the grain boundaries as a result of this driving force is formed. These grain boundaries are migrating drastically; the smaller grains disappear immediately compared with the surrounding bigger grains. Simulations with a 2000x2000 square matrix are used to develop the grain growth depicted in Figure 3. Periodic boundary conditions are used to obtain the borders of nearby grains. Grain-orientation tracking ensures all grains have the same orientation as their first or second closest neighbors, which can be accomplished by keeping track of each grain's first and second close neighbors [19].

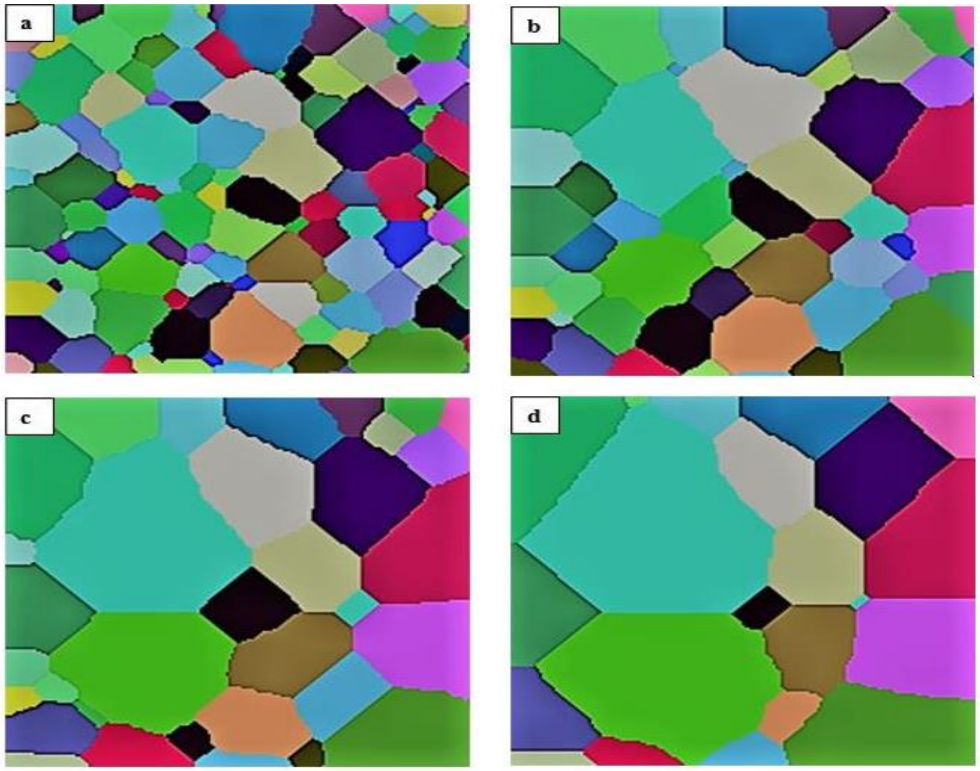


Figure 3. Grain growth kinetics when N=2000, Q=64, and f=0 at various MCS (a) 10000 MCS, (b) 30000 MCS, (c) 60000 MCS, and (d) 100000 MCS

Grain Growth Under Static Particles

The Hamiltonian, which represents the surface energy of the grain boundaries, falls continuously during grain growth, owing to a decrease in the grain boundary area. If we assume that the initial matrix is filled with random numbers so that there are no two like neighbors, the total Hamiltonian of the system is calculated as $2N^2$, where N is the matrix size, Suppose at each instant of grain growth, the Hamiltonian is calculated. In that case, the drop in the Hamiltonian is the difference between 2N2 and the Hamiltonian at any moment. Figure 4 shows the decrease in the Hamiltonian energy continuously as MCS increases. The Hamiltonian energy was calculated by metropolis algorithm, and if this value is constant for 5000 MCS, we declare the stagnation of the grains, Calculate the Limiting grain size under maximum surface fractions (0.1%), and also declare optimum MCS value (100000 MCS)

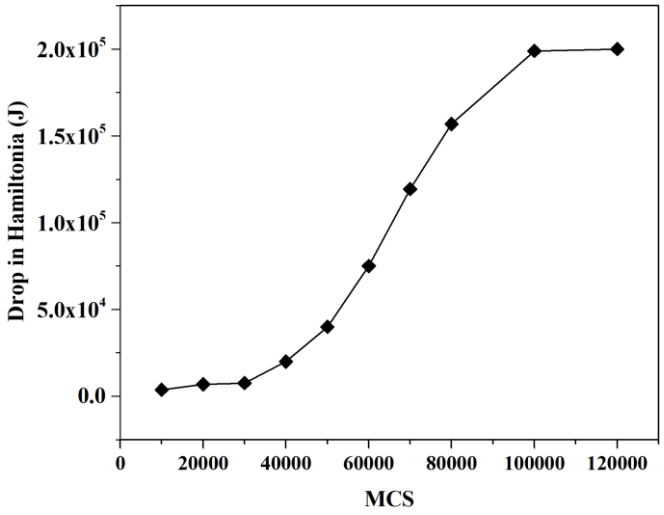


Figure 4. Drop-in Hamiltonian energy (J) vs. MCS When f=0.1

The simulations were performed on a 2D square matrix with an array size (N) of 2000×2000 and Q-states (grain Orientations) 64 by using standard Monte Carlo algorithms [17] to randomize the simulation completely. The static particles of one pixel present in the matrix are achieved by giving the value Q=0. The second phase particles were also provided a one-pixel homogeneous structure and turned solid. The nearly linear relation between the R(mean) and MCS with various surface fractions static particles was studied as shown in Figure 5.

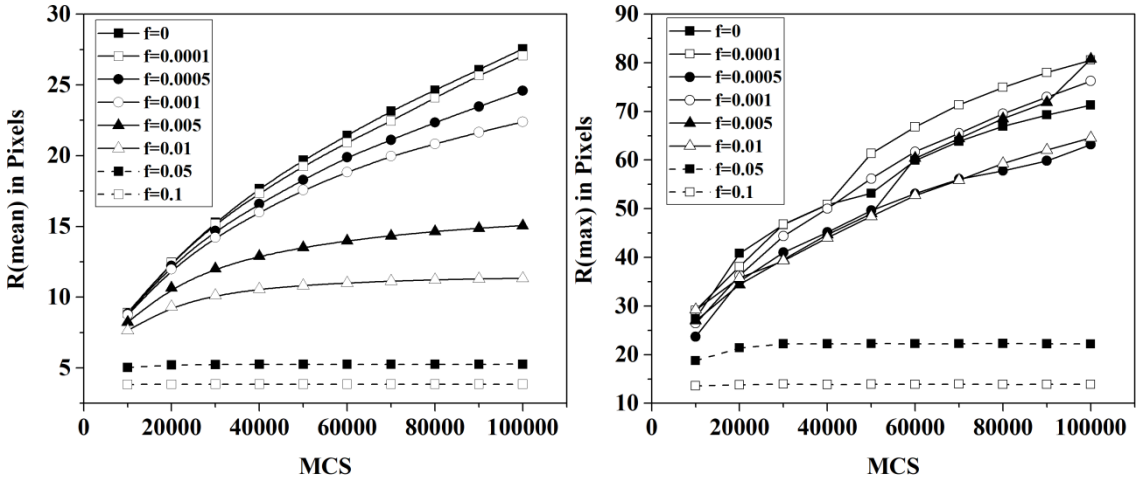


Figure 5. R (mean) (in pixels) vs. MCS for N = 2000 at Q = 64 and Figure 6: R (max) (in pixels) vs MCS for N = 2000 at Q=64.

First individual grains area data was computed through the simulation. Thereby, the R(mean) value was calculated using sqrt (A/π) with all dimensions in pixels. The rate at which R(mean) values drop with higher values of f and increases with more iteration (MCS). The lower fraction of second phase particle led to a higher grain growth rate. A greater proportion of second phase particles associate with grain boundaries at higher values of f. Thus, in such situations, Zener pinning is more operational than at lower values. The grain radius grows at a slower rate. Figure 6 shows the variation of the maximum grain radius with MCS for various values of f, and comparing both figures result in normal grain growth

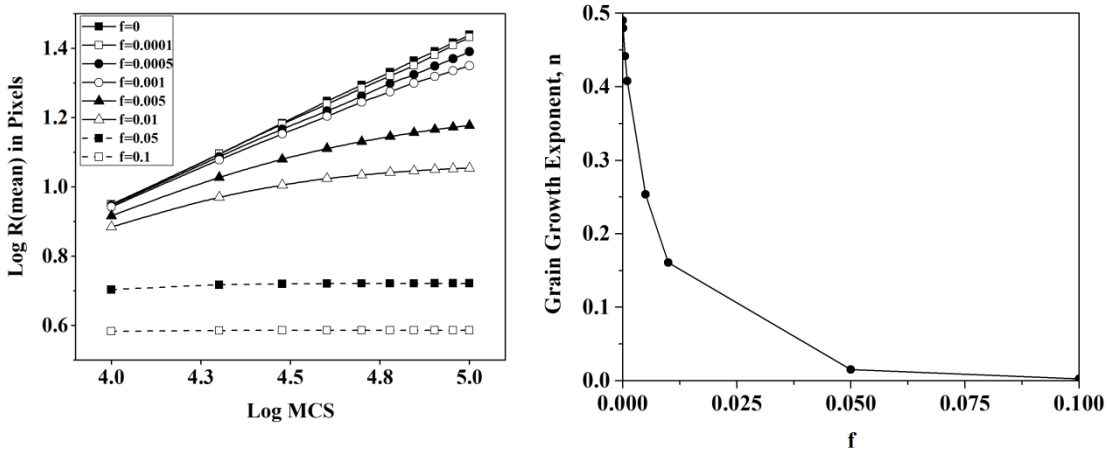


Figure 7. LogR (mean) vs MCS for N = 2000 at Q = 64 and Figure 8. N vs. surface fraction, f, for N = 1000, Q = 64.

We can see that the maximum grain size for each surface fraction is only around three times the Rmean, a typical feature of average grain growth. Figures 7 indicate R(mean) vs. MCS ton log scale, and figure 8 illustrates grain growth exponent (n) vs. f., which can be used to study grain growth kinetics. The grain growth factor has a value of n=0.48 (m=2) at f=0, which is equal to the experimentally determined value of n=0 .5 [20] However, when the static particles increases led to a drop in the grain growth exponent significantly. Figure 6 shows that grain growth is challenging to achieve due to the substantial surface percentages. The percentage of

static particles inert on the grain boundary versus MCS was computed as shown in Figure 7. The immobile particles that cling to the grain's sides were counted. The MCS rise at the lower level percentages was maintained at high-level Monte Carlo steps, indicating that the number of particles engaging the grain size was large when the surface fractions were higher. We know from Gibbs–Thomson equation

$$P = \frac{2\gamma}{R} \tag{4}$$

The keywords are ΔP and R the same way as before. Where R is the radius of the grains, P is the pressure drop at the grain boundary interface, and γ is the surface energy of the grains, and Gibb's free energy equation.

$$\delta g = \frac{Vm2\gamma}{R} \tag{5}$$

The change in pressure around the grain size and Gibb's free energy change are approximately equal to the grain radius. As a result, for small R values, both ΔP as well as δg is higher, implying grain growth is more vital.

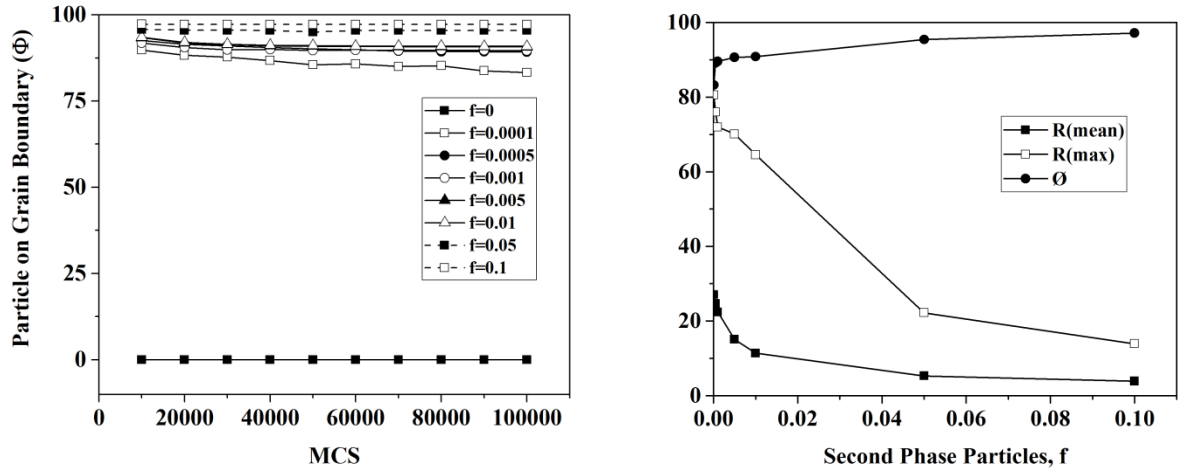


Figure 9. Φ vs MCS for N = 2000 at Q= 64 and Figure10. Variation of R (mean), R (max) and Φ vs f. for N = 2000 at Q=64.

Because the grain radius is smaller at the start of grain refinement, a comparatively higher driving force results in particles being emitted from the grain sizes at higher speeds [21], as the iterations are strengthened, for all purposes, the force decreases when there is a start of restricting grain size, and Ø stagnates. Figure 10 shows precisely how, with the rise in surface fraction, R (mean) and R(max) drop off, while Ø increases f, showing an asymmetrical relationship with R(mean) and R(max).

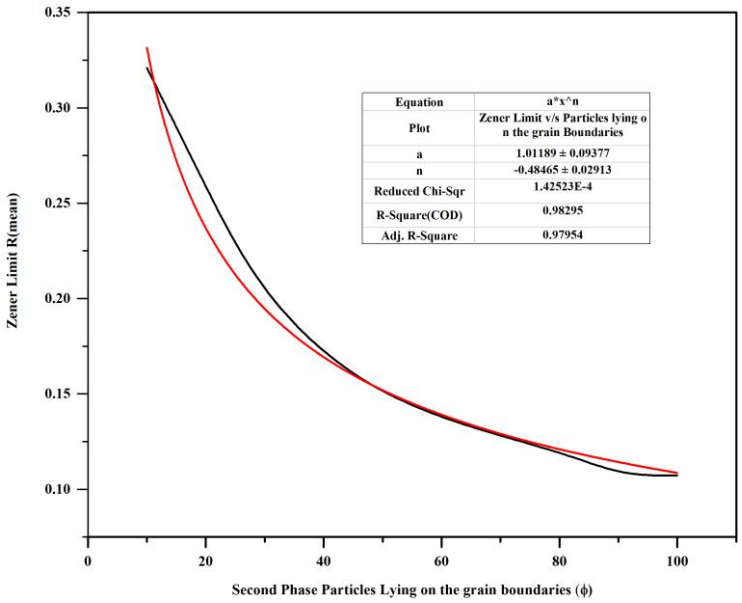


Figure 11. Relation between second phase particles lying on the grain boundary vs. Zener limit R (mean)

The grain growth exponent calculated with limiting grain size is 0.48, as shown in figure 11 and experimentally proved by [21] that the value of grain growth exponent for polycrystalline materials is 0.5. We got the R 2, 98%. The simulated grain growth exponent value is equal to the experimental value.

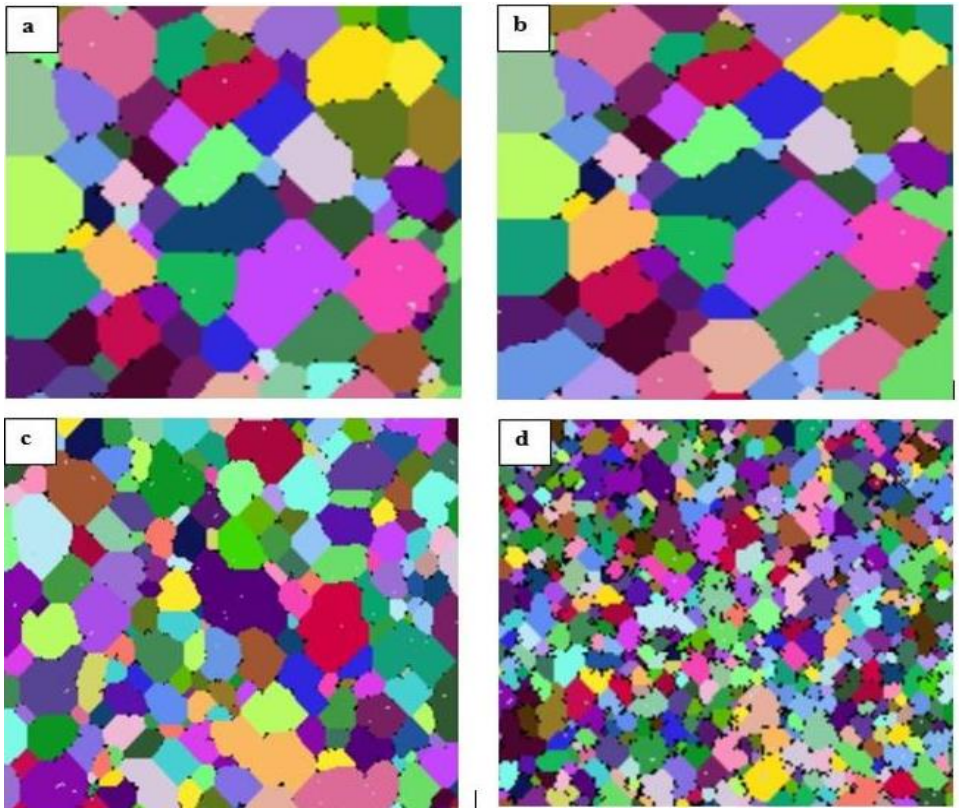


Figure 12: (a) N = 1000, Q = 64, f = 0.0001, (b) N = 1000, Q=64, f=0·001and(c) N=1000, Q=64, f=0·01. (d) N=1000, Q=64, f=0·1

A few images of microstructures that are simulated demonstrate their resemblance to real ones in figure 12 (a-d) (at MCS=100,000 and different values of f). Micrographs display an equal grain structure distribution, displaying static Zener particles in Figure 7(a-d). It can also be noted that, with an increase in fractions of the second phase particles, the grain sizes decrease by an average of 100,000 MCS. Evolving microstructures' self-similarity, it is also possible to detect this feature of grain growth in the three digital micrographs.

Unfortunately, experimental methods for acquiring digital microstructures are not always successful in achieving the resolution required to capture the significant geometric characteristics of the microstructures. The inability to undertake a full microstructure assessment and material activity recognition, such as modal testing based on numerical modeling may be limited by the frequency of microstructural characteristics ignored due to inadequate resolution.

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CONCLUSIONS

The Metropolis algorithm is considered to form an excellent base. However, Java provides excellent software support for researching the evolution of microstructure in polycrystalline materials. It was found that an optimum size of matrix 2000, Q-states 64, and 100000 MCS are desirable for better results while carrying out Monte Carlo simulation of grain growth in two dimensions. In a polycrystalline material, the grain growth exponent was determined to be 0.48. Still, with a high surface fraction of 0.1, the value plummeted virtually to zero. Simulation has accomplished a very well distribution of grain size, microstructures, and homogenization of the microstructure. The surface fraction of second phase particles inert on the grain boundaries obeys the inverse square root dependency. Grain growth kinetics of specific materials with the addition of varying second phase particles can be studied in future.

REFERENCES

[1] Y. Liu, T. Baudin, and R. Penelle, "Simulation of normal grain growth by cellular automata,"Scripta Materialia, vol. 34, no. 11, 1996.

[2] T. M. Rodgers, J. D. Madison, V. Tikare, and M. C. Maguire, "Predicting Mesoscale Microstructural Evolution in Electron Beam Welding,"JOM, vol. 68, no. 5, pp. 1419–1426, 2016.

[3] D. J. Srolovitz, M. P. Anderson, P. S. Sahni, and G. S. Grest, "Computer simulation of grain growth—II. Grain size distribution, topology, and local dynamics,"Acta Metallurgica, vol. 32, no. 5, pp. 793–802, 1984.

[4] E. A. Lazar, R. D. MacPherson, and D. J. Srolovitz, "A more accurate two-dimensional grain growth algorithm,"Acta Materialia, vol. 58, no. 2, pp. 364–372, 2010.

[5] D. J. Srolovitz, G. S. Grest, and M. P. Anderson, "Computer simulation of recrystallization—I. Homogeneous nucleation and growth,"Acta Metallurgica, vol. 34, no. 9, pp. 1833–1845, 1986.

[6] F. J. Humphreys and M. Hatherly, "Recrystallization and Related Annealing Phenomena". Elsevier, 2021.

[7] D. J. Srolovitz, M. P. Anderson, G. S. Grest, and P. S. Sahni, "Computer simulation of grain growth-III. Influence of a particle dispersion" Acta Metallurgica, vol. 32, no. 9, pp. 1429–1438, 1984.

[8] M. P. Anderson, D. J. Srolovitz, G. S. Grest, and P. S. Sahni, "Computer simulation of grain growth—I. Kinetics" Acta Metallurgica, vol. 32, no. 5, pp. 783–791, 1984.

[9] Y. Saito and M. Enomoto, "Monte Carlo Simulation of Grain Growth," ISIJ International, vol. 32, no. 3, pp. 267–274, 1992.

[10] J. W. Martin, R. D. Doherty, and B. Cantor, Stability of Microstructure in Metallic Systems. Cambridge University Press, 1997.

[11] R. Zheng and B.-G. Liu, "Stable two-dimensional ferromagnets made of regular single-layered lattices of single-molecule nanomagnets with perpendicular anisotropy," Journal of Applied Physics, vol. 106, no. 5, pp. 054316, 2009.

[12] Z. Liu and O. Ciftja, "A quantum simulation approach for a three-dimensional Ising spin model—Comparison to mean-field theory," AIP Advances, vol. 7, no. 5, pp. 055103, 2017.

[13] S. Mishra and T. DebRoy, "Non-isothermal grain growth in metals and alloys," Materials Science and Technology, vol. 22, no. 3, pp. 253–278, 2006.

[14] B. Radhakrishnan and T. Zacharia, "Monte Carlo simulation of grain boundary pinning in the weld heat-affected zone,"Metall Mater Trans A, vol. 26, no. 8, pp. 2123–2130, 1995.

[15] Y. J. Kim, S. K. Hwang, M. H. Kim, S. I. Kwun, and S. W. Chae, "Three-dimensional Monte-Carlo simulation of grain growth using triangular lattice,"Materials Science and Engineering: A, vol. 408, no. 1, pp. 110–120, 2005.

[16] N. Metropolis and S. Ulam, "The Monte Carlo Method,"Journal of the American Statistical Association, vol. 44, no. 247, pp. 335–341, 1949.

[17] Stickler, Benjamin A., and Ewald Schachinger. "Markov-Chain Monte Carlo and the Potts Model," In Basic Concepts in Computational Physics, pp. 275-286. 2014.

[18] Panzarino, Jason F., and Timothy J. Rupert. "Tracking microstructure of crystalline materials, a post-processing algorithm for atomistic simulations," pp. 417-428, 2014.

[19] N. P. Louat, "On the theory of normal grain growth," Acta Metallurgica, vol. 22, pp. 721– 724, 1974

[20] L. B. Kong et al., "Grain Growth and Microstructure Development," in Transparent Ceramics, L. B. Kong, Y. Z. Huang, W. X. Que, T. S. Zhang, S. Li, J. Zhang, Z. L. Dong, and D. Y. Tang, Eds. Cham: Springer International Publishing, pp. 519–579, 2015.

[21] El-Khozondar, Rifa J., Hala J. El-Khozondar, G. Gottstein, and A. Rollet. "Microstructural simulation of grain growth in two-phase polycrystalline materials," Vol. 29, no. 1, 2006.