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Phase field modeling; the materials science, mathematics and computational aspects

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Module No.18
Lecture No.73
Grain growth

Welcome grain growth is another problem which is also related to curvature effect, which is related to grain boundary energy, which is like any other interfacial energy except that it is an interfacial energy between the same phase, so why does the grain structure or grain boundaries come about? So we can understand it.

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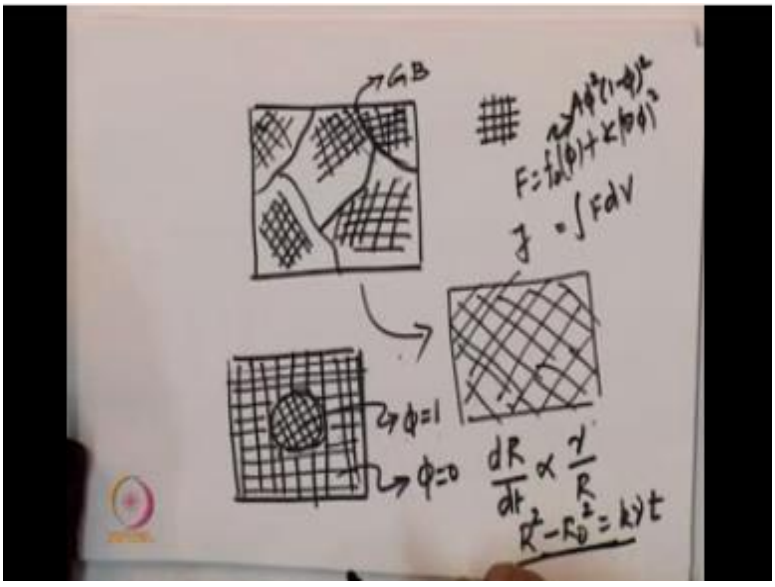

Suppose if you look at crystal, and let us say it is a cubic crystal, or let us take in two dimensional versions of its which is all squires, so you can think of taking a graph sheet, so suppose if you have different parts, of a system where the graph sheet is aligned in different ways right? So, this alignment is basically that I have this unit cells okay, different pieces of this is rotated in different angles.

So some of them could be for example you know like this, and this could be rotated by some angle, and let us say that then I would get that. So this kind of the orientation of the unit cell in different parts this happens because this could be a nuclei, which formed like this and it started blowing, another new clay formed like this and that started growing another nuclear form like this that started growing, so when they meet you can see that there, will be a mismatch.

These mismatched regions are what are known as grain boundaries, so the interface between two different orientations is known as a grain boundary, and there is an excess free energy associated with the grain boundary, this excess free energy the system can get rid of if all of these grain boundaries go away, and everywhere for example the system chooses one of these variants so the least energy state is of course a single crystal, which is oriented say like this.

So all the grains are oriented like this okay, so all unit cells if they become oriented like this then there are no these boundaries between differently oriented regions, so the system can get rid of the excess interfacial energy associated with the grain boundaries, so that is why grain growth happens, okay and it is possible to model as you can see the order parameter for modelling grain growth is non-conserved one, because they were one two three four five orientations here, all of it has become one orientation here.

And moreover because we are using periodic boundary conditions, I would like to start with a grain structure initial grain structure, which is also periodic. So to do that let me consider this particular case, let me say that I have a big rain, in which there is an embedded small grain okay.

So let us say that this grain has, orientation of the unit cells like this whereas the other grain has orientation like that. So this region is the grain boundary and that is the excess energy region, now I am going to represent this region by $\phi = 1$, and this region by $\phi = 0$, so we have

an order parameter to describe the microstructure, and it is known that the curvature and the interfacial energy is what decides, how this grain growth is going to take place? In fact one can show that the rate of change of the radius of this grain, is proportional to γ / R, okay.

So it is equal to some K γ / R, and if you integrate you will see that $R^2 - R_0^2$, k γ t, okay so this is the solution, so this is what we are going to, that means that this grain is going to shrink with time, and so that is what we want to see, so we have used the order parameter and I am going to use the free energy to be the same, like we used in the Alanson equation, so f 0 (ϕ) +s k $(\Delta\phi)^2$, so $\int$Fdv, is basically the free energy functional, and this f0(ϕ), I am going to take as a ϕ^2 1 - v^2 okay.

Why because there are only two grains, if there are many different orientations you need as many Arab order parameters as there are orientations, okay so we will look at the more generalized case, where let us say we have some five or six other parameters, like in this case but in that case then we have to solve using finite difference technique, because there is no periodic boundary condition. You know this orientation and that orientation do not match but if you want to use periodic boundary condition then we have to take the initial structure in such a way, that it is assistant with periodic boundary condition.

In any case so we have the order parameter, we have the free energy functional we know that we have to write the Alanson equation, and so except for the initial profile this problem is now the same as the one in which we were looking at the domain structure evolution in an order disorder system.

So I am going to take the 2d Alanson phosphate transform problem, that we solved in the last class, I am going to change the initial profile just I am going to make it is similar to the Connelly Hilliard case that we discussed, one circular grain embedded in the other grain and I want to see as time goes by what happens to this grain structure? Okay so let us go to the code.

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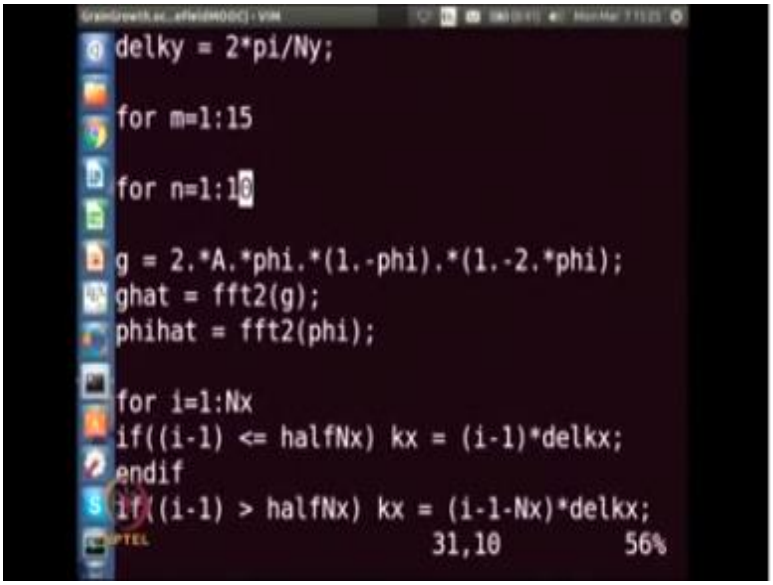

So I have copied the 2D ACFFT as grain growth, .OCT so we will do the same modification, so we will again look at 64 by 64 problem, because it is a form or easier and faster, and I am going to take this half and x half and y up here, so that it is easier for me to define the, so I am going to say if i - half NX *I - half NX k + J - half NY (j- half NY< R *R) then the ϕ is going to be 1, else if phi(i,j) = 0.

And if now I also need to define R, so let me define R to be a size 15, is equal to 15 okay, so we have defined the initial profile, which is circular profile, so it will plot this, and then it will proceed the evolution everything is the same, and it is going to keep plotting this composition everyone's in some number of time steps, so let us change that also so let us say that so let us make it something like 12 or 15 and every 10 steps once ok. So let us run this code okay.

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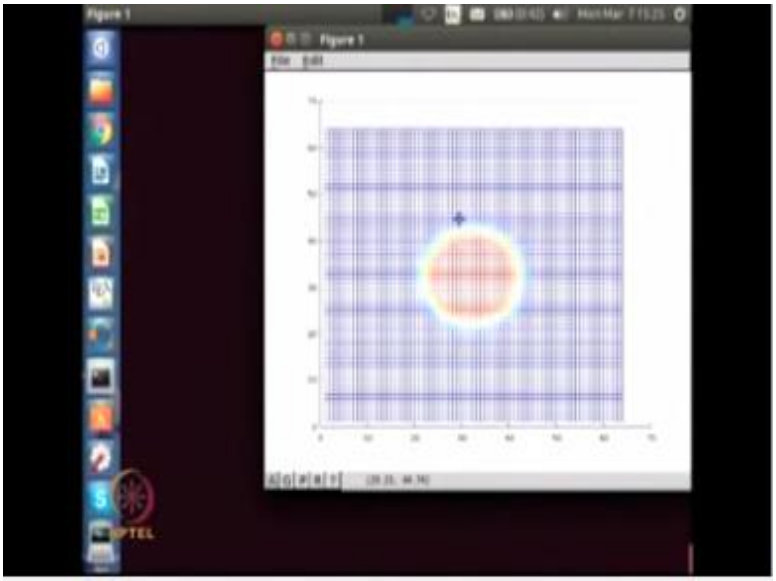

So I have an initial profile and you can see that an interface is set up and this precipitate is shrinking so every five time units ones I am plotting, and you can see in the micro structure that this is shrinking, because dr / dt is proportional to 1 / r.

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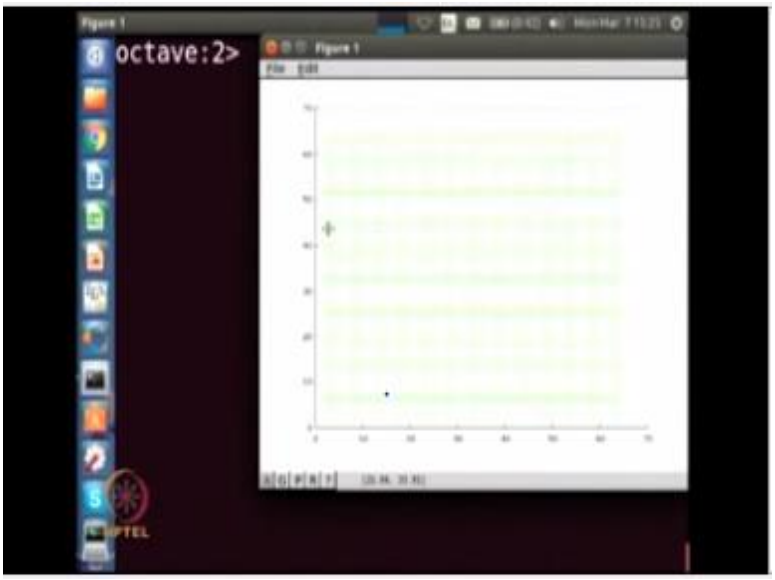

As the precipitate becomes smaller the shrinking also happens to be very fast, so let us run once more, so it is very beautiful so this keeps shrinking bigger precipitate takes longer to shrink,, and as it becomes smaller and smaller the shrinking rate is also high, because it goes as 1 / r so smaller r means faster growth rate or shrinking rate, and you see that it disappears.

So this is what the grain growth is. So we can actually also look at the quantitative information so we can look at the size of this shrinking grain. as a function of time square it plot it as a function of time then if the analytical result is correct. And if the phase field model captures the analytical result then that r squared versus T curve will be a straight line. R 2- R_0^2/ T.

So by looking at the slope of that curve, then we can determine the constant and in fact because we know that it is proportional to interfacial energy, we know how to calculate the interventional energy, so we can even identify what that constant is and compare it with the available analytical solutions.

So we have looked at two cases, one is based on Cornelia equation the other one is based on khan Alan equation, both of them are related to what is known as capillary effect or interfacial energy effect, in both cases it is the curvature of the interface that plays a key role

in the micro structural evolution, in both cases the phase field model is able to capture what is known from other analytical results in the case of con Hilliard for example.

I showed you that the change in composition that we measure from our numerical simulations is what you would expect from an analytical study, so it tells us that the phase field equations in the proper limit give us the proper sharp interface solutions, and in the case of grain growth also it is possible to study this in a more quantitative manner we will not do it, so I am leaving it as a tutorial.

So you can take the script you can identify where the interfaces, you can calculate the diameter of the precipitate at various times, for and hence the radius and you can square it you can plot R^2-R_0^2 as a function of time, and look at how the curve looks like, so that is a tutorial or an exercise problem, and we will go look at a more general grain growth scenario sometime later in the course because that means solving.

So till now we have been solving only one equation so, solving real grain growth problem or grain growth problem which looks similar to what it looks in real life would mean, taking large number of equations and solving them and so that can become a little bit problematic if you are doing it using octaves, so it is better to do that using C program or something.

But we will at least look at a case where there is more than one grain, them in more than two grains so we will look at this on 34 grain scenario, so we can we can do that sometime later towards the end of this course, so now that we have shown the phase field equations and how they can capture some of the interesting physics like the assumption or grain growth or spin or decomposition or order disorder domain evolution etcetera.

We can also go look at slightly more complicated scenarios, and how the micro structural evolution is captured by phase field model, so that is what we will do for the rest of this course so from this point onwards all that we are going to do is to make the equations more complicated or solve more than one equation, or have more sort of nonlinear interaction between equations are make the evolution equation more complicated, so most of the core of faithful modelling is already over, so we are going to look at more complex scenarios and how they help us model the microstructure, so that is what we will do in the rest of this course thank you.

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