

Computer Simulation Through Diffuse interface of Two Grains of Different Geometries in 2D

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Abstract

A grain is a crystal within the polycrystal, which usually does not have a regular shape; and, a grain boundary is a zone of transition between different crystalline orientations of the adjacent grains. Here we discuss the diffuse-interface description for movement of grain boundaries and assurity of the diffuse interface field model in explaining curvature driven microstructural evolutions. In this study, we only consider two dimensional systems with isotropic grain boundary energy. Specifically, we report results from our studies on two grains of elliptical geometries in 2-D and the effect of various simulation parameters on the results. There are a variety of computer simulation methods to study grain growth; for example, models such as boundary dynamics model, vertex models, Potts model, Voronoi tessellation and models based on mean field theories (see Ref. 9). In this report, we use diffuse-interface models of the type proposed by Chen and co workers (see Ref. 9-11). In this section we summarise the salient features of as well as some of the pertinent results from the diffuse interface models.

1. Introduction

A grain is a crystal within the polycrystal, which usually does not have a regular shape; and, a grain boundary is a zone of transition between different crystalline orientations of the adjacent grains.

Grain boundaries are regions of disorder. This disorder results in an increase in the internal energy due to the broken, unsatisfied or unequilibrated bonds at the grain boundaries. However the increase in the entropy associated with the disorder at the grain boundary is not large. Hence, as compared to a single crystal, a polycrystal with grain boundaries has a higher (positive excess) free energy. So, grain limit movement happens in polycrystalline materials to decrease the all out grain limit region and the abundance free vitality related with them; this procedure is alluded to as grain development

In polycrystalline materials the microstructure, i.e, the sizes, shapes and strategy of grains, essentially chooses the mechanical properties; for instance, using an equation like Hall–Petch, it can be shown that the yield stress is inversely proportional to the grain size. So, as the grains become smaller and smaller, the material becomes more and more strong. Hence grain growth can lead to changes in the properties of the materials and is an important area of study both from an industrial and fundamental points of view.

Some salient analytical results

According to Neumann and Mullins (Ref. 2-3), in 2-dimensions, the individual grain area change with respect to time doesn't rely upon the size or geometrical state of the grain, however depends just on its number of sides. This condition is applicable when the grain boundary energy is isotropic and the triple junctions are at equilibrium, i.e. at the points where three grains meet the boundaries make an angle of 120° :

$$\frac{da}{dt} = \frac{m\gamma\pi}{3}(n-6), \quad (1.1)$$

where a and n are the area and the number of sides of grains, γ and m are the energy of the grain boundaries and mobility.

- Grains grow when $n > 6$; that is, when the number of sides of grain are greater than six.
- Grains contract when $n < 6$; that is, when the number of sides are less than six.
- Grains neither grow nor contract if $n = 6$; that is, when the number of sides are six.

The above result of Neumann and Mullins can also be understood if we consider the grain growth as a curvature driven process. If a grain boundary is curved, the atoms on the concave side have lower potential than those on the convex side. That is, the atoms are less tightly bound by neighbouring atoms on the convex surface. Thus, if the system is kept at a high enough temperature which gives enough mobility, thermal movements will gradually transfer the atoms from the grain with a more convex surface to a grain with a more concave surface. Since little grains will in general have surfaces with more keen convexity, they will progressively vanish by nourishing the bigger grains. The net impact is grain development.

In interface motion theories, the grain boundary motion in term of V is

$$V = B\Delta u,$$

$$V = B\sigma_{gb}\Omega(\lambda_1 + \lambda_2), \quad (1.2)$$

where, Δu = Chemical potential difference per atom across the
boundary.

Ω = Atomic volume

B = Mobility

$\lambda_1 + \lambda_2$ = Mean curvature

σ_{gb} = Grain boundary energy

Diffuse interface modeling of normal grain growth

Both experimentally and from simulations, it is known that grain growth can in general be classified as of two types: normal and abnormal grain growth; see for example (Ref. 4). As shown schematically in Fig. 1.2 and 1.3 below, under normal growth of grain, the size of grains increases slowly, and the grain size distribution is unimodal. During abnormal grain growth the mean grain size changes first a little, if at all, and thereby increase rapidly; the initial stage of very little or no growth is known as incubation period. In this report, we only study normal grain growth.

There are many different types of models of grain growth. These can broadly be classified as atomistic and continuum models. Continuum models may again be broadly classified as sharp and diffuse interface models. In the sharp-interface models the grain limits are unique geometrical surfaces having properties, for example, region, bend, free energy, and portability. Such models are reviewed in (Ref. 5-7).

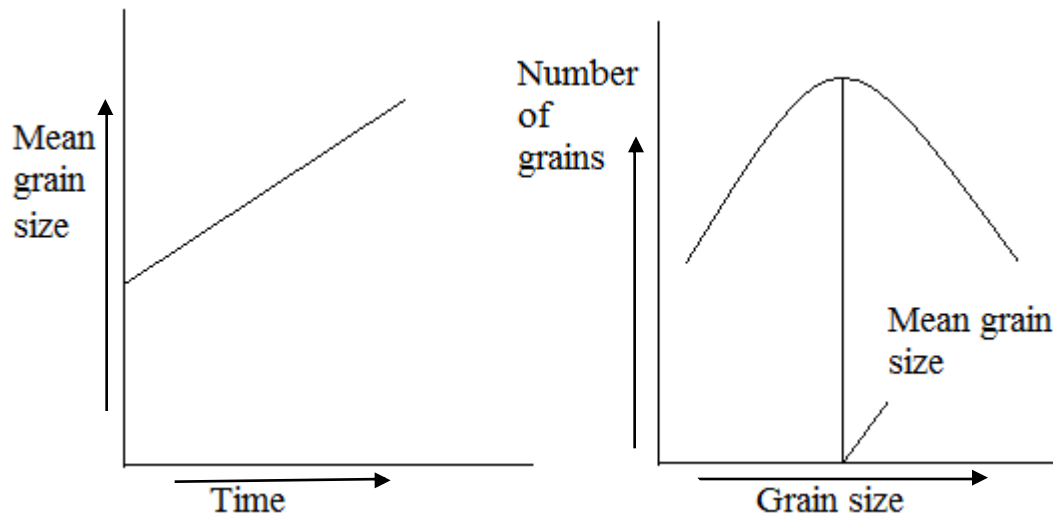


Fig.1.2 Normal grain growth

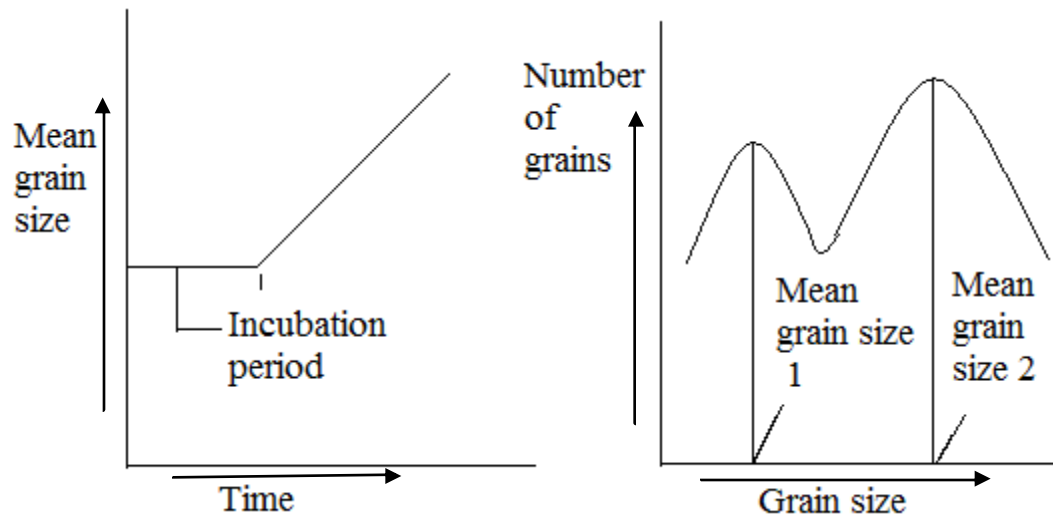


Fig.1.3 Abnormal grain growth

In diffuse interface model the main feature is diffuse of grain boundaries with limited thickness. This is like the hypothetical treatments of antiphase space limits by Allen and Cahn (see Ref. 8). The grain limit vitality is naturally presented through the inclination vitality terms in the free vitality practical. One fundamental preferences approach is that a self-assertive microstructure

can be often treated as the inter-faces are not solitary surfaces requiring inconvenience of moving limit conditions as in the sharp-interface depiction, however only a district where the fields have high slopes (see Ref. 9).

2. Theoretical Formulation and Numerical Implementation

In the diffuse interface model, a polycrystalline characteristic is depicted as many orientation field variables as there are distinct grains (see Fig. 2.1 below where we schematically show the description of a system with seven grains); these field variables recognize the various directions of the grains and are nonstop elements of spatial position and time. For every grain, the corresponding orientation field variable has a constant value of unity inside the grain but changes to zero outside the grain over the thickness of the grain boundary. The worldly development of these field factors, and hence the microstructural advancement and grain development energy are described by the time-dependent Ginzburg- Landau (TDGL) equations.

2.1 The diffuse-interface model

Let us consider a subjective polycrystalline microstructure portrayed by a lot of direction field factors like

$$\eta_1(r), \eta_2(r), \dots, \eta_p(r),$$

where p is the number of possible orientations. The absolute free vitality of such a framework as far as all the direction field factors and their inclinations can be written as:

$$F = \int [f_o(\eta_1(r), \eta_2(r), \dots, \eta_p(r)) + \sum_{i=1}^p \frac{k_i}{2} (\nabla \eta_i(r))^2] d^3 r \quad (2.1)$$

where $i=1, 2, \dots, p$, and f_o (free local energy density as a component of field variables η_i), and k_i (gradient energy coefficients).

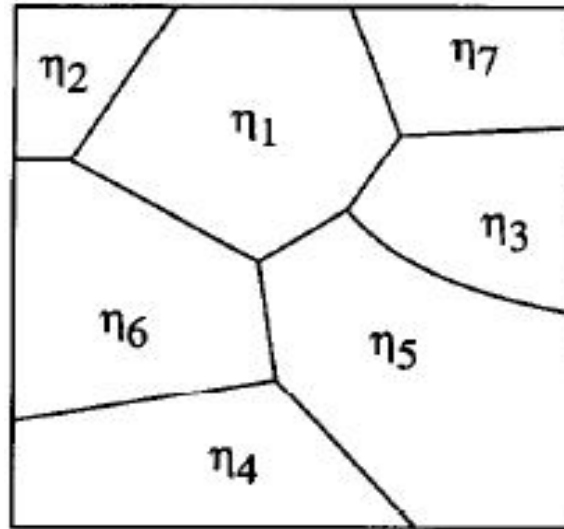


Fig.2.1. Diagram of microstructure showing 7 grains using 7 orientation field variables

In present study, to begin with, we consider the two grain case of one grain embedded in another; hence, there are two continuous field variables η_1 and η_2 , corresponding to the two orientations. In such a case, the free total energy of the inhomogeneous framework as a component of the two direction field factors and their inclinations is:

$$F = \int [f_o(\eta_1(r), \eta_2(r)) + \sum_{i=1}^2 \frac{k_i}{2} (\nabla \eta_i(r))^2] d^3 r . \quad (2.2)$$

The main requirement for f_0 is that it has two (since $p=2$) degenerate minima with equal depth, f_{\min} located at $(\eta_1, \eta_2) = (1, 0)$, and $(0, 1)$ in the 2D space.

Since the direction field factors are non-rational amounts, their neighbourhood development rates are straightly relative to the variational subsidiary of the all out free vitality as for the nearby direction field variable, i.e. governed by the Ginzburg - Landau equations,

$$\frac{\partial \eta_i(r,t)}{\partial t} = -L_i \frac{\delta F}{\delta \eta_i(r,t)}, \quad i=1, 2, \dots, p \quad (2.3)$$

where L_i is Relaxation co-efficients, time as t and Free total energy as F). For the two grain case we have two equations:

$$\frac{\partial \eta_1(r,t)}{\partial t} = -L_1 \frac{\partial F}{\partial \eta_1(r,t)}$$

$$\frac{\partial \eta_2(r,t)}{\partial t} = -L_2 \frac{\partial F}{\partial \eta_2(r,t)}$$

If we substitute for the free energy expression in the above equations, we obtain the equations for the evolution.

Thus, for our case, the evolution of the orientational order parameter fields η are described by,

$$\frac{\partial \eta_1(r,t)}{\partial t} = -L_1 \frac{\partial}{\partial \eta_1(r,t)} \left[\int [f_0(\eta_1, \eta_2) + \frac{k_1}{2} (\nabla \eta_1)^2 + \frac{k_2}{2} (\nabla \eta_2)^2] d^3r \right],$$

$$\frac{\partial \eta_2(r,t)}{\partial t} = -L_2 \frac{\partial}{\partial \eta_2(r,t)} \left[\int [f_0(\eta_1, \eta_2) + \frac{k_1}{2} (\nabla \eta_1)^2 + \frac{k_2}{2} (\nabla \eta_2)^2] d^3r \right],$$

Putting $f_0(\eta_1, \eta_2) = -\frac{\alpha}{2} (\eta_1^2 + \eta_2^2) + \frac{\beta}{4} (\eta_1^4 + \eta_2^4) + 2\gamma (\eta_1^2 \eta_2^2), \quad (2.4)$

where α , β and γ are positive constants

we obtain,

$$\frac{\partial \eta_1}{\partial t} = -L_1[-\alpha \eta_1 + \beta \eta_1^3 + 4\gamma \eta_1 \eta_2^2 - k_1 \nabla^2 \eta_1]$$
$$\frac{\partial \eta_2}{\partial t} = -L_2[-\alpha \eta_2 + \beta \eta_2^3 + 4\gamma \eta_2 \eta_1^2 - k_2 \nabla^2 \eta_2].$$

Initial and boundary conditions:

In our model calculations, when we embed a grain inside another, for the initial profile (that is, profile at $t=0$) of the continuous field variables η_1 and η_2 , we assume the following: η_1 is unity in the embedded grain (while η_2 is 0) while it is the other way around for the other grain.

$$\eta_1(x, t = 0) = 1 \text{ and } \eta_2(x, t = 0) = 0 \text{ only inside the embedded grain.}$$

On the outside of the embedded grain $\eta_1(x, t = 0) = 0$ and $\eta_2(x, t = 0) = 1$. We use periodic boundary conditions on the simulation domain which is the natural boundary condition to use since our numerical implementation is based on Fourier transforms as described below.

2.2 Numerical implementation

We use a semi-implicit Fourier spectral technique to solve the equations of microstructural evolution. To do so, we first (spatially) Fourier transform the evolution equations, and use a forward difference scheme for the time evolution.

$$\frac{\partial \eta_1}{\partial t} = \frac{\eta_1^{t+\Delta t} - \eta_1^t}{\Delta t}, \tag{2.5}$$

$$\frac{\partial \eta_1}{\partial t} = L_1 \alpha \eta_1 + k_1 L_1 \nabla^2 \eta_1 - L_1 \beta \eta_1^3 - 4L_1 \gamma \eta_1 \eta_2^2.$$

Similarly,

$$\frac{\partial \eta_2}{\partial t} = L_2 \alpha \eta_2 + k_2 L_2 \nabla^2 \eta_2 - L_2 \beta \eta_2^3 - 4L_2 \gamma \eta_2 \eta_1^2.$$

Taking $h_1(\eta_1, \eta_2) = -L_1 \beta \eta_1^3 - 4L_1 \gamma \eta_1 \eta_2^2,$ and,

$$h_2(\eta_1, \eta_2) = -L_2 \beta \eta_2^3 - 4L_2 \gamma \eta_2 \eta_1^2$$

we obtain,

$$\frac{\partial \tilde{\eta}_1}{\partial t} = L_1 \alpha \tilde{\eta}_1 + k_1 L_1 \nabla^2 \tilde{\eta}_1 + \overline{h_1}(\eta_1, \eta_2), \tag{2.6}$$

where,

$$\nabla \tilde{\eta}_1 = -i\kappa \tilde{\eta}_1$$

$$\nabla \nabla \tilde{\eta}_1 = (-i)^2 \kappa^2 \tilde{\eta}_1 = -\kappa^2 \tilde{\eta}_1$$

$$\frac{\tilde{\eta}_1^{t+\Delta t} - \tilde{\eta}_1^t}{\Delta t} = L_1 \alpha \tilde{\eta}_1^{t+\Delta t} - k_1 L_1 \kappa^2 \tilde{\eta}_1^{t+\Delta t} + \overline{h_1}(\eta_1, \eta_2)^t$$

$$\frac{\tilde{\eta}_2^{t+\Delta t} - \tilde{\eta}_2^t}{\Delta t} = L_2 \alpha \tilde{\eta}_2^{t+\Delta t} - k_2 L_2 \kappa^2 \tilde{\eta}_2^{t+\Delta t} + \overline{h_2}(\eta_1, \eta_2)^t$$

Finally, we get

$$\tilde{\eta}_1^{t+\Delta t} = \frac{\tilde{\eta}_1^t + \overline{h_1}(\eta_1, \eta_2)^t}{1 + \Delta t(-L_1 \alpha + k_1 L_1 \kappa^2)}, \tag{2.7}$$

and $\tilde{\eta}_2^{t+\Delta t} = \frac{\tilde{\eta}_2^t + \overline{h_2}(\eta_1, \eta_2)^t}{1 + \Delta t(-L_2 \alpha + k_2 L_2 \kappa^2)}.$

Coding

The following results are obtained using a C code which is a modified version of a code of M. P. Gururajan, which is available online (see Ref. 13). I have downloaded this code, which is meant for solving the Allen-Cahn equations for order-disorder transformations (using the freeware fastest fourier transform to the west of pacific-- FFTW). I have modified it to do grain growth simulations for one grain inside the another. This modification involves, changing the initial conditions in this program, modifying the formulation with increased numbers of parameters (two instead of one), and, doing the calculations for two orientation field variables instead of one.

Simulation parameters

In all our simulations we use the following values for the various parameters (unless specified otherwise).

Table 2.1 Simulation parameters

Case :	$n_x = n_y$	256	512	1024
	$\Delta x = \Delta y$	1	0.5	0.25
	$\alpha = \beta = \gamma$	1	1	1
A.Elliptical	$k_1 = k_2$	1		
	$L_1 = L_2$	1		

3. Results and discussions

In this report, we discuss the time evolution of elliptical grain boundary in different embedded grains:

3.1 Microstructures

In Fig. 3.1 (a-d), we show the evolution of microstructural for a grain with elliptical boundaries embedded in another; similarly. While the elliptical ones move in such a way that as time proceeds the embedded grains decrease in area; finally, they will disappear leaving behind a single grain. This trend is in agreement with what we expect from the curvature driven growth. Further, the differences in time for the complete disappearance of the embedded grains in the elliptic cases is a reflection of the differences in the mean curvature at various points on the boundary in these cases; it is not so in the case of the elliptic boundary. Finally, the elliptical one becomes more and more circular as time proceeds. This is also expected because we have assumed isotropic grain boundary energy and hence for a given area a circular shape minimizes the grain boundary length.

Fig.3.1. Microstructural evolution for a grain with elliptical boundaries embedded in another.

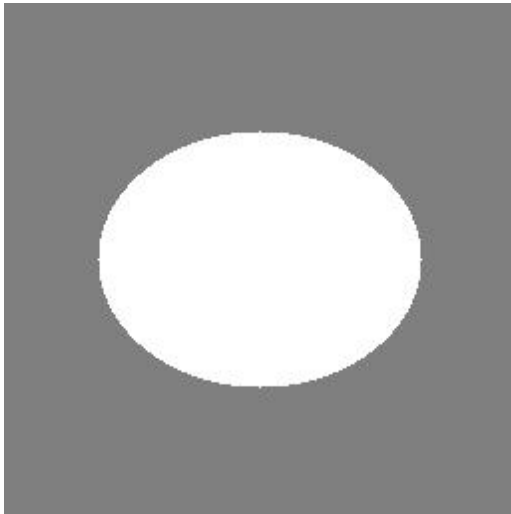


Fig.(a) Elliptical grain inside the another at $t=0$,

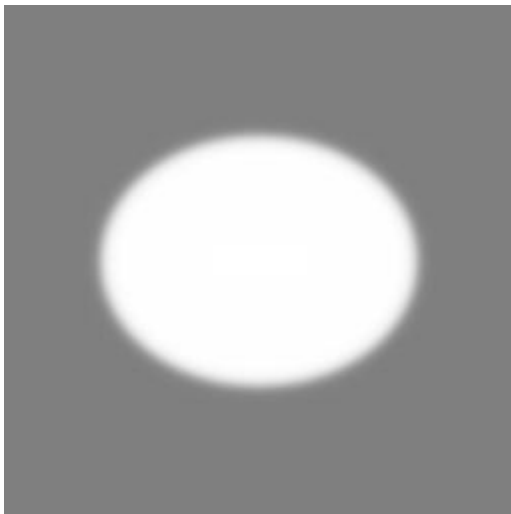


Fig. (b) At $t=5000$,



Fig. (c) At $t=11000$,

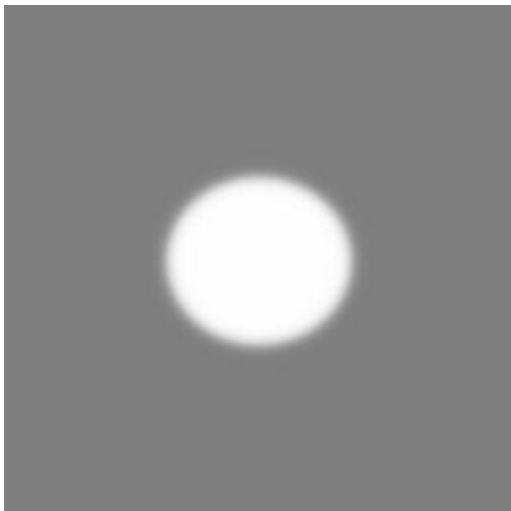


Fig. (d) At $t=15000$,

3.2 Positions of the grain boundaries

Using a similar analysis it is also possible to locate the position of the grain boundary along the x-axis from the centre of the simulation cell towards the right hand side. The plots of such positions of the grain boundary as a time dependent is shown in Fig. 3.2 for elliptical boundaries. From these plots also, it is clear that the interface moves in elliptical grain cases

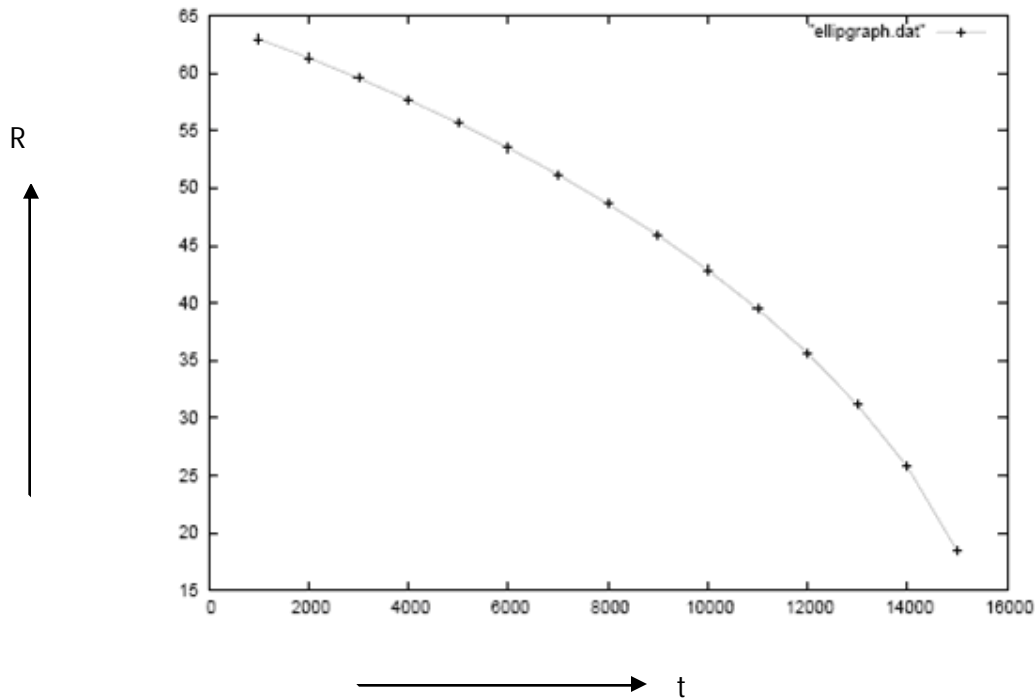


Fig.3.2 . Graph of interface position (R) versus time (t) for an elliptical grain.

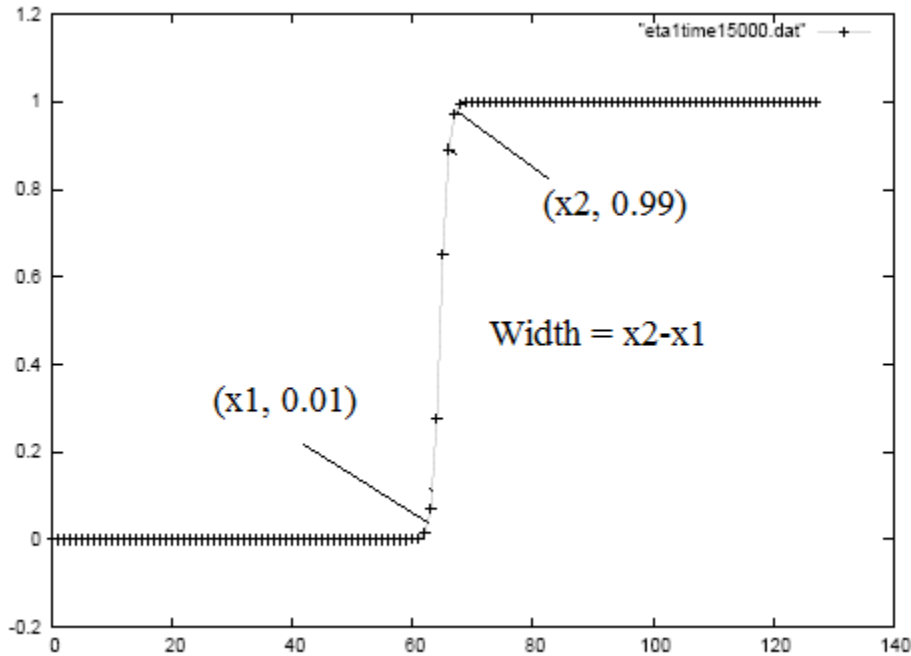


Fig.3.3 Interface profile for determining the width of the interface.

3.3 Widths and Energies of the boundaries

In Table 3.1 we show the effect of grid refinement as well as gradient energy coefficient on the interface widths. In this case we consider the flat grain boundary to avoid any errors due to the grain boundary movement. After the boundary becomes diffuse, say after 15000 time steps, we consider the interface profile (see Fig. 3.3). From this profile, we identify two points – one above 0.5 and another below 0.5. Knowing the values of the grid position for these two points and the values of the order parameter at these two grid positions, one can calculate the exact point of the grid at which the order parameter profile takes a value of 0.99 and 0.01. For example, in the figure shown above, we have taken the grid point 65 and 67; for these two points, the value of the order parameter, read from the data files are 0.3655870 and 0.7290936 respectively. Now, knowing two points, say, (x_1, y_1) and (x_2, y_2) , a straight line can be fit; or, in other words,

we use a straight line interpolation to identify the interface position, put $y = 0.99$, we get $x = 68.43549746$. Also put $y = 0.01$, we get $x = 63.04357335$. The difference between these two values gives the width of the interface.

In Table 3.1, we show the calculated interface widths for three pairs of gradient energy coefficients (see the columns 3-5). It is well known that in this models the interface width scales as the square root of the gradient energy coefficient (see Ref. 14 for example). In Table 3.2 we give the scaled widths ($\frac{w}{k^{0.5}}$) for the different simulations. From these values it is clear that the numerical simulations (a) are not well resolved for $k_1 = k_2 = 1$; (b) the finer discretization of the grids leads to better values. Further from these values it is also clear that for $k_1 = k_2 = 4$ and $k_1 = k_2 = 8$, even a coarse grid gives reliable widths.

Table 3.1

Calculation of the grain boundary width with different value of gradient energy coefficients.

Total Grid Size: $n_x = n_y$	Gradient Energy Coefficients k_i	256	512	1024
Grid Spacing: $\Delta x = \Delta y$		$\Delta x = \Delta y = 1$	$\Delta x = \Delta y = 0.5$	$\Delta x = \Delta y = 0.25$
Relaxation Coefficients: L_i		$L_1 = L_2 = 1$	$L_1 = L_2 = 1$	$L_1 = L_2 = 1$

Width	$K_1 = K_2 = 1$	3.193146075	5.3919256	11.67026495
	$K_1 = K_2 = 4$	5.39192411	10.24001336	20.99285939
	$K_1 = K_2 = 8$	7.36703627	14.96650479	29.370556

Table 3.2

Scaled grain boundary widths

Total Grid Size: $n_x = n_y$ Grid Spacing: $\Delta x = \Delta y$ Relaxation Coefficients: L_i	k_i Gradient Energy Coefficients	256 $\Delta x = \Delta y = 1$ $L_1 = L_2 = 1$	512 $\Delta x = \Delta y = 0.5$ $L_1 = L_2 = 1$	1024 $\Delta x = \Delta y = 0.25$ $L_1 = L_2 = 1$
Scaled width	$K_1 = K_2 = 1$	3.19	5.39	11.67
	$K_1 = K_2 = 4$	2.69	5.12	10.44
	$K_1 = K_2 = 8$	2.60	5.29	10.38

The grain limit vitality starts from the slope vitality terms $(\nabla \eta_i)^2$ which are non zero just in region of the grain boundaries and the local free energy density which has higher values compared to the interior regions of the grain. According to Cahn and Hilliard (see Ref. 15 for example), the energy σ_{gb} of flat grain-boundary among orientation i & j ($i \neq j$) described as:

$$\sigma_{gb} = \int_{-\infty}^{+\infty} [f_0(\eta_i, \eta_j) - f_{\min} + \frac{k_i}{2} \left(\frac{d\eta_i}{dx}\right)^2 + \frac{k_j}{2} \left(\frac{d\eta_j}{dx}\right)^2] dx ,$$

Where f_{\min} is the local free energy density in the interior regions of the grain. Note that the grain-boundary energy, thus, is nothing but the extra free energy of in-homogeneous systems than a homogeneous system with an equilibrium value of either η_i or η_j . For a given f_0 , the boundary energy and thickness vary with k_i and k_j . The smaller the k_i and k_j , thinner is the boundary region, and smaller is boundaries between different grains.

In Fig.3.10 we show the grain boundary energy (calculated using the expression below) as a component of time for the flat boundary using all the three discretizations listed in Table 3.1. From the figure unmistakably the grain boundary energy stabilizes within the first 200 time steps in all the three cases and to the same value.

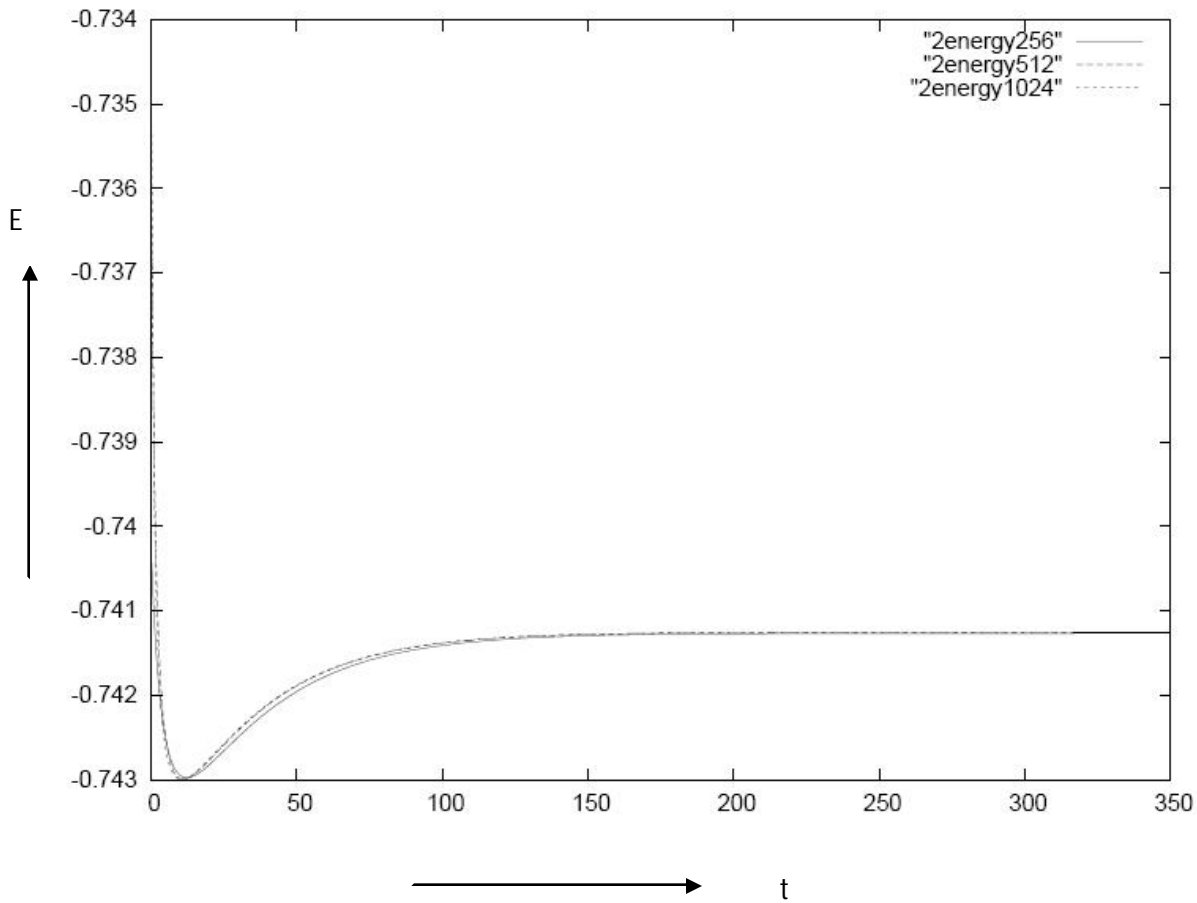


Fig.3.10. Graph of energy (E) versus time (t).

4. Conclusions

1. We have implemented a Fourier spectral code in C to do diffuse interface simulations of 2-D grain growth.
2. Our numerical simulations are in adequate responses along with some of available analytical results; for example, the growth is curvature.

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