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A MONTE CARLO SIMULATION IN GRAIN GROWTH: KINETIC IN PRESENCE OF INCOHERENT PARTICLES

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Abstract

In this paper, a modified Monte Carlo simulation is developed for studying grain growth in presence of stable incoherent particles. The aim is to introduce the calculation method (with C^{++}) applied to the particles problem, to pick out the grain local behavior, to evaluate the grain growth exponent and to determine the abrupt transition between normal and stagnant microstructure. We deal with 2D microstructures with a constant particle diameter and different particle area fraction.

Keywords: *Monte Carlo simulation, growth, grains, particles, microstructure.*

Résumé

Une version modifiée de la technique de simulation Monte Carlo est développée pour étudier la croissance des grains en présence de particules incohérentes et stables. Les modifications introduites dans la méthode de calcul (en C++) permettent de considérer le problème des particules en introduisant le comportement local des grains, d'évaluer le coefficient de la cinétique de croissance et de déterminer la transition entre la croissance normale et la stagnation. Nous traitons le problème avec des microstructures en 2D, avec différentes fractions de particules de même diamètre.

Mots clés: *Simulation Monte Carlo, croissance, grains, particules, microstructures.*

S. GUESSASMA
N. ROUAG
Département de Physique
Faculté des Sciences
Université Mentouri
Constantine, Algérie

ملخص

تم تطوير تقنية محسنة لمحاكاة Monte Carlo و ذلك لدراسة نمو الحبيبات مع وجود جزيئات غير ملتحمة و مستقرة. يهدف هذا البحث إلى إدخال طريقة الحساب (C^{++}) المطبقة على مشكل الجزيئات و على التصرف الموضعي للحبيبات، وإلى تقييم معامل حركية النمو، و كذلك إلى تحديد انتقال المفاجئ من النمو العادي إلى ركود البنية المجهرية. نتعامل مع بنية مجهرية نوع 2D ذات نسب مختلفة لجزيئات ثابتة القطر.

الكلمات المفتاحية: *محاكاة Monte Carlo، نمو، الجزيئات، حبيبات البنية المجهرية.*

Grain growth was widely investigated since 1949, earlier theoretical [1-5] and statistical [6-7] developments were unable to introduce correctly the local features of the grain growth. They often consider an average behavior in which grain size is assumed to be the unique growth process variable. An other approach of the problem was considered this last two decades giving interesting results. It consists of Monte Carlo simulation technique [8-10] that allows an access to process information at a deep level, i.e. considering a probabilistic evolution of atoms blocs (sites) by memorizing each bloc state in a sample (extension of the Ising Model). Other approaches were also considered like vertex delimited Network [11-12] or Cellular Automata [13] (for an overview of simulation methods applied to recrystallization see for example [14-15]). Monte Carlo technique appears to be the most flexible tool and is easy to build up. It permits a wide investigation over the most important parameters influencing the growth problem and best of all, it fits remarkably a great range of experimental data [16-17]. We are interesting in developing this method for the fine particles influence in grain growth. These particles are known for their drag action that leads to stagnation [18-22] and this aspect depend strongly on the amount of particles present and of the efficiency of the pinning process.

If the Q Potts model, soap froth or vertex model are in good agreement with classical predictions concerning the normal kinetic of growth [15-17], the main difficulty is to test the validity of analytical equations in presence of the particle restraining force. There is steal a doubt that the efficiency of the drag effect proved in 2D microstructures can be found in 3D. All the factors considered in normal growth may be reviewed, these can be role of curvature and boundary anisotropy. In addition, some hypothesis in MC method may be clearly discussed like anisotropy due to discretization or the evolution criterion. Finally, the role of each particle parameter may be considered also (particle shape,

distribution). Our contribution to the method was to include shape effect [23], boundary anisotropy [24] and distribution nature in both 2 and 3 dimensions. In order to introduce our work, we present only the calculation method as described in the abstract.

I- PROCEDURE

I.1- Introduction

The microstructure is divided in a discrete triangular network containing (200x200) sites. Each site is assigned an arbitrary orientation Q_i (Fig.1) in the range of [0,64].

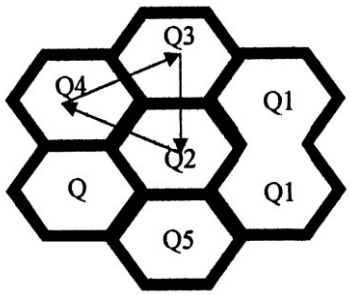


Figure 1: Triangular Lattice representing a 2D microstructure, each cell (site) is assigned on orientation Q_i. Sites having the same orientation are part of the same grain; particles are single sites (Q) not allowed to switch orientation.

Neighbour sites of the same orientation are part of the same grain unlike they are separated by a boundary segment of constant energy (no influence of the boundary nature is treated here). Hence the total energy of the system is:

$$E = \frac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{6} j\left(1-\delta_{Q_iQ_j}\right) \qquad (1)$$

where j is the boundary energy constant, i.e. the energy associated with the boundary segment in the model, N is the number of sites of the microstructure.

The evolution is regarded as the successful reorientation process decreasing the total energy, each site should only have the orientation of his neighbours, the configuration obtained after one reorientation is accepted with the normalised probability (1):

$$P(\Delta E) = \frac{1}{1+e^{\Delta E/kT}} \qquad (2)$$

see for example [25].

In fact, a bulk site has not the right to change orientation because this action increases the system energy, when selecting such site we simply avoid the test and increment the loop to count properly the Monte Carlo steps. Though, this consumes time calculation but it reduces the fluctuations occurring at high temperature procedures.

Particles introduced randomly at the beginning as single sites are not allowed to change orientation and present an interface of same energy as that of boundaries.

Time is quoted in, arbitrary units of Monte Carlo steps, one step corresponding to (N-N_p) reorientation attempts, where N and N_p are respectively the total number of sites and particles in the sample.

I.2- The basic idea

The temporal evolution of a particles system (sites) in respect to energetic constrains can be described by a corresponding evolution in a phase space of N dimensions (if the degree of freedom of each constituent is the orientation in a 2D microstructure). For simplicity, this space is regarded as a discontinuous space in which we construct a fine scaled grid, in order to track the system evolution. One has to determine the points the system pass through, this is in fact not possible because of the great points number that a computer has to store (Q^N) (if we say for example Q orientations for N sites). Instead of this, we randomly pick out the grid points, the evolution is then viewed as the successful passage from one point to an other. In fact, the passage to some point (state) correspond meanly to N reorientation attempts in the sample. In our modified Monte Carlo simulation, selected points from the phase space are not completely random ones. We have worked with the so called the importance sampling method [26] which correspond to a real contributor points selection. Because the site reorientation corresponds to a boundary passage, the final result is to get the orientation of a neighbouring site which is a part of a growing grain. In that way, the trial is realised only from the nearest neighbour orientations, this generate a Markov chain (succession of most probable states) with a significant accuracy and a real correspondence with the growth problem. The validity of such choice will be discussed elsewhere, here we simply argue on the fact that a diffusive behaviour is adopted for the grain growth may meet this idea of a deterministic motion of grain boundaries.

However, the statistical approach presents some drawbacks:

- Where in reality everywhere in the sample we can find atoms jumps (singly or in groups) occurring at the same time, this is not practically fully translated in the Monte Carlo method, since the probability for this action (which correspond to probability summation of the reorientation attempts at that time) is very small, even if in the new configuration, there is some truth in the transition. This means exactly that we are not able to obtain rapid convergence to thermal equilibrium.

- Time quoted in Monte Carlo method is not a real time corresponding to a deterministic evolution, even if we are able to plot a temporal variation. This time is not well representative because of choosing sites to be units of the sample: a site is a volume of a material which is chemically and physically homogeneous, details on what happens through the site are not allowed, so time is not accessible in a continuous manner. This can be a significant problem if we are concerned by the dynamic interaction of particles with boundaries, where the resolution of the system does not permit a good estimation of quantities such the Zener drag.

- The initial state is one of the consistent problems in the Monte Carlo technique. The deterministic nature of the method comes from specifying an initial state from which all the evolution will be determined, according to energetic

factors. Even if time is sufficient and the grid is well scaled, situation, grain boundaries are jagged with grain

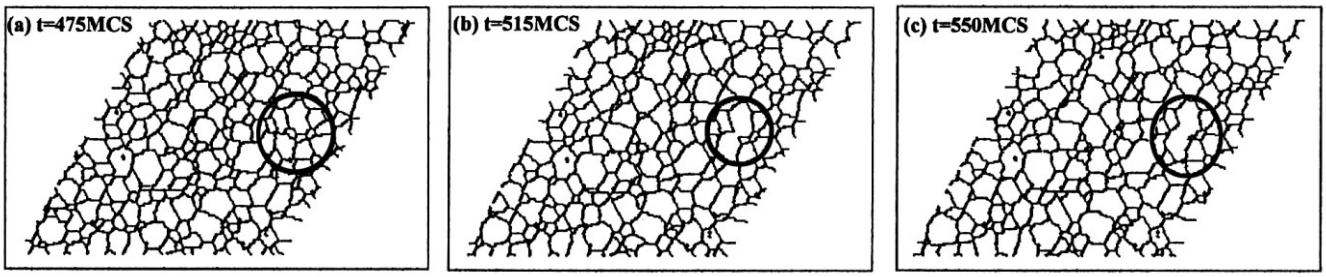


Figure 2: Temporal evolution at ~0K of a microstructure with 1% particle fraction area, showing discontinuous growth (merging growth) occurring when two grains of same orientation come in touch, these microstructures are taken from a video sequence of 1000 MCS in the rate of 1 image/5MCS.

In addition, anisotropy due to a site morphology choice can introduce some mathematical corrections, that have no clear physical sense: for example, we must attenuate this anisotropy by considering an interaction over the nearest sites neighbours.

I.3- Influence of simulation time and pseudo number generator

The base of the procedure is a parallelism between statistical configuration and probabilistic behaviour. Choosing long time simulation is better to encounter the reality, but this is also expensive in time calculation and is not always available. Concerning the grain growth, the acceptance of configurations leading to an increase in energy is determined by the probability $P(\Delta E)$ (Equation 2).

I.4- Influence of choosing the representative number of orientations Q

At it was first examined by Anderson et *al.* [8], choosing a little number to represent the orientation spread leads generally to a growth with merge, this occurs when two grains with the same orientation come in touch, the boundary separating them disappears, giving an increase in grain dimensions (Fig.2). This situation has no sense because, even in the case of small misorientations (<1°), the boundary exists and no rotation of grains here is possible. In order to deal with this problem, one can assume a very stable grain boundary to separate such grains. This does not mean a significant decrease in the mean radius evolution if a random grain distribution is assumed. In addition, choosing the number of orientations up 64 is sufficient to represent adequately the grain boundary distribution, even if boundary energy degeneracy is not taken into account.

I.5- Influence of temperature

Grain growth is a thermally activated phenomenon, this means an increase in temperature enhances the process. However, temperature is rather taken as a disorder parameter in simulation. It enters to the procedure via equation (1); it is interesting to see there is a limiting case in which temperature plays a reverse role. At higher T, configurations leading to an increase in energy are more and accepted (Fig. 3) shows microstructures reflecting such

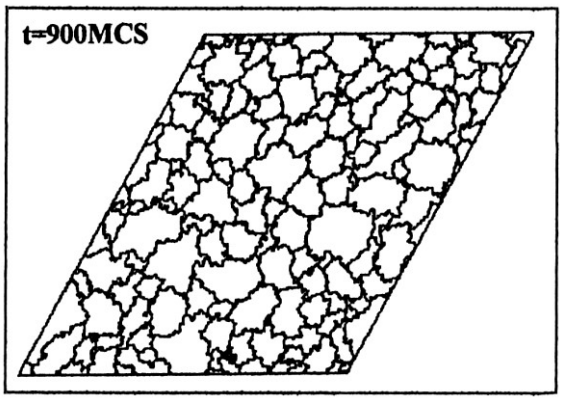


Figure 3: Microstructure at 2000K without particles at 900 MCS showing temperature effect on grain morphology.

sizes which indicates the important statistical weight of a none disappearing grains. So at high T, the procedure gives none realistic configuration because of fluctuations maintain in time, which states a limit for real behaviour in respect to temperature. All simulations presented here are undertaken at ~ 0K, this is of course an abstraction to a real process, but it is useful when we want to suppress all states increasing energy.

I.6- Real dimension of sample sites

Depending on what the simulation is applied, one can define his own scale, the manner can be [28] the evaluation of properties studied on both physical and model units (ex. stored energy per site and per cm^3). When finding a property constant value, we just express it in both units systems to find the correspondent site size. In our case, we have started from the particle diameter. If we are not interesting in particle shape, than one site/particle is some what sufficient, if we also admit a fine particle to be between 0,001μm-0,1μm, and a good representative grain population of 1000 grains, we need approximately 40.000 sites to start. In this regard, a care must be taken for the initial microstructure and the time spent to get pinned configuration.

II- DISCUSSION AND RESULTS

In order to perform the study, we realised growth

sequences representing evolutions up to a time of 2000MCS.

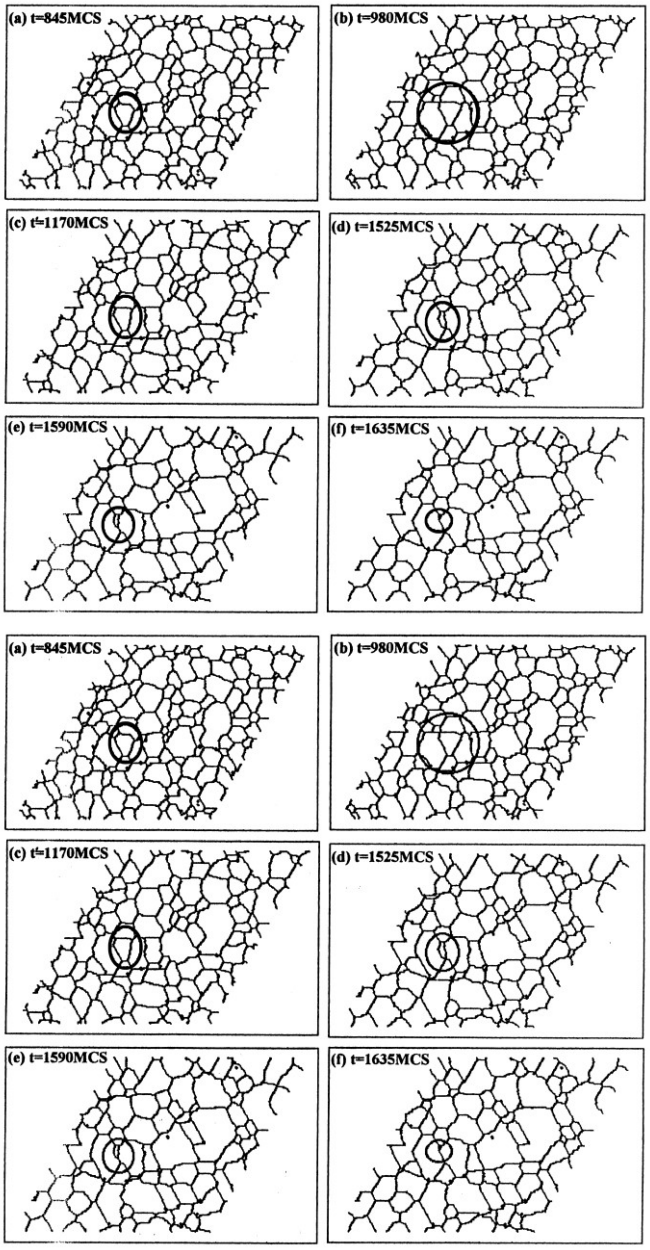
II.1- Mechanism of grain shrinkage

According to Von Neumann, grains with less than 6 sides are unable to grow, a relation ship of the form is reported (3):

$$\frac{dA}{dt} = C(N-6) \tag{3}$$

where A is grain area, N number of sides and C a constant.

Although this relation does not incorporate curvature which is the responsible of the driving pressure, it fills approximately the topological features of growth in 2D. A real description should also take into account the explicit effect of the neighbouring grains. Figure 4 describes quantitatively the evolution of a microstructure in respect to the later condition.



aid of relation (3) since particles presence leads to significant changes in grain shape.

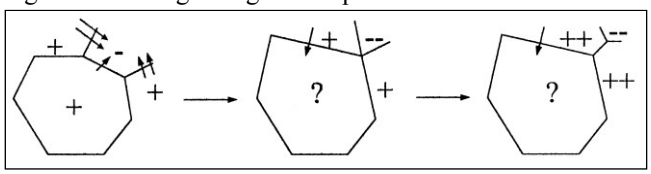


Figure 5: Competition in gaining new sides in the growth mechanism: (+) growing grain, (-) shrinking one and (?) a none determinate (strings indicate boundary displacement sense).

II.2- Grain exponent

Since the driving force is proportional to the mean curvature and assuming a linear relation between migration rate and the driving pressure, we find easily the general relation expressed as follows (4):

$$A = kt^{2n} \tag{4}$$

where n is the grain exponent (some authors prefer $1/n$), n = 0.5 corresponds to parabolic low.

Many authors tried to evaluate n and to verify the parabolic low [9,30-35]. Some results [36] revealed the controversy about such measure, and both experimental and simulation methods gave different results. It is still put in doubt that n = 0,5 can be observed by the majority of refined metals, its value is suspected to lie between [0,1-0,5]. Figure 6-a shows the mean grain area as a function of time for an evolution without particles. The grain exponent calculated from six runs is found to have a mean value of 0,41. Figures 6-c,d show the corresponding microstructure which exhibits the characteristic of a normal growth compared to real microstructure of pure Fe. The distribution scaled with the mean size is time invariant (figure 6-b) and the largest grain size is not far away from the mean one.

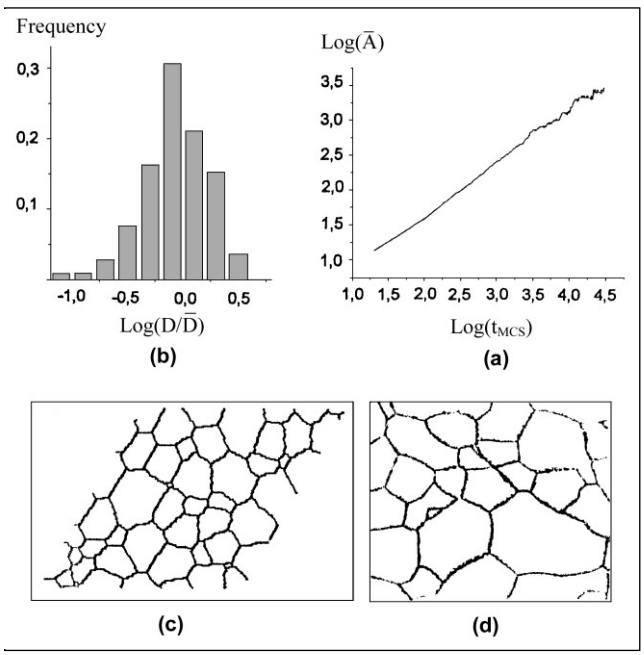


Figure 6: Results concerning grain growth without particles at ~0K: **(a)** plot mean grain area as function of time. **(b)** grain size distribution. **(c)** corresponding microstructure at t=3000MCS. **(d)**

for comparison a polished and etched section of pure Fe (taken from [10]).

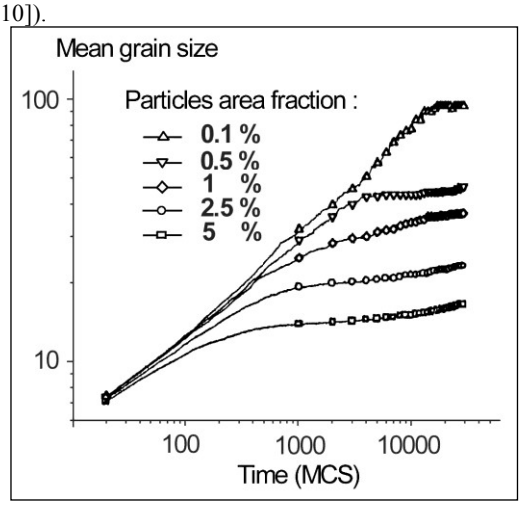


Figure 7: Plot of mean size (arbitrary unit) as function of time in logarithmic scale for several area fractions.

Figures 7, 8, 9 show results obtained for various particle area fractions (f_s = 0,1; 0,5; 1; 2,5; 5 %). The growth rate is found to be slower according to the pinning pressure, that decreases the total driving force and depending on f_s, but no quantitative variation is permitted with the few number of *fs* chosen, the average value was found to be at 0,35.

II.3- Stagnation

The passage from the normal growth to stagnation is related to the amount of particles present. Figure 7 shows the average grain diameter evolution with time. Figures 8 (a,b,c,d) presents the final microstructure obtained.

The final grain size is found to be related to *fs* (figure 9) as shown in relation (5):

$$A_f \propto \sqrt{f_s} \qquad (5)$$

However, this relation is followed with a wide scatter and an exact expression cannot be viewed. Also it seems that for small fractions the limiting grain size is not best represented by the non-correlated relation (relation 4) as it is the case for large fractions.

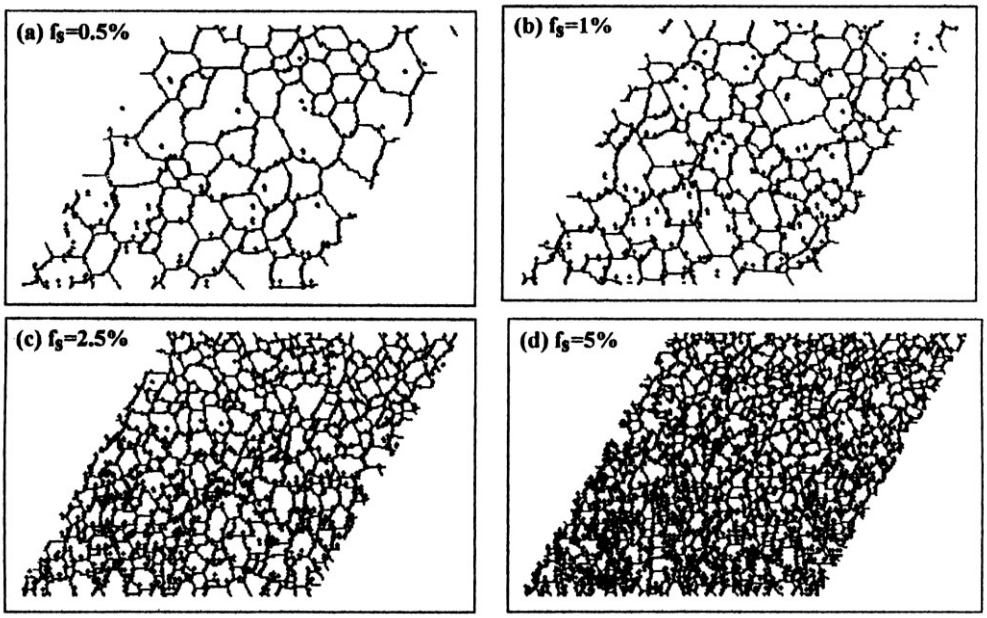


Figure 8: Stagnation microstructure for divers area fraction corresponding to some evolution shown in figure 7.

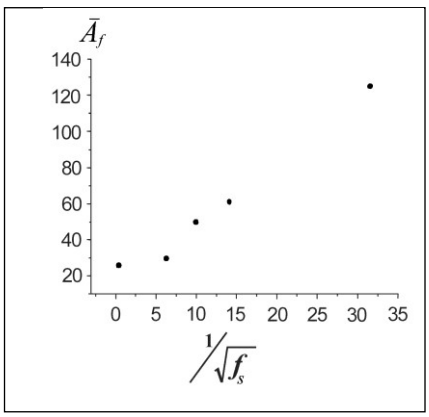


Figure 9: Scatter graph of the final grain size as function of particle fraction.

CONCLUSION

In conclusion, we have tried to present our modified Monte Carlo technique applied to grain growth, this powerful method allows the study of several aspects of growth, the local behaviour of grains which is difficult to interpret with other models is easily followed. The resolution of the current procedure is not sufficient to represent accurately the particles problem, but a n observed successfully and a grain exponent of 0,55 have been reported, the final grain size is found to have square root variation with area fraction expected for large particle fractions.

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