MANIPULATING THE METROPOLIS ALGORITHM TO YIELD GRAIN GROWTH KINETICS OF REAL METALS - A MONTE CARLO SIMULATION ATTEMPT

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Abstract

A modification to the Metropolis algorithm, which drives Monte Carlo (MC) simulation of grain growth, is suggested here. Though MC simulation allows for study of effects of variables on growth kinetics and growth inhibition in ways not possible by experimentation, the method has been largely limited to the understanding of these phenomena with a generic metal in mind rather than a specific one. During MC simulation, variables such as time, temperature and grain size have only their simulation equivalents considered and are assumed the same for all materials. The present work manipulates the Metropolis algorithm in such a way that it mimics growth kinetics of known metals, as observed through experimentation. We propose Kalale-Bhat-Mukherjee-Kashyap (KBMK) factors, which help yield precise grain growth exponents. This, along with other results relating length and time scales between real and simulated microstructures, can pave the way for an effective Material-Specific MC simulation of grain growth in future.

Keywords: Metropolis Algorithm, Hamiltonian, Grain growth exponent, MCS, KBMK factors

1. INTRODUCTION

The Monte Carlo (MC) technique using the Metropolis algorithm was first adapted by Anderson et al [1] in the 1980's for the simulation of microstructure evolution. This along with Srolovitz et al [2] for 2D grain growth and the later extension to 3D grain growth by Anderson et al [3] pioneered renewed research in recrystallization and grain growth using the various computational techniques. Since then computer simulation of grain growth has come a long way with major contributions towards its progress made by several research scientists [4 - 11] from around the world, to name a few Grain growth studies with respect to its kinetics, growth inhibition due to Zener pinning, abnormal grain growth, etc., have all been extensively investigated through MC simulation over the years. But all such simulations carried out till date has been with reference to a generic material, without name or number. Though MC simulations have been able to investigate the effects of different variables on grain growth, which otherwise would be very difficult in experimentation, they have not been able to allow for comparison with real materials and their microstructures. Ultimately if Monte Carlo simulations have to be used in predicting grain size, either during grain growth or in pinned regimes, material specificities may have to come into picture, owing to varied reactions of the materials to the principle operating variables *viz.* time and temperature. For material-specific Monte Carlo simulations of grain growth to become a reality, the following challenges have to be met from a broad perspective:

1) To achieve specific grain growth exponents by controlling the rate at which simulated grains grow.
2) To convert the simulation time scale to real time, for the material in question.
3) To adjust the length scales between simulated and real microstructures.
4) To correlate simulation and real temperatures.

An initial attempt therefore has been made in this work to address the first of the four conditions mentioned above. This has been achieved through the manipulation of the Metropolis algorithm which drives the MC simulation.

1.1. Metropolis Algorithm

The Monte Carlo method is a stochastic computer simulation technique applied to study grain growth and related phenomena. While analytical models predict ensemble characteristics of microstructure evolution in polycrystalline materials, algorithm-based computer simulations have helped generate snapshots of microstructure evolution with time. Applying this simulation route to metallography, both local and ensemble properties of the microstructure may be determined. Quite a few computer simulation methodologies have been tried over the years, and among them, the Monte Carlo method is one of the most effective techniques employed to simulate evolution of microstructure in polycrystals. This method was initially developed for studying the diffusion of neutrons in fissionable materials but was adapted for grain growth studies since the underlying processes were both stochastic in nature.

In its basic form, the procedure for MC (Potts model) simulation of grain growth and based on Metropolis Algorithm [1] is as follows:

1) The basic lattice type is first chosen i.e. square or triangular. We have considered a square lattice.

2) A square matrix of size '*N*', populated with random numbers, is then generated, using an appropriate coding platform. These numbers range from *1* to *Q*, where *Q* stands for the number of grain orientations in the digitally evolving microstructure.

3) Among the N^2 elements present in the matrix, a random element is chosen and is compared with all its nearest neighboring elements, which in the case of square lattice is eight.

   If *i* = element randomly picked,

   j = any of the eight neighboring elements that *i* is compared with

   then,

   $\partial_{ij} = 0$ *if* $i \neq j$

   $\partial_{ij} = 1$ *if* $i = j$

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

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

4) The *Q*-value of the chosen element is now flipped into a new random element, and in its place, the Hamiltonian (E_2) is calculated again for the new element using equation (2). This then gives the energy change, $\Delta E = E_2 - E_1$.

5) If $\Delta E \leq 0$, the change is accepted

   else if $\Delta E > 0$, the change is rejected.

6) In the above process steps *3* to *5* form one iteration of the algorithm. Each iteration is then repeated 'N^2' times to constitute one Monte Carlo Step (*MCS*).

From the above procedure it is understood that each Monte Carlo step iterates the Metropolis algorithm N^2 times which means that there are N^2 attempts to swap spins and also to reduce the system energy which is the Hamiltonian. If, instead of N^2 attempts in each *MCS*, a different number of attempts are made, the rate at which Hamiltonian reduces, and therefore the rate at which grains grow, could be controlled. If N^2 is multiplied by a fraction, having values between *0* and *1*, the rate at which grains grow would exactly behave the way that we want it to. Since most known and important materials have been tested for growth kinetics through experimentation, their grain growth exponents (*n*) are well established [12]. For example, the grain growth

exponent (*n*) of Aluminum is 0.25 [13], that of Iron is 0.4 [14], and the value for tin is 0.5 [15]. Keeping this as the starting point the Metropolis algorithm was manipulated to yield precise grain growth exponents in the simulated grain growth environment as well. In order to obtain significant grain growths in simulation environment, the Metropolis algorithm had to be run millions of times in case of each metal.

2. RESULTS AND DISCUSSIONS

Simulations were run on a *1000 x 1000* matrix considering square lattice and under periodic boundary conditions while the code was developed on JAVA platform. It was coded in such a way that instead of N^2 iterations which would make one *MCS*, a fraction of it was considered. **Table1** gives a list of many such values which when taken as a fraction of each *MCS,* would control grain growth rate during simulation and hence yield the required grain growth exponent values. We wish to call them Kalale-Bhat-Mukherjee-Kashyap factors or *KBMK* factors.

Table 1 Kalale-Bhat-Mukherjee-Kashyap (*KBMK*) factors to yield different '*n*' values

Grain growth exponent *(n)*	*KBMK* factors	Grain growth exponent (n)	*KBMK* factors
0.1958	0.0005	0.3168	0.02
0.2033	0.00055	0.3444	0.05
0.2101	0.0006	0.3798	0.1
0.2223	0.0007	0.3999 (Fe)	0.15
0.233	0.0008	0.4204	0.2
0.2418	0.0009	0.4413	0.3
0.2504 (Al)	0.001	0.4487	0.4
0.3357	0.005	0.4539	0.5
0.3343	0.006	0.4591	0.58
0.3248	0.01	0.4965 (Sn)	2

KBMK factors share an exponential relationship with grain growth exponent (n) and can be approximated as,

$$KBMK\ factor = exp\ \hat{}\ (\ 29.32n - 13.9\ ) \quad (2)$$

Using eq. 2 we can substitute the grain growth exponent value of any metal as n and the resulting *KBMK* factor can be multiplied to N^2 of the Metropolis algorithm to achieve grain growth as applied to a known material. Simulations were run for varying number of MCS (which is the simulation equivalent of time) to allow for grain growth, and at each juncture the average grain size (R (mean)) was found through coding. From theory, Burke and Turnbull [16] have given us the equation which relates the average grain size and time as,

$$R\ (mean) = k\ t^{1/n} \quad (3)$$

Where t = time, n = grain growth exponent and k = constant of proportionality.

Applying the above equation to simulation, and replacing time with MCS, we can find n as the slope of the curve of *log (R (mean)) vs. log MCS,*

$$\text{Grain growth exponent, } n = log(R\ (mean))\ /\ log\ MCS \quad (4)$$

Figure 1 shows the engineered *log R (mean)* vs. *log MCS* curves for specific materials, where *R (mean)* is the average grain size at any point of grain growth as dictated by the number of *MCS* at that juncture. The slopes of these curves yield grain growth exponent of that curve, and in this case, that of the particular material. It

should be noted here that this is perhaps the first work to attempt achieve specific grain growth rates in simulated regimes.

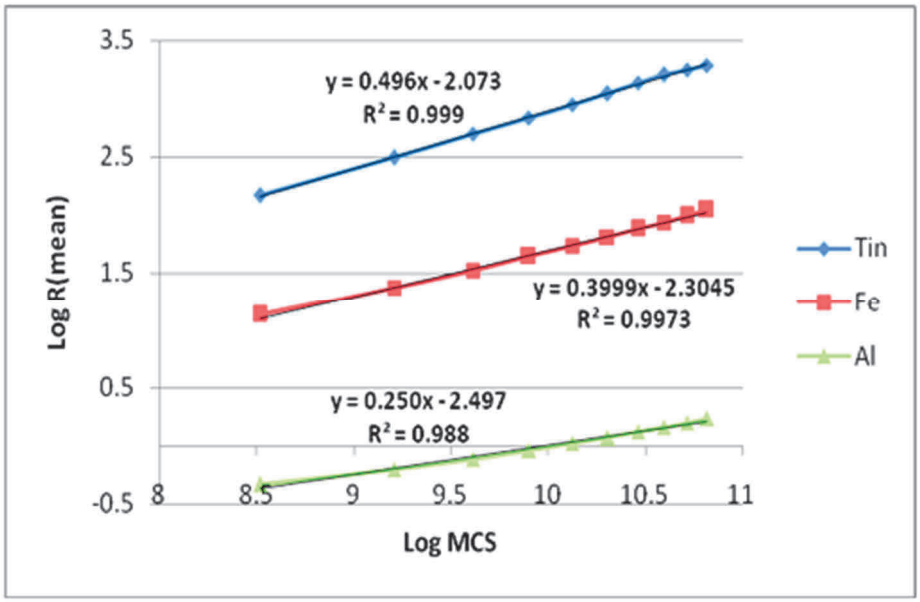

Figure 1 Material-specific grain growth rates

Thus all simulations carried out to investigate various grain growth parameters can now be related to specific materials rather than a generic one. This, we are sure, will open up new roads towards grain growth studies of specific and industrially important materials.

The second step towards achieving material-specific MC simulation of grain growth is to convert simulation time to real time and vice-versa. Saito [17], Saito and Enomoto [18], Haghighat and Taheri [19], and so on, have addressed the issue of establishing a relation for conversion of the simulation time to real time, in different ways. Saito and Enomoto [18], especially, have suggested an idea, based on the diffusion-controlled mechanism of grain growth, for converting *Monte Carlo Steps* to real time. According to this conversion, the real time value in seconds for one *MCS* was given by,

$$1(MCS) = \frac{d^2}{6DQ}\ seconds \tag{5}$$

Where,

D = grain boundary diffusion coefficient,

d = simulation lattice constant

Q = *Q-States* of grain orientations.

On the third condition required for achieving material-specific MC simulation, i.e. towards adjustment of length scales, Rollett et al [20] have analyzed the relationship between grain size in the Monte Carlo model and physical grain sizes, although in the realm of recrystallization and not grain growth. Nosonovsky et al [21], and more recently Lim et al [22], too, have worked on the issue of scaling relationships between physical time/length and the MC step/cell size.

Thus our contribution towards achieving grain growth exponents of known materials through MC simulation can be combined with others' contribution to overcome challenges mentioned earlier and move towards material-specific MC simulation of grain growth in future.

3. CONCLUSIONS

Monte Carlo simulation of grain growth was carried out in such a way that the resultant grain growth rate imitated growth kinetics of known metals. This was achieved by introducing KBMK factors, which is our contribution to available literature, as a modification tailored into the Metropolis algorithm. Through this work we are able to achieve grain growth comparable to known materials in simulated regimes as well. Combining this with work proposed by others in the domains of relating length, time and temperature between real and simulated microstructures, more meaningful material-specific research in microstructure evolution can be achieved in the coming years.

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REFERENCES

[1] ANDERSON, M. P., SROLOVITZ, D. J., GREST, G. S., SAHNI, P.S. Computer simulation of grain growth Kinetics-I. *Acta Metallurgica*, 1984, vol. 32, pp. 783-792.

[2] SROLOVITZ, D. J., ANDERSON, M. P., SAHNI, P. S., GREST, G. S. Computer simulation of grain-growth: II. Grain size distribution, topology, and local dynamics. *Acta Metallurgica*, 1984a, vol. 32, pp. 793-802.

[3] ANDERSON, M. P., GREST, G. S., SROLOVITZ, D. J. Computer simulation of grain growth in three dimensions. *Philosophical Magazine*, 1989, vol. B59, no. 3, pp. 293-329.

[4] MIODOWNIK, M., HOLM, E. A., HASSOLD, G. N. Highly parallel computer simulations of particle pinning: Zener vindicated. *Scripta Materialia*, 2000, vol. 42, pp. 1173-1177.

[5] ZOLLNER, D., STREITENBERGER, P. Three-dimensional normal grain growth: Monte Carlo Potts model simulation and analytical mean field theory. *Scripta Materialia*, 2006, vol. 54, no. 9, pp. 1697-1702.

[6] ROBERTS, C. Grain growth and the Zener pinning phenomenon: A computational and experimental investigation. *Ph. D thesis*, Carnegie Mellon University, 2008.

[7] PHANEESH, K. R., BHAT, A., MUKHERJEE, P., KASHYAP, K. T. On the Zener limit of grain growth through 2D Monte Carlo simulation. *Computational Materials Science,* 2012, vol. 58, no. 6, pp. 188-191.

[8] PRINZIO, C. L. D., DRUETTA, E., NASELLO, O. B. More about Zener drag studies with Monte Carlo simulations. *Modelling and Simulation in Materials Science and Engineering,* 2013, vol. 21, no. 2, pp. 025007-025015.

[9] NISHINAGA, T. *Handbook of Crystal Growth-Fundamentals, Thermodynamics and Kinetics.* Volume 1, Part A, 2nd ed. Elsevier, The University of Tokyo, Japan, 2014.

[10] MASON, J. K., LIND, J., Li, S. F., REED, B. W., KUMAR, M. Kinetics and anisotropy of the Monte Carlo model of grain growth. *Acta Materiala,* 2015, vol. 82, no. 1, pp. 155-166.

[11] ZOLLNER, D., STREITENBERGER, P., RIOS, P. R. Shedding some light on the early grain growth regime: About the effect of the initial microstructure on normal grain growth. *Computational Materials Science,* 2016, Vol. 113, no. 15, pp. 11-20.

[12] HUMPHREYS, F. J., HATHERLY, M. *Recrystallization and Related Annealing Phenomena.* Elsevier Pergamon, UK, Second edition, 2005.

[13] GORDON, P., EL BASSYOUMI, T. A. *Transactions of Metallurgical Society,* A.I.M.E., 1965, vol. 223, pp. 391.

[14] HU, H. Grain growth in zone-refined iron. *Canadian Metallurgical Quarterly*, 1974, vol. 13, pp. 275 - 286.

[15] HOLMES, E. L., WINEGARD, W. C. Grain growth in zone-refined tin. *Acta Metallurgica.* 1959, vol. 7, pp. 411 - 414.

[16] BURKE, J. E., TURNBULL, D. Recrystallization and grain growth. *Progress in Metal Physics,* 1952, vol. 3, pp. 220-292.

[17] SAITO, Y. The Monte Carlo simulation of microstructural evolution in metals. *Material Science & Engineering,* 1997, vol. A223, pp. 114 - 124.

[18] SAITO, Y., ENOMOTO, M. Monte Carlo simulation of grain growth. *ISIJ International,* 1992, vol. 32, pp. 267 - 284.

[19] HAGHIGHAT, S. M., KARIMI Taheri, A. Investigation of limiting grain size and microstructure homogeneity in the presence of second phase particles using the Monte Carlo method. *Journal of Material Processing Technology,* 2008, vol. 195, pp. 195 - 203.

[20] ROLLETT, D., LUTON, M. J. Computer simulation of dynamic recrystallization. *Acta Metallurgica,* 1992, vol. 40, pp. 43 - 55.

[21] NOSONOVSKY, M., ZHANG, X., ESCHE, S. K. Scaling of Monte Carlo simulations of grain growth in metals. *Modeling & Simulation in Material Science & Engineering*, 2009, vol. 17, pp. 13 - 22.

[22] LIM, H., ABDELJAWAD, F., OWEN, S. J., HANKS, B. W., FOULK , J. W., BATTAILE, C. C. Incorporating physically-based microstructures in materials modeling: Bridging phase field and crystal plasticity frameworks. *Modeling & Simulation in Material Science & Engineering,* 2016, vol. 24, no. 4, pp. 045016.