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Grain Growth Inhibition By Second Phase Particles: A Two-Dimensional Monte Carlo Computational Study

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Abstract

A comprehensive 2D simulation was performed on a square lattice under the influence of a second phase particle to validate the Zener limit. The effect of matrix sizes from 100 to 10,000 was examined on R(lim), R(max), Scaling constant(k), and impurities lying on the grain boundaries (ϕ). In addition, the optimum matrix size N=2000 under various second phase particles and Q states were investigated. The particle-pinned regimes developed a unique relationship between the Zener limit and the fraction of second phase particles resting on the grain boundary, i.e., $R_{(limit)} = \frac{1}{e^{\phi}}$*. It was observed that the particle fraction is proportional to the determined limiting grain size. The homogeneity and distribution of grains were observed to obey the lognormal behaviour.*

Keywords: *Q-States, second phase particles, matrix size, Grain size Distribution, Zener limit, and scaling constant.*

1.0 Introduction

Smith and co-workers have studied the evolution of grain growth under second-phase particles over the years since the initial work in 1948 [1]. The principles of microstructure interpretation in terms of interaction between second phase particles and moving grain boundaries due to limiting grain sizes have been explained before. The pinning pressure induced by the second phase particles would counteract the driving pressure that exists owing to grain boundary curvature [1]. Since this happens, it would be impossible for normal grain growth to proceed. As a result, the grain size would reach a maximum radius [1], given by

$$R_{(limit)} = \frac{4r}{3f} \quad \ldots (1)$$

Where *R(lim)* is the maximum grain radius under the influence of second phase particles, r is the mean size of second phase particles, and f is the area fraction of the second phase particles. In developing the equation to approximate the limiting grain size possible, Zener made certain assumptions, which have led to proposals of altering the equation.

$$R_{(limit)} = k\frac{r}{f^m} \quad \ldots (2)$$

Where *k* represents the constant value, i.e. $k = \frac{4}{3}$ and *m*=1, equation 2 transforms to the Smith-Zener equation. Investigation of the limiting grain size through the simulation route began with pioneering work by Srolovitz et al. in 1984 [2]. The 2D grain growth kinetics was carried out using Monte Carlo simulation. Exploration of the Zener limit through the

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simulation route has, since then, gathered enormous attention. However, simulations continue being performed to understand the limiting grain size, including this research work. The various values for the pinned grain size proposed by researchers over the years have been summarized in Table 1 in chronological order. The Smith-Zener equation for the theoretical limit of the grain size is also given in the table to compare with the simulation result. Srolovitz [2] carried out a 2D Monte Carlo simulation on a triangular lattice on a modest matrix of size 150×150. The value obtained for the limiting grain area A(lim), which is scaled inversely with the volume fraction of the particles and can be approximated to the effect that the limiting grain radius is inversely proportional to the square root of the volume fraction. Doherty et al. [3] also arrived at similar limiting grain size values while carrying out a computer simulation of 2D microstructure but with a non-random distribution of particles. The authors chose non-random distribution since it was reasoned that random distribution of particles led to a more than random interaction of the particles with the grain boundaries in a simulated atmosphere.

Hazzledine and Oldershaw [4] carried out a 2D simulation and proposed a value R(lim) almost equal to its predecessor. Hassold et al. [5] performed a similar study employing MC simulations to study the influence of second phase particles on a triangular lattice of 200×200. They gave a value for the Zener limit, as shown in Table 1. Finally, Gao et al. [6] investigated the effect of second phase particles on a 500×500 triangular matrix of size using 2D simulations. They gave the Zener limit value as shown in Table 1. Mohseni introduced the degree of contact between grain boundaries and second phase particles to predict the grain size limit in the presence of second phase particles. The degree of contact increased during grain growth and reached a stable value when the grain structure was pinned [16]. Although the initial location of second Table 1: Zener limit modifications over the years through 2D simulation

Table 1: Zener limit modifications over the years through 2D simulation

Sl. No.	Author(s)	Year	R(lim)
1	Smith [1]	1952	$\frac{1.33r}{f}$
2	Srolovitz *et al.* [2]	1984	$\frac{r}{f^{0.5}}$
3	Doherty *et al.* [3]	1987	$\frac{1.7r}{f^{0.5}}$
4	Hazzeldine *et al.* [4]	1990	$\frac{1.8r}{f^{0.5}}$
5	Hassold *et al.* [5]	1990	$\frac{0.6r}{f^{0.55}}$
6	Gao *et al.* [6]	1997	$\frac{0.59r}{f^{0.52}}$
7	Kad *et al.* [7]	1997	$\frac{1.41r}{f^{0.5}}$
8	Soucail *et al.* [8]	1999	$\frac{1}{(f)^{0.5}}$
9	Huang *et al.* [9]	2006	$\frac{1}{f^{0.5}}$

Second phase particles did not have a significant contribution to the pinning of grain boundaries without considering the measure for the degree of contact (R), Gao et al. [6] obtained a limiting grain size use approximately equivalent to that obtained by Harsold et al [5] as shown in Table 1. Kad and Hazzledine [7] carried out 2D MC simulations on 2000×2000 matrix size in a square and triangular lattice under various shapes of second phase particles. They hypothesized that the square root of 'f' scaled inversely with the pinned grain size. Furthermore, they observed that the stagnant grain shape did not depend strongly on the precipitate shape, but the stagnant grain size had a weak dependency.

Soucail et al. [8] carried out a 2D MC simulation on a 2000×2000 triangular lattice under surface fractions from 0.0001 up to 0.1. They introduced a new variable ϕ into the Zener equation. They proposed that the Zener limit scale is inversely proportional to the square root of the product of ϕ and f (Table 1). However, the effect of ϕ on the limiting grain size has been discussed earlier by Srolovitz et al. [8], Doherty et al. [3] and Huang et al. [9] carried out 2D Potts model simulations on a 200×200 lattice. They observed that pinned grains are found to obey a and $R(lim) \propto \frac{1}{\sqrt{f}}$ relationship fora range of particles in the presence of randomly distributed impurities with fractions varying from 0.0001 to 0.1.

2.0 Methodology

2.1 Monte Carlo simulation by Potts model

Potts model, based upon the Metropolis algorithm and a normal boundary condition, was used in the present study, and the Monte Carlo simulation is a reputable method to study grain growth [2], [11-12]. Therefore, I disregarded the impact of lattice temperature and conducted the simulations at a steadystate, i.e., T=0. Originally, the continuum microstructure appears as a square matrix with arbitrary integers ranging from 1 to Q, where Q indicates the orientations of the grains. Next off, the number of dissimilar neighbors is calculated by selecting an arbitrary matrix aspect and contrasting it to its closest neighbors. Next, the previously selected element, the once minor (?) is a larger chosen element, is flipped. Finally, we tally up the number of people who have unrelated neighbors. Suppose the unlike neighbors of the flipped items (DE) are the same or different from the original elements (DE). Flipped element replaces the original matrix. That is until something better is found, the initial element remains. When N and MCS are the matrix size

and measure of time, respectively, one Monte Carlo step is formed. Second phase particles bring random static components into the matrix that do not participate in grain coalescence but prevent it from occurring.

2.2 Hardware and software

More than a hundred million iterations were required to allow for grain growth and the evolution of microstructures under different input variables by using a powerful computer. As a result, a system with the following specifications was explicitly created to run all simulations. A Dell OptiPlex 7070 Tower Desktop Computer was built for adaptability, flexibility, and enhanced performance. It was driven by a 3.0 GHz Intel Core i7-9700 Eight-Core CPU that can be increased to 4.7 GHz, enabling it to run several programmes simultaneously. Furthermore, the 64GB of 2666 MHz DDR4 RAM assists to guarantee smooth multi-tasking and also permits the computer system to access frequently-used data promptly. Programmes, particularly for such an application, are purely a function of CPU memory interaction speed. Therefore, this combination was the fastest available in the market.

The present code, on which the results of this research work are presented, is entirely on the Java platform. The code generated is very efficient, highly parallel, and super-fast in execution. For example, it takes about 1 minute for a 2000×2000 size matrix with a Q-state value of 64 to run 1,000 Monte Carlo steps, which means that 4×10^9 iterations of the Metropolis algorithm would have been accomplished. Some salient features of the code are (1) The code was written in JAVA (JDK version SE 14.0.2) using freeware, Eclipse (4.16.0). (2) The code was parallelized, permitting all 4 processors to be used throughout the simulation. Achieved this by splitting the array into four smaller sections and creating a thread to process each section while ensuring that the size is divisible by 4.3. used multiple threads in the code to carry out parallel processing, utilizing all four cores effectively. The cores did not present any artificial boundary conditions since no matrix subsection was allotted to one core. Also, as we see from the results later, the grains have grown quite generously across all cores and have extended grain boundaries at various angles. (4) Grain area estimations were additionally parallelized, with the choice to create the needed documents after a particular variety of runs. (5) coded the option to self-terminate a simulation trial upon no change in the Hamiltonian for a specific number of iterations for stagnation cases. saved files by specifying the gap between the file hold in terms of MCS.

The simulation, on the other hand, took almost two weeks to complete. It required 280 hours of non-stop CPU usage only to keep the 10000×10000 matrices static. Used the code to keep track of the limiting grain size. It was also written to automatically end the simulation when the Hamiltonian value did not change for 1000MCS consistently, as determined by the Metropolis method. Therefore, only computed the limiting grain size once to avoid wasting CPU time at the simulation conclusion. Consequently, the drop in Hamiltonian, which directly indicates grain growth, was regarded as an indication of grain growth stagnation. Therefore, the 2D simulation was performed on irregularly sized impurity particles with a start count of 10 MCS. Converting selected grains into impurities and allowing them to spread randomly over the matrix until the desired percentage of impurities is attained. Every impurity is static. Furthermore, except for inert particles, the simulation continues with the remaining grains and begins initially; since the impurity sites are fixed, and their area is preserved, they do not participate in the lattice reorientation process. Another way, cannot to acquire impurities outside of the impurity region. Impurity particles obstruct grain movement locally when grain size decreases, making unpinning difficult.

3.0 Results and Discussions

This research work found that Monte Carlo simulations of smaller-sized matrices (≤ 500) have been the primary focus of two excerpts: Kad et al. [7] and Soucail et al. [8], having dealt with matrices 2000×2000. To prevent the influence of the matrix size on the experiment outcome and ensure accurate results, researchers should choose a pinned grain size of R(lim) that is smaller than one-third of the matrix size [13]. When smaller matrices are used and run to stagnation with low surface percentages of second phase particles, their grain sizes increase. As a result, they are likely to have minimum size restrictions violated.

After determining the best-sized matrix to use, the next step was to examine the Zener limit carefully. Since sample values for Q – State were constant a 64 and the percentage of second phase particles (f) at 0.1, ran a wide range of matrix sizes (varying from 100 to 10,000). The calculated parameters were averaged across three attempts for all matrix sizes within 2000. In addition to the previously mentioned parameters, R(max), k, and ϕ were considered. The value Q is fixed to zero for all second phase particles, distinguishing it from Q – State values. The particle was defined as being within a grain of particles of the same Q – State surrounding it. Otherwise, it was meant to be located on the grain boundary. Fig.1(b) shows that the largest grain size is around 3 times the Zener limit at stagnation, as seen in Figure 1(a). it indicates normal grain growth. But, more importantly, all the parameters constrain behaviour at larger matrix sizes ($N \geq 2000$). However, the variations involving smaller matrix sizes seem to be normal. This monitoring follows the results obtained by Kad et al. [7]. They recommend that the 500 minimum matrix size required

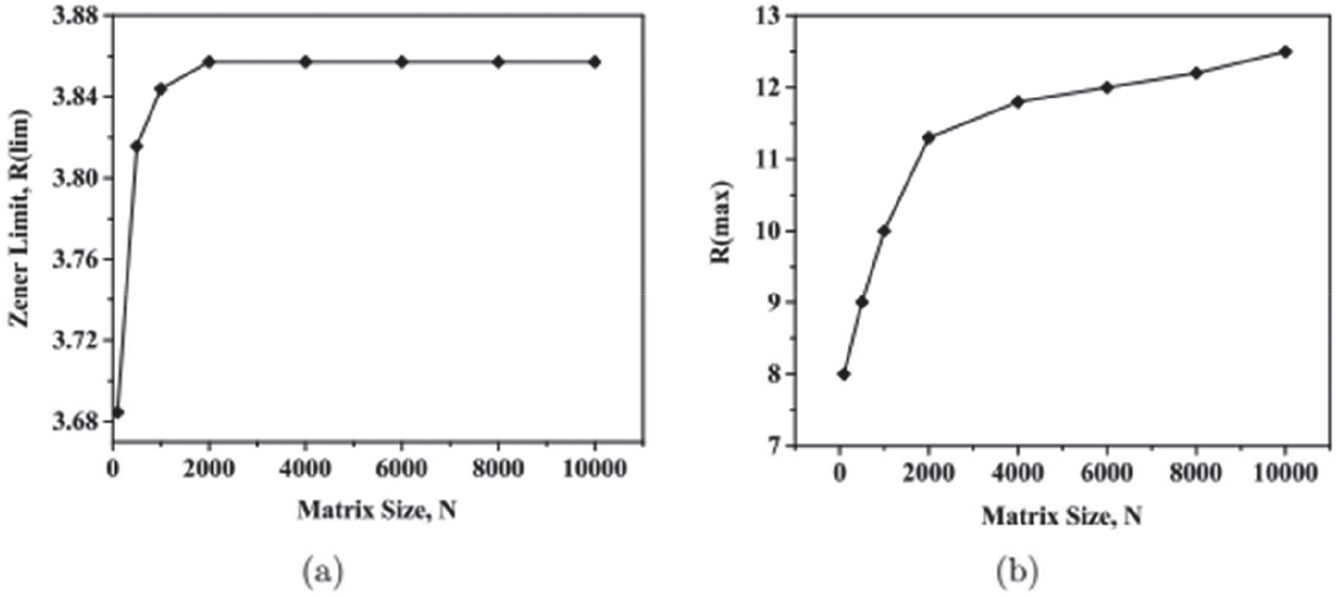

Figure 1: Effect of (a) matrix size vs. R(lim) and (b) matrix size vs. R(max) under the influence of second phase particles

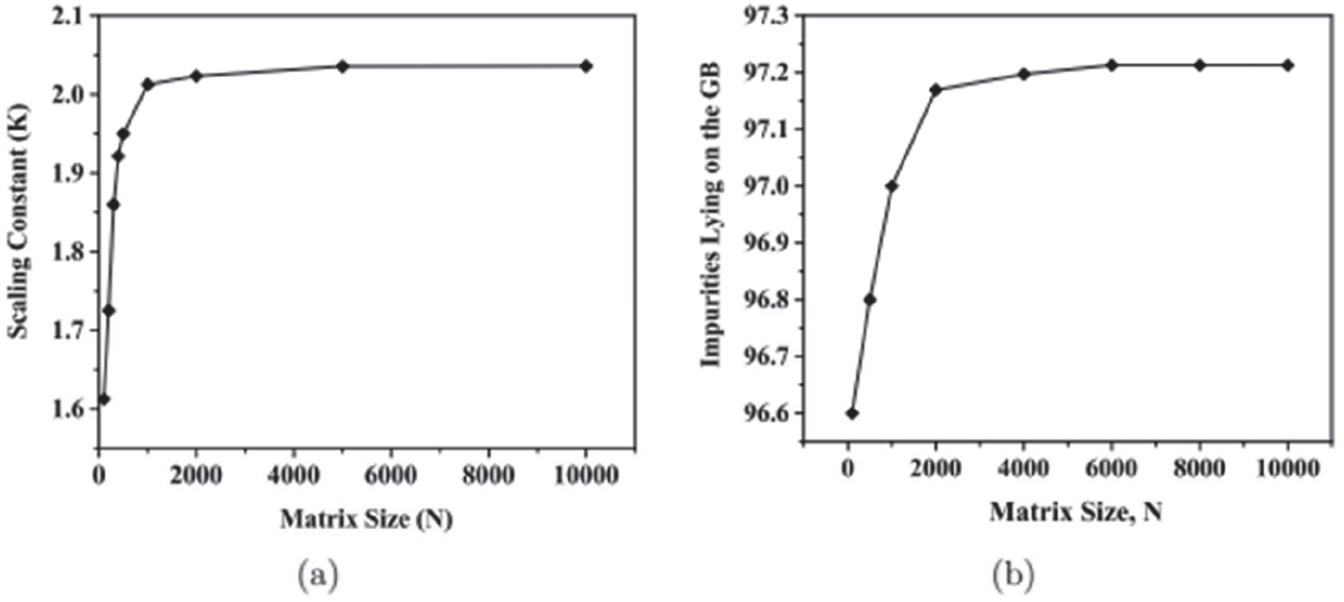

Figure 2: Effect of (a) matrix size vs k and (b) matrix size vs ϕ under the influence of second phase particles

for more reliable simulation results eliminates any disagreeable results. However, it is better to decide on a larger matrix size ($N \geq 2000$) to bring out a Monte Carlo likeness of grain growth in this particular research study. Figure 2(a) indicates the scaling constant against the various matrix sizes, and the calculated k value is 2, which is near the theoretical value. Figure 2(b) indicates that second-phase particles lying on the grain boundary increase with matrix size increases. which concludes the normal grain growth behaviour under second phase particles.

The Q-States 32, 64, and 128 are run to stagnate for various surface fractions ranging from f=0.001 to 0.1 using optimum matrix size N=2000. Figure 4 indicates that various Q-States have only a minor influence on the grain size. The inverse square root dependency correlation between the R(lim) and 'f', is shown in Figure 3. The R(lim) contributes to the power-law and a good interdependence with R^2=0.9952. The Zener limit equation can also be modified as follows:

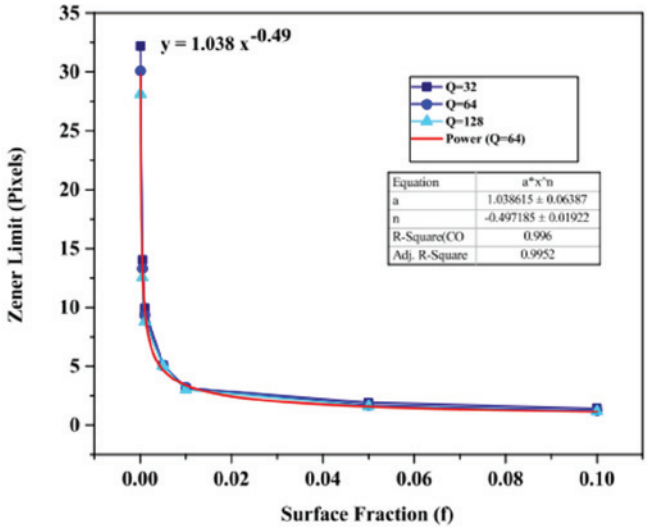

Figure 3: Zener limit vs f for different Q-States

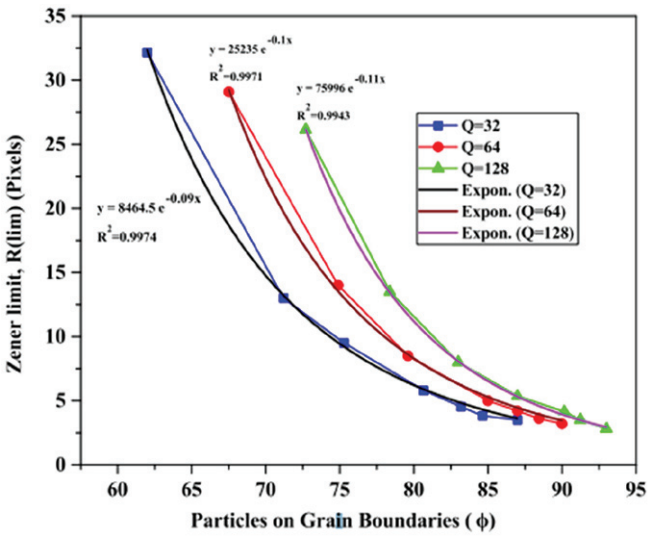

Figure 4: The Zener limit vs ϕ for different Q-States.

$$R_{(limit)} = \frac{1.038r}{f^{0.49}} \quad ...(3)$$

k is approximately unity, equation (3) rewritten as,

$$R_{(limit)} = \frac{r}{\sqrt{f}} \quad ... (4)$$

The new Zener limit value was achieved, and it is close to the value recommended by Srolovitz et al. [2], as shown in Table 1. The key distinction is that Srolovitz employed a triangular lattice in their study, while the present work used a square lattice. Figure 4 depicts the relationship between the limiting grain size and ϕ under various surface fractions 'f' Figure 3 shows that the Zener limit varies inversely and exponentially with ϕ. Thus, the Zener limit seems to vary as $\frac{1}{\sqrt{\phi}}$ and it conflicts with the conclusions of Soucail et al. [8]. Stearns and Harmer [14], [15] revealed that the correlation between R(lim) and ϕ is linear, which contradicts the exponential correlations proposed above. According to current findings, ϕ increases exponentially as 'f' increases. Higher 'f' values result in lower R (lim) values and a greater grain boundary area; therefore, this is the case. Thus, ϕ increases even though R(lim) varies nonlinearly as an 'f' function.

Microstructures of pinned regimes are shown in Figure 5 (a–c) with essential information. The images show that the average grain size reduces as the surface percentage of second phase particles increases. In addition, because grain boundary pinning is improved at higher values of 'f', the number of Monte Carlo steps necessary to achieve stagnation lowers as particle fraction increases. Figure 6 shows the frequency distributions of the normalized grains,

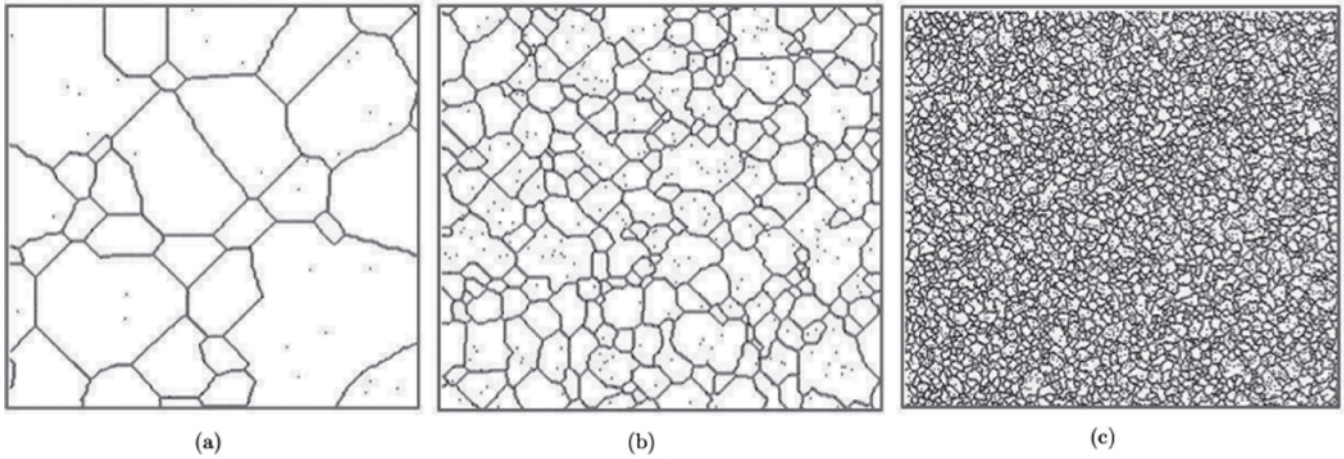

Figure 5: Pinned microstructures: (a) N=2000, Q=64, f=0.001, MCS (at stagnation)=5,86,076, (b) N=2000, Q=64, f=0.01, MCS (at stagnation)=2,20,225 and (c) N=2000, Q=64, f=0.1, MCS (at stagnation)=59,589

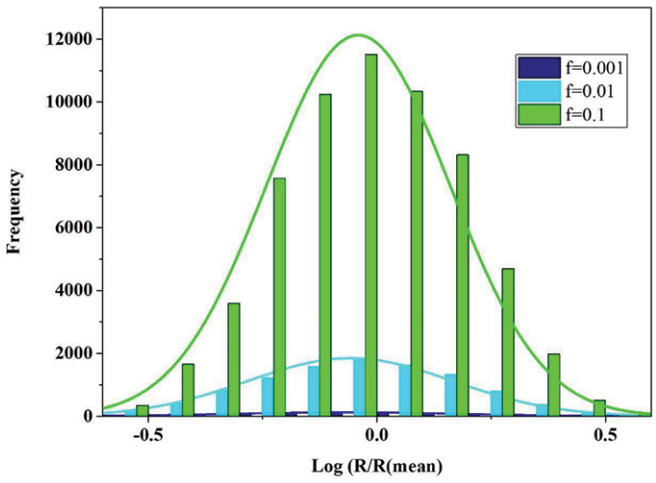

Figure 6: Comparison of grain size distributions, at stagnation, for various particle fractions when N=2000, Q=64.

on a log scale, at stagnation, and the effect of various second-phase particle fractions. Stagnated grain sizes are much bigger in lower surface fractions of particles. In contrast, they are much 9 smaller and thus greater in number for higher particle fractions. Therefore, the grain distributions show a higher frequency of grains for higher 'f' values. It is very well established from the graph that simulated microstructures show lognormal behaviour under the influence of all particle fractions, thereby validating the simulations carried out.

4.0 Conclusions

The followings are major conclusions from the current research work, which involved large-scale Monte Carlo simulations of grain growth under second-phase particles in polycrystalline materials by a two-dimensional computational method:

- It was found that the size of the matrix had a significant impact on the grain size limit. The optimal matrix size, N=2000, was determined after examining several growth characteristics. Moreover, Monte Carlo simulations of grain growth were recommended to use this method.
- The extensive 2D simulation was carried out under various matrix sizes, Q-state and second phase particles which resulted in a modified Smith Zener equation was proposed as $R_{(limit)} = \frac{1.038r}{f^{0.49}}$
- A unique relationship was proposed between the Zener limit and the fraction of particles lying on the grain boundaries, i.e., $R_{(limit)} = \frac{1}{e^{\Phi}}$. It is based on 2D simulation results.
- It was found that the two-phase materials had excellent results in grain size distribution, uniformity, and visual depiction of simulated microstructures.

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6.0 References

1. Smith, C. S. (1948): Grains, phases, and interfaces: An introduction of microstructure. *Trans. Metall. Soc.* AIME, 175, 15-51.
2. Srolovitz, D. J., Anderson, M. P., Grest, G. S., & Sahni, P. S. (1984): Computer simulation of grain growth-III. Influence of a particle dispersion. *Acta metallurgica,* 32(9), 1429-1438.
3. Doherty, R. D., Srolovitz, D. J., Rollett, A. D., & Anderson, M. P. (1987): On the volume fraction dependence of particle limited grain growth. *Scr. Metall.*; (United States), 21(5).
4. Hazzledine, P. M., & Oldershaw, R. D. J. (1990): Computer simulation of Zener pinning. *Philosophical Magazine A*, 61(4), 579-589.
5. Hassold, G. N., Holm, E. A., & Srolovitz, D. J. (1990): Effects of particle size on inhibited grain growth.
6. Gao, J., Thompson, R. G., & Patterson, B. R. (1997): Computer simulation of grain growth with second phase particle pinning. *Acta Materialia*, 45(9), 3653-3658.
7. Kad, B. K., & Hazzledine, P. M. (1997): Monte Carlo simulations of grain growth and Zener pinning. *Materials Science and Engineering: A*, 238(1), 70-77.
8. Soucail, M., Messina, R., Cosnuau, A., & Kubin, L. P. (1999): Monte Carlo simulation of Zener pinning in two dimensions. *Materials Science and Engineering: A*, 271(1-2), 1-7.
9. Zhang, Z., Wu, Q., Grujicic, M., & Wan, Z. Y. (2016): Monte Carlo simulation of grain growth and welding zones in friction stir welding of AA6082-T6. *Journal of Materials Science,* 51(4), 1882-1895.
10. Srolovitz, D. J., Anderson, M. P., Sahni, P. S., & Grest, G. S. (1984): Computer simulation of grain growth—II. Grain size distribution, topology, and local dynamics. *Acta metallurgica*, 32(5), 793-802.

11. Anderson, M. P., Srolovitz, D. J., Grest, G. S., & Sahni, P. S. (1984): Computer simulation of grain growth–I. Kinetics. Acta metallurgica, 32(5), 783-791.
12. Rollett, A. D., Srolovitz, D. J., Anderson, M. P., & Doherty, R. D. (1992). Computer simulation of recrystallization-III. Influence of a dispersion of fine particles. *Acta metallurgica et materialia*, 40(12), 3475-3495.
13. Miodownik, M., Holm, E. A., & Hassold, G. N. (2000): Highly parallel computer simulations of particle pinning: Zener vindicated. *Scripta materialia,* 42(12), 1173-1177.
14. Stearns, L. C., & Harmer, M. P. (1996): Particle Inhibited Grain Growth in AI_2O_3 SiC: I, Experimental Results. *Journal of the American Ceramic Society*, 79(12), 3013-3019.
15. Stearns, L. C., & Harmer, M. P. (1996): Particle Inhibited Grain Growth in Al2O3 SiC: II, Equilibrium and Kinetic Analyses. *Journal of the American Ceramic Society,* 79(12), 3020-3028.
16. Mohseni, M., Eivani, A. R., Vafaeenezhad, H., Jafarian, H. R., Salehi, M. T., & Zhou, J. (2021): An experimental and theoretical investigation of the effect of second-phase particles on grain growth during the annealing of hot-rolled AZ61 magnesium alloy. *Journal of materials research and technology*, 15, 3585-3597.