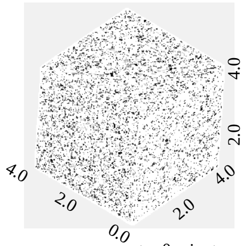
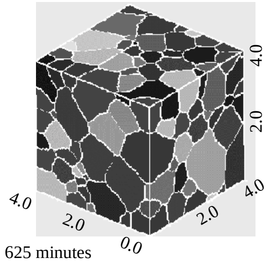
Computer Simulation of Grain Growth By Monte Carlo Method

Zone-Refined Iron



T = 923 K



t = 0 minutes

t = 625 minutes

Computer Simulation of Grain Growth By Monte Carlo Method

Why study grain growth?

How does it occur?

What is Monte Carlo method?

Grain Growth Study

Why?

- Most metal processing involves grain size changes
- Grain size changes affect strength, toughness and corrosion resistance
- Changes in grain structure also have significant impact on susceptibility to cold cracking and reheat cracking

Basic Definitions

Annealing (isothermally heating) a cold-worked metal =>
Recovery and Recrystallization => Grain Growth

- **Recovery**
  Dislocation motion relieves stored internal strain energy, as a result of enhanced atomic diffusion at elevated temperature. Physical properties like electrical and thermal conductivities are recovered to their pre-cold-worked values.
- **Recrystallization**
  Formation of a new set of strain-free and equiaxed grains having low dislocation densities. The new grains form as very small nuclei and grow until they completely replace the parent material.

Driving force - difference in internal energy between the strained and the unstrained material.

Basic Definitions

- **Grain Growth**

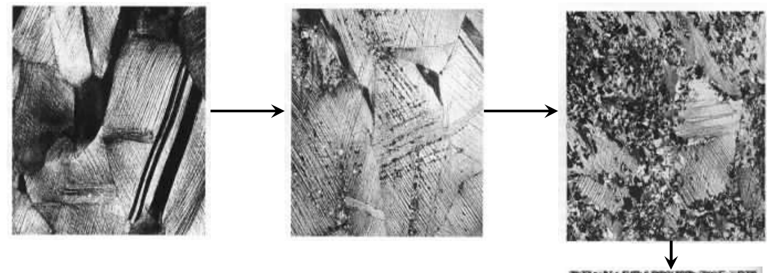
  Continued growth of strain-free grains after recrystallization
  More growth at higher temperatures and longer times.

  Driving force – Reduction in grain boundary energy due to decrease in total grain boundary area

  Process - Occurs by the migration of grain boundaries. (short range diffusion of atoms from one side of the boundary to the other.)

  - Large grains grow at the expense of smaller ones that shrink.

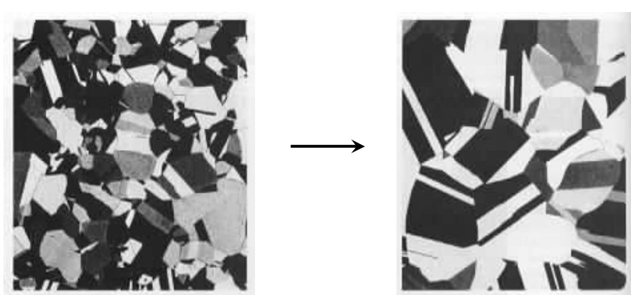
Basic Definitions



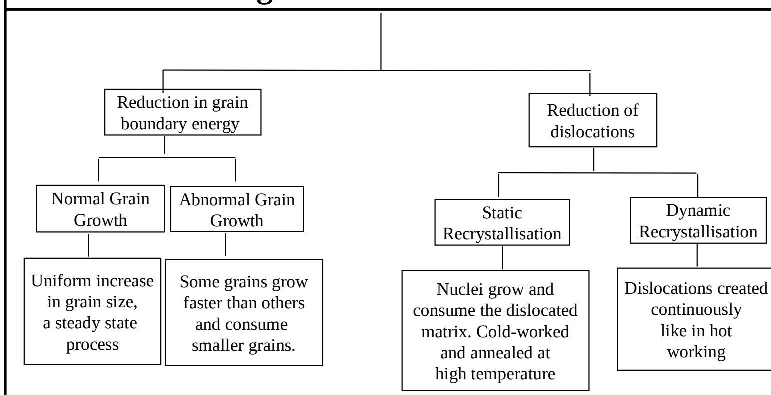
Recrystallization

Basic Definitions

Normal Grain Growth



Driving Force in Grain Growth



Grain Growth Study

How?

- Analytical equations - give quantitative information making some assumptions
- Computer simulations - relax some of the assumptions and make the calculations more realistic
- Both the methods initially studied Normal Grain Growth

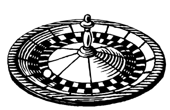
Why Monte Carlo simulation?

- Grain growth results from the interaction between the topological requirements and the forces driving boundaries to migrate, to reduce boundary curvature and hence area and energy
- Thus no grain can ever be treated as an isolated entity but should always be seen in relation to its neighboring grains
- The assumption that the grains are spherical ignores that adjacent grains share common boundaries leading to a connected assembly of mutually interacting grains

What is Monte Carlo Method?

It solves mathematical and physical problems by simulation of random quantities

Roulette wheel is a simple mechanical device for obtaining random quantities

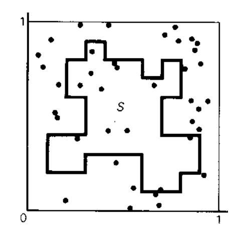


Does not help one to win at Roulette

Example: compute the area of figure S

S is contained completely within the unit square

Randomly choose N points within the square. Number lying within S is M



(area S/area of unit square) = M/N

In this figure, M= 12 and N= 40; M/N = 0.3

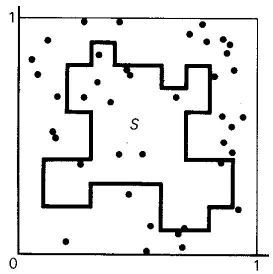
True area = 0.35 x area of unit square

Monte Carlo (MC) Algorithm

A process of producing a random event

The process is repeated N times

The results of the trial are averaged



Error = $\sqrt{D/N}$

D is a constant and N is number of trials

Monte Carlo (MC) Algorithm

In this case, D = S(1-S) = 0.35(1 - 0.35) where S is the area

Error = $\sqrt{D/N} = \sqrt{0.23/40}$ **= 0.076**

How to reduce error?

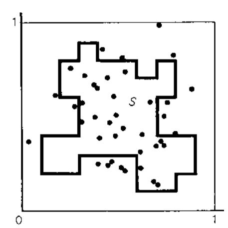
N must be increased by a factor of 100 to reduce error by a factor of 10

Monte Carlo (MC) Algorithm

Imagine this figure hanging on the wall as a target

Darts are aimed at the center

They strike the target at N random points



Can these points be used to calculate the area?

In this figure, M= 24 and N= 40; M/N = 0.6, which is almost twice the actual area (0.35)

When darts are thrown with skill, results are bad

Monte Carlo (MC) Algorithm

Results are good only when the points are not "simply random", but in addition, "uniformly distributed"

So we need to be familiar with the definition of random variables and some of their properties.

Random variables

Random: Any process that proceeds without any discernible aim or direction

Discrete random variables

Distribution of random variables:

$$X = \begin{pmatrix} x_1 & x_2 & x_3 & \ldots\ldots & x_n \\ p_1 & p_2 & p_3 & \ldots\ldots & p_n \end{pmatrix}$$

x_1 x_2 x_3 ….. x_n are possible values of X
p_1 p_2 p_3 ….. p_n are corresponding probabilities

Expected value of a variable

Probabilities must satisfy two conditions:

$p_i \geq 0$ and $p_1 + p_2 + p_3 + \ldots. + p_n = 1$

Expected value of X or mathematical probability of variable X is called E(X)

$$E(X) = \sum_{i=1}^{n} x_i\, p_i$$

To illustrate its physical meaning, we write it in the following form:

$$E(X) = \sum_{i=1}^{n}(x_i\, p_i) / \sum_{i=1}^{n} p_i$$

E(X) is in a way the average value of X with more probable values added with larger weights

Expected value of a variable

$$E(X) = \sum_{i=1}^{n}(x_i\, p_i) / \sum_{i=1}^{n} p_i$$

E(X) is in a way the average value of X with more probable values added with larger weights

If masses m_1, m_2, m_3, …., m_n are distributed on the x-axis at the points x_1, x_2, x_3, …., x_n, the abscissa of the center of gravity of the system is given by:

$$x = \sum_{i=1}^{n}(x_i\, m_i) / \sum_{i=1}^{n} m_i$$

Note that the sum of all masses do not add to 1

Expected value of a variable

E(X + c) = E(X) + c

E(X + Y) = E(X) + E(Y)

E(cX) = cE(X)

Observe a variable X many times and obtain values: x_1, x_2, x_3, …., x_n. The arithmetic mean of these numbers will be close to E(X)

$$E(X) = (1/n)\sum_{i=1}^{n} x_i$$

The spread of the values around the average E(X) is called the variance of X

Variance of a variable

Variance of X, Var (X) = $E((X - E(X))^2)$

$= E(X^2 - 2E(X)\,X + (E(X))^2)$

$= E(X^2) - 2(E(X))^2 + (E(X))^2$

$= E(X^2) - (E(X))^2$

Let us consider a random variable X

$$X = \begin{pmatrix} 1 & 2 & 3 \ldots\ldots & 6 \\ 1/6 & 1/6 & 1/6 \ldots\ldots & 1/6 \end{pmatrix}$$

E(X) = (1/n) $x_i = (1 + 2 + 3 + 4 + 5 + 6)/6 = 3.5$

Var (X) = $E(X^2) - (E(X))^2$
$= (1^2 + 2^2 + 3^2 + 4^2 + 5^2 + 6^2)/6 - (3.5)^2 = 2.917$

Variance of a variable

Now let us consider a random variable Y

$$Y = \begin{pmatrix} 3 & 4 \\ 1/2 & 1/2 \end{pmatrix}$$

E(Y) = (1/n) $y_i = (3 + 4)/2 = 3.5$

Var (Y) = $E(Y^2) - (E(Y))^2$
$= (3^2 + 4^2)/2 - (3.5)^2 = 0.25$

E(Y) = E(X) but Var (Y) < Var (X)

This could have been anticipated, since the values of Y differ from 3.5 only by ±0.5, while for X the spread can reach ±2.5

Continuous random variables

A random variable is continuous if it can take any value in some interval [a,b]

Let (a',b') be an arbitrary interval contained in [a,b]

The probability that X lies in the interval (a',b')

P(a'<X<b') = $\int_{a'}^{b'} p(x)dx$

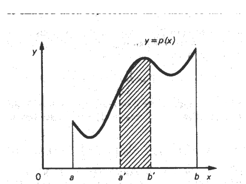


Fig. 2.2

p(x) must satisfy two conditions similar to discrete variables

Continuous random variables

Two conditions: p(x) ≥ 0 and $\int_a^b p(x)dx = 1$

Expected value E(X) = $\int_a^b xp(x)dx$

E(f(X)) = $\int_a^b f(x)p(x)dx$

Let p(x) = 1 for all values of x between 0 and 1

E(G) = $\int_0^1 xp(x)dx$ **= $(x^2/2)\Big|_0^1$ = 1/2**

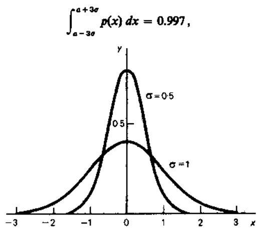
Var (G) = $\int_0^1 x^2 p(x)dx$ **- $(E(G))^2$= $(x^3/3)\Big|_0^1$ - 1/4 = 1/12**

Normal random variables

A random variable having the density:

$$p(X) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left[-\frac{(x-a)^2}{2\sigma^2}\right]$$

$$\text{Max } p(X) = \frac{1}{\sigma\sqrt{2\pi}}$$



The area under the curve p(x) is 1

It is possible to show that E(Z) = a and Var (Z) = σ^2

P(a - 3σ <Z< a + 3σ) = 0.997

Monte Carlo Method

We want to determine some unknown quantity m

We try to devise a random variable X with E(X) = m

Let Var (X) = v^2

Consider N independent random variables X_1, X_2, …., X_N, with distributions identical with that of X

Consider the sum $S_N = X_1 + X_2 + …. + X_N$

$E(S_N) = E(X_1 + X_2 + …. + X_N) = Nm$ => a

$Var(S_N) = Var(X_1 + X_2 + …. + X_N) = Nv^2$ => σ^2

Monte Carlo Method

$P(Nm - 3v\sqrt{N} < S_N < Nm + 3v\sqrt{N}) = 0.997$

$P(m - 3v/\sqrt{N} < (S_N/N) < m + 3v/\sqrt{N}) = 0.997$

We can rewrite this relation in the following form

$$\mathbf{P}\left(\left|\frac{1}{N}\sum_{i=1}^{N} X_i - m\right| < \frac{3v}{\sqrt{N}}\right) = \mathbf{0.997}$$

This relation is very important for the MC method. Gives us a method of calculating m and an uncertainty of estimation

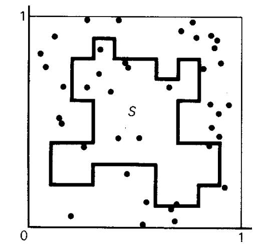
When the value is m calculated from arithmetic average of random values, the probability is high (0.997) that the error will be less than $3v/\sqrt{N}$

Error analysis

Calculation of area

Result of a single trial

X_j = 1, if the random point lies in S
0, if the random point lies outside S



Estimate area S as $\sum x_j/N$

Distribution of X_j: $\mathbf{X_j} = \begin{pmatrix} \mathbf{0} & \mathbf{1} \\ \mathbf{1-S} & \mathbf{S} \end{pmatrix}$

$$\mathbf{E(X)} = \sum_{i=1}^{n} x_i p_i = 0(1-S) + 1(S) = S$$

$Var(X) = E(X^2) - (E(X))^2$
$= 0^2(1-S) + 1^2(S) - (S)^2 = S(1-S) = v^2$

$$\mathbf{Error} = v/\sqrt{N} = \sqrt{S(1-S)/N}$$