Evolving Close-to-Real Digital Microstructures in Polycrystalline Materials
A Monte Carlo Simulation Approach

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Keywords: Monte Carlo Simulation, Metropolis Algorithm, Al-4% Cu, Annealing, Simulated Microstructure.

Abstract: For more than three decades now simulation of recrystallization and grain growth phenomena in annealed metals have been studied through a variety of computer modeling techniques including that of Monte Carlo (MC) simulation. In this study, we have been able to show the efficiency of the MC technique by evolving simulated microstructures comparable very closely to real microstructures. The real microstructures were generated in about a 50% cold-worked alloy of Al-4% Cu (Duralumin) annealed to various degrees. The digital microstructures were evolved through a 2D simulation of a square lattice using Potts model Monte Carlo simulation technique based on the Metropolis algorithm. Through our work we have been able to show the close similarity between microstructures of real metals and microstructures digitally evolved through simulation, perhaps for the first time, thereby validating the MC technique as an efficient computer simulation tool for grain growth studies.

1 INTRODUCTION

Annealing is an important heat treatment process carried out widely in the industry during mechanical and thermal processing of cold-worked polycrystalline materials. During this process, metals undergo three stages of microstructural and behavioral transformation - recovery, recrystallization and grain growth. While the first two stages are driven by the energy stored in the metals during cold working, grain growth is driven primarily by the reduction of excess energy stored in the grain boundaries (Humphreys and Hatherly, 2005). The final microstructure in a polycrystalline material, i.e., the grain size & its distribution, grain shape & its geometry, depends largely on the extent of grain growth that has taken place which in turn is influenced by time, temperature and the presence of second phase particles.

The microstructures of polycrystalline materials carry valuable information which helps predict their mechanical behavior through study of their grain shapes and sizes. The average grain size, especially, has a profound effect on the strength of materials, as given by the Hall-Petch equation. The average grain size of polycrystals are known to vary according to degree of growth driven by curvature on the one hand, and on the other hand stunted by the presence of second phase particles. The study of growth and stagnation of grain size in polycrystals has been widely aided by the simulation approach of generating digital microstructures, which follow the basic guide lines of formation of real microstructures.

Microstructures of metals resulting from normal grain growth is distinguished by two characteristics – the first is the presence of microstructural homogeneity, in the sense that the size of the largest grain present in the ensemble is only 2.5 – 3 times bigger than the average grain size of the microstructure. The second characteristic is the time invariance of the grain size distribution which suggests self-similarity in grain shapes and sizes at different stages of grain growth (Anderson et al., 1984). Both these conditions of normal grain growth found in real microstructures have been sufficiently displayed in simulated microstructures by many researchers through MC simulation studies

Phaneesh K., Bhat A., Mukherjee G. and Kashyap K..
Evolving Close-to-Real Digital Microstructures in Polycrystalline Materials - A Monte Carlo Simulation Approach.
DOI: 10.5220/0005531401180124
In *Proceedings of the 5th International Conference on Simulation and Modeling Methodologies, Technologies and Applications* (SIMULTECH-2015), pages 118-124
ISBN: 978-989-758-120-5

(Srolovitz et al., 1984; Saito, 1997; Wang et al., 2009 and Phaneesh et al., 2013). These studies also show the statistical similarity between microstructures generated in real materials and microstructures generated through MC simulation. But what has not been very well demonstrated is the grain shapes in simulated microstructures imitating the grains in the real microstructures. Through our work, and perhaps for the time according to our studies, we have been able to show a stark similarity between certain grains of digital and the real microstructures, and in the process, validate further the relevance of MC simulation technique in grain growth studies. What is exceptional here is the fact that the digital microstructures that have been selected for comparison have been drawn from various combinations of parameters such as various surface fractions of static second phase particles *(f)* which inhibit grain growth, variation in matrix sizes *(N)* which represent the sample material surfaces, different Q states which represent grain orientations, various simulation temperatures *(kT)* which act as effects of higher temperatures during simulation, various stages of grain growth as given by Monte Carlo steps *(MCS),* and so on. Thus this is a comprehensive comparison between digital microstructures drawn from a large simulation domain and some real microstructures generated from a very commonly used non-ferrous alloy, Duralumin.

2 THE MONTE-CARLO METHOD OF SIMULATION

The Monte Carlo method is a probabilistic computer simulation technique used to study grain growth and related phenomena. While analytical models predict ensemble characteristics of microstructural evolution, computer simulations have helped to generate snapshots of the evolving microstructure with time. Using the computational version of metallography, both local and ensemble properties of the microstructure may be determined from these snapshots. Among a few computer simulation methodologies which have been evolved over the years, the Monte Carlo method is one of the prominent techniques employed to simulate microstructural evolution in crystalline materials. This method was developed by Ulam et al., (1947) for basically studying the diffusion of neutrons in fissionable materials. But adaptation of Monte Carlo technique using Potts model for the simulation of microstructure was first introduced by (Anderson et al., 1984 and Srolovitz et al., 1984) for two-dimensional grain growth and extended to three-dimensional grain growth by Anderson et al., (1989).

The procedure for Monte Carlo Potts model simulation of grain growth based on Metropolis Algorithm is as follows:

1. Choose the lattice type i.e. square or triangular. It is square in our case.
2. A square matrix of size '*N'* is then generated, which contains all its elements as random numbers ranging from 1 to Q, where Q stands for the number of grain orientations.
3. Among the N^2 elements present in the matrix, a random site is chosen and is compared with all its nearest neighboring elements, which is eight in case of square lattice.

If *i* = element randomly picked, and *j* = any of the eight neighboring elements that *i* is compared with, then,

$$\partial_{ij} = 0 \text{ if } i \neq j$$
$$\partial_{ij} = 1 \quad \text{if } i = j$$

where ∂_{ij} = Kroneckar delta, a relative interaction energy value between one element and any other neighboring element. The Hamiltonian (E_1) is then calculated for the chosen element by the following relation,

$$(E_1) = -J \sum_i^n [\partial si \, \partial sj - 1] \quad (1)$$

where J (> 0) is an interfacial energy constant of the system and *n* the total number of lattice sites in the system.

4. The grain orientation corresponding to the chosen element is changed into a new random element in its place and the Hamiltonian (E_2) is calculated again for the new element using equation (1), and then giving the energy change,

$$\Delta E = E_2 - E_1 \quad (2)$$

5. If $\Delta E \leq = 0$, the change is accepted else if $\Delta E > 0$, compute probability

$$p = exp\ (-\Delta E/kT) \quad (3)$$

where k = Boltzmann constant, and, T = temperature
If $r < p$ where r is a random number generated and uniformly distributed between *0 & 1*, the change is still accepted, else, rejected.

The entire steps from 3 to 5 form one iteration and are repeated 'N^2' times, which then constitute one Monte Carlo Step (*MCS*), which is the measure of time in simulation. Also, in the current paper,

simulations have been carried out at both *kT=0* and at values *1>kT>0*, under periodic boundary conditions. It is to be noted here that the term *kT* in simulation replaces both the Boltzmann constant and the temperature as an assumed combined product. The term *kT* generally takes a value between 0 and 1 and represents the thermal energy of simulation. It is analogous to the thermal energy of experimental systems but not directly related (Janssens et al., 2007). Just as in the real world, when a phase change is imminent when a metal is heated beyond a critical temperature, there is a critical value for the term KTs, beyond which the microstructure evolution through simulation seizes and a disordered state sets in.

3 EXPERIMENTAL HARDWARE AND SOFTWARE

All the experiments were carried out on a specially built system with 16 GB ram, INTEL CORE 15-2500K-6M-3.3 GHZ Processor and a Asus P8H67-MLE Motherboard B3 Model. The code was written on a Java Core Eclipse platform and close attention was paid to memory management since very large arrays were run. The code invokes generation of massive random numbers which was achieved through the JAVA virtual machine (JVM).

Random number generation plays a crucial role in the process of computer simulation of grain growth. Since computers are basically calculating machines, and use deterministic algorithms to generate random numbers, they basically produce pseudo random numbers, unless and until they are accessing some external device such as a gamma ray counter or a clock. The very foundation of Monte Carlo method lies on generation of robust and long range random numbers, especially since certain simulation trials have to last millions of Monte Carlo Steps, preferably without repeating the sequence. The JAVA virtual machine (JVM) has a reliable random number generator based on linear congruential algorithm and can produce billions of random numbers (2^{48}, to be precise) on the trot, before it repeats the sequence.

4 RESULTS AND DISCUSSIONS

In this work, Al-4% Cu samples, initially hot extruded to about 50%, were annealed at a recrystallization temperature of 480^0C, and held for various durations such as 1, 2, 3, 4 and 10 hours. They were then polished with emery sheets (with grit sizes 80 – 1200) and etched with Keller's reagent (2.5% HF, 1.5% HNO_3, 1% HCl, rest ethanol) for 10 seconds. They were then washed in running water and dried with methanol and hair dryer. The microstructures were observed under a microscope and snapshots were taken, at magnifications of 50x, 100x, 200x, etc. Al-4% Cu was selected because upon annealing the alloy precipitates fine second phase particles of $CuAl_4$ which pin grain boundaries and stagnate the average grain size.

On the other hand, simulations were run on various matrix sizes with different quantities of second phase particles randomly interspersed to represent polycrystalline materials. The matrices were processed with millions of steps of the Metropolis algorithm simulating grain growth which takes place in metals during annealing. Simulated grain structures were captured at different stages of grain growth evolution of various matrix samples and selected portions of these microstructures have been used for pictorial comparisons with real microstructures. Pictures from stagnation stage, which refers to a stage where no more evolution is possible due to grain growth inhibition by second phase particles, have also been used in the comparison.

Table 1 shows pictorial comparisons between various real microstructures on the left hand side, and, the simulated microstructures on the right hand side. The first set of pictures shown in Figure 1(a) and 1(b) allows for a comparison between an *Al-4%Cu* alloy annealed at 480^0 *C* for *one* hour, and photographed at *100x* magnification, with a portion of the simulated microstructure evolved with a square matrix of size *(N) 1000 x 1000*, a *Q-state* value of *16*, with zero percent of second phase particles representing a pure metal and finally a certain stage in grain growth as represented by the number of Monte Carlo steps of *50,000*.

Figures 2(a) and 2(b) show the comparison between the same alloy annealed for two hours with a digital microstructure having parameters *N=1000*, *Q=64*, *f=0.001*, *kT=0.5* and *MCS=1,394,926* (at stagnation). The selected crystal surface is based on *1000 x 1000* matrix with an assumed *64 (Q)* grain orientations. A value of *f=0.001* means that a surface fraction representing *0.1%* of the surface of the microstructure is occupied by second phase particles each having a size of one unit being randomly distributed throughout the matrix. These static particles are shown as tiny dark spots in the

digital photos. Such second phase particles are also present in the real microstructure of the Al-4% Cu alloy but cannot be seen under normal metallurgical microscope and at lower magnifications. These second phase particles pin the grain boundaries and stagnate them from growing any further. This is observed both in reality as well as in Monte Carlo simulation making it another valid reason for adopting this technique. Figure 2(b) here represents the stagnated stage of grain growth in simulated environment. A value of $kT=0.5$ means that a higher temperature effect (but which cannot be equated to an exact real temperature) is introduced into grain growth under simulation. It is very well known that grains grow faster at higher temperatures and higher values of kT show the same effect as well. Finally grain growth has been stagnated due to inhibition of grain boundaries by second phase particles at more than a million steps of the algorithm, which is equivalent to passage of time in simulation.

It should be, however, noted here that there are no conclusions made to equate the simulation samples to the real alloy samples but an effort is made towards realistic representation of actual microstructures through computer simulation. At current levels of research, simulated microstructures just represent generic metals and not particular alloys. But future research may well be represent real alloys through their simulated counterparts. This opens the door for understanding grain structures of real metals and their grain growth better.

All the rest of the photos from Figure 3 to Figure 8 show comparison between real and simulated grain regimes under different parameters but show excellent shape similarities between certain grains on either side. Figures 3(a) and 3(b) show a comparison between two vertices on either side by encircling them. According to theory (Smith, 1952) three grains meeting at a vertex should be at an angle of 120^0 to each other for a stable grain structure. This could very well be seen in the vertices encircled and also in all real and simulated microstructures further validating the technique.

Table 1: Comparison between Real and simulated microstructures.

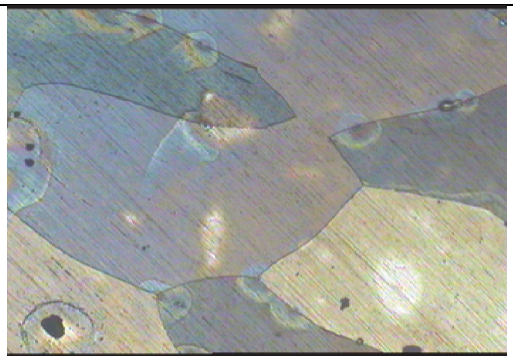
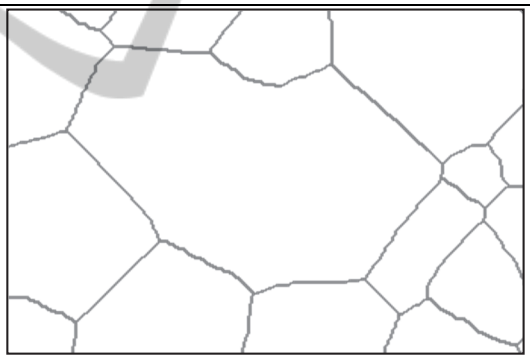
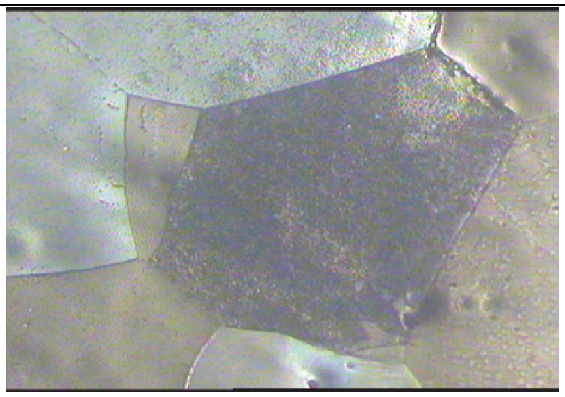
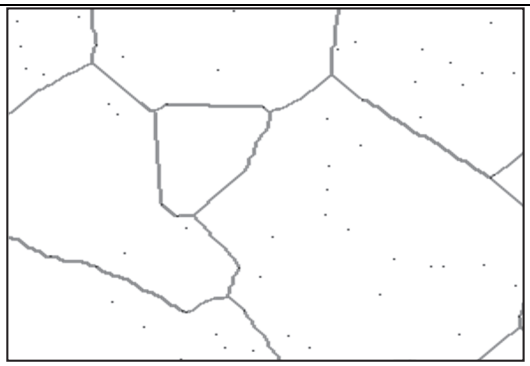
Real microstructures from annealed Al-4% Cu alloy	**Simulated microstructures**
 Figure 1(a): Annealed at 480^0 C for 1hr, at 100x.	 Figure 1(b): N=1000, Q=16, f=0, MCS=50000.
 Figure 2(a): Annealed at 480^0 C for 2hr, at 100x.	 Figure 2(b): N=1000, Q=64, f=0.001, MCS=1394926 (at stagnation).

Table 1: Comparison between Real and simulated microstructures. (cont.)

Real microstructures from annealed Al-4% Cu alloy	Simulated microstructures

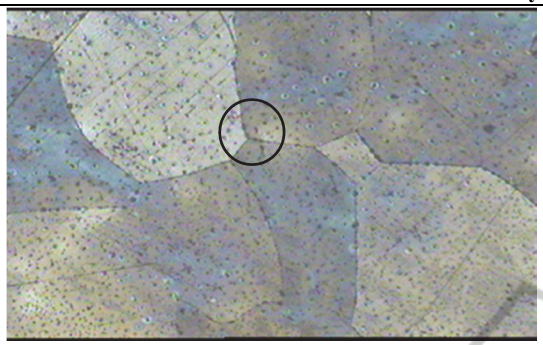
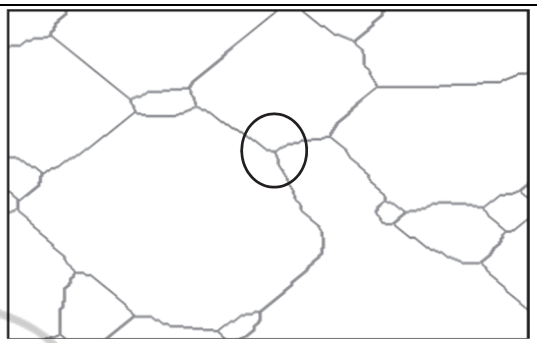

	

Figure 3(a): Annealed at 480^0 C for 3hr, at 100x.	Figure 3(b): ***N***=1000, *Q*=32, *f*=0, *MCS*=50000.

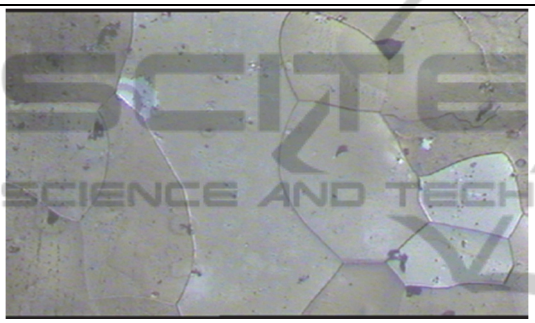



Figure 4(a): Annealed at 480^0 C for 3hr, at 100x.	Figure 4(b): *N*=1000, *Q*=32, *f*=0, *MCS*=50000.

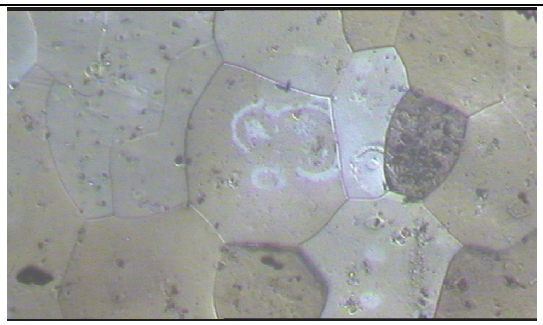
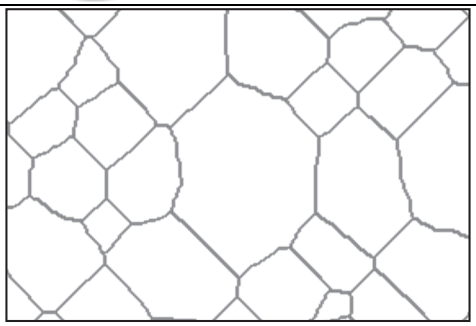

	

Figure 5(a): Annealed at 480^0 C for 3hr, at 100x.	Figure 5(b): *N*=1000, *Q*=32, *f*=0, *MCS*=50000.

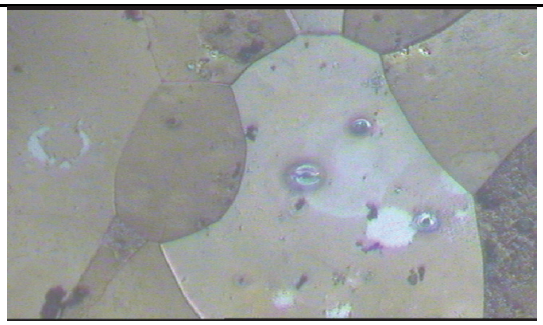
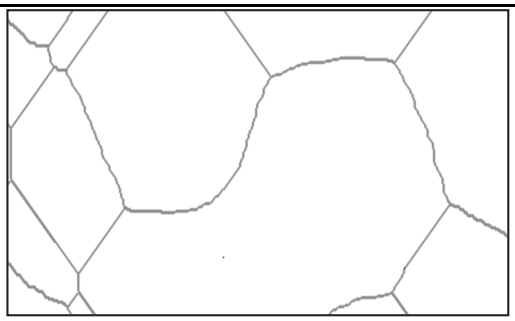
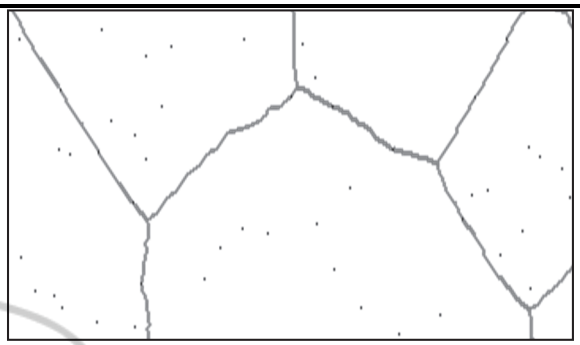

	

Figure 6(a): Annealed at 480^0 C for 3hr, at 200x.	Figure 6(b): *N*=1000, *Q*=64, *f*=0.001, *MCS*=60000.

Table 1: Comparison between Real and simulated microstructures. (cont.)

Real microstructures from annealed Al-4% Cu alloy	Simulated microstructures
	
Figure 7(a): Annealed at 480^0 C for 4hr, at 200x.	Figure 7(b): N=1000, Q=64, f=0.001, kT=0.4, MCS=1589026(stagnation).

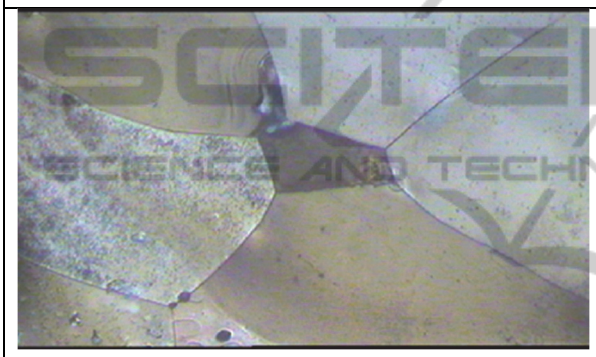



Figure 8(a): Annealed at 480^0 C for 10hr, at 50x.	Figure 8(b): N=1000, Q=64, f=0.001, kT=0.4, MCS=1589026(stagnation).

5 CONCLUSIONS

This work has been able to show close similarity between microstructures generated after annealing a prominent non-ferrous alloy and the simulated microstructures evolved by the Monte Carlo simulation technique. The striking closeness especially between certain set of grains between real and simulated microstructures enhances the validity of the MC technique to investigate grain growth and its inhibition in polycrystalline materials. The 120^0 angle vertices found in stable grain structures in real metals can also be seen prominently in digital structures. But it should be iterated here that the comparison only allows for the topological and grain shape similarities between the two sets of micrographs and no other comparisons are made with respect to their evolution *vis-a-vis* time and temperature. It is an ongoing work to relate real and simulated microstructures on all parameters so that MC simulation can be applied to particular alloys as against generic as is being done now.

ACKNOWLEDGEMENTS

Acknowledgements are due to - Visvesvaraya Technological University, Karnataka, India, which funded this project (*No. VTU/Aca/2009-10/A-9/11417*); Dr. S. Y. Kulkarni, Principal, Dr. Ramesh Rao, Prof. & Head, Dept of Mechanical Engineering, M. S. Ramaiah Institute of Technology, Dr. R. Chandrashekar (rtd.), MSRIT, Bangalore; Dr. K. N. B. Murthy, Principal, Dr. C. S. Ramesh, P E S Institute of Technology, Bangalore.

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