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

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Module No.21
Lecture No.79
Grain boundary grooving II

Welcome we are modeling the grain boundary grooving problem so we have seen the free energy, we have seen the initial microstructure that we need to construct and we have seen the evolution equations so here is a octave script that does this problem so as usual we start with clear all clc and clf so to clear everything from the memory figure and so on more is off so that when the microstructure becomes available it will be immediately plotted.

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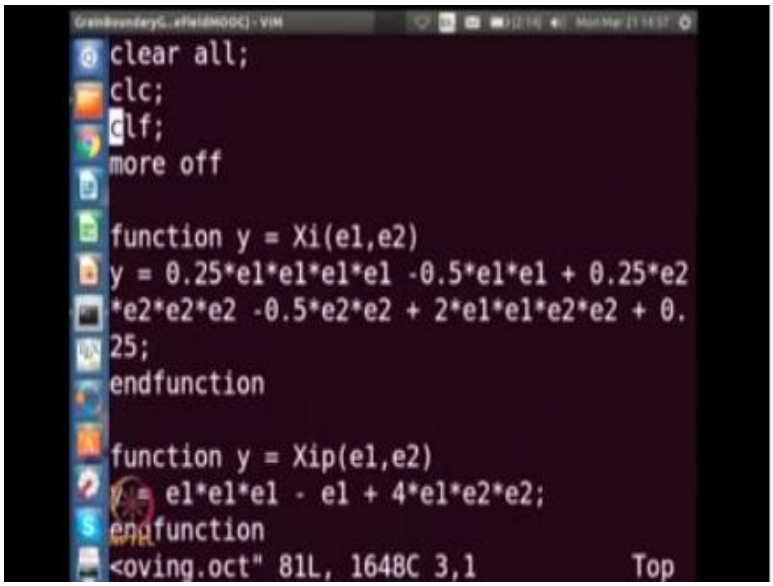

We define this function Xi, Xi has e1 e2 values and we saw that it is $\eta 1^2$ or phi $1^2/4$ - phi $1^2/2$ so that is why it is 0.2 and 0.5 and similarly $phi2^2/4 – phi2^2/2 + 2\ phi1^2\ phi2^2$ +0.25 so this is what we defined the Xi function as so that is what I have implemented. Now when we take the variational derivative with respect phi1 or phi2, then we also need the variation the derivative of this function with respect to either phi 1 or phi 2 but this function is symmetric in phi1 and phi2.

So we can manage to do the calculation with just one function so this is what this Xi prime basically is so if you differentiate this for example this is power 4 so 4 will come four times 0.25 is going to become 1 and this is e1 cube so that is this minus similarly 2 will come that is 1 and e 1 plus in this case so $e1^2$ so that will become 4 e1 $e2^2$ and if you differentiate with respect to e2 you have to just flip the variables here, you have to call this as e2 and this as e1 then you will get it $e2^3$ - e2 + 4 e1 $e2^2$.

So that way this function can do both the derivatives then I have defined the kappa c kappa phi1 kappa phi 2 like I said kappa c is 1 kappa phi 1 v 2 are one-third and the constant Z A B is that they are all one and we are going to do it on a 64 x 64 mesh with dx as one. So, I is first need to define the three variable C phi 1 phi 2, so they are all initially assumed to be 0 then I go to the

each point in the domain and if the first quarter or the fourth quarter, if I am there then I am going to make C to be 1 because that is where the solid is.

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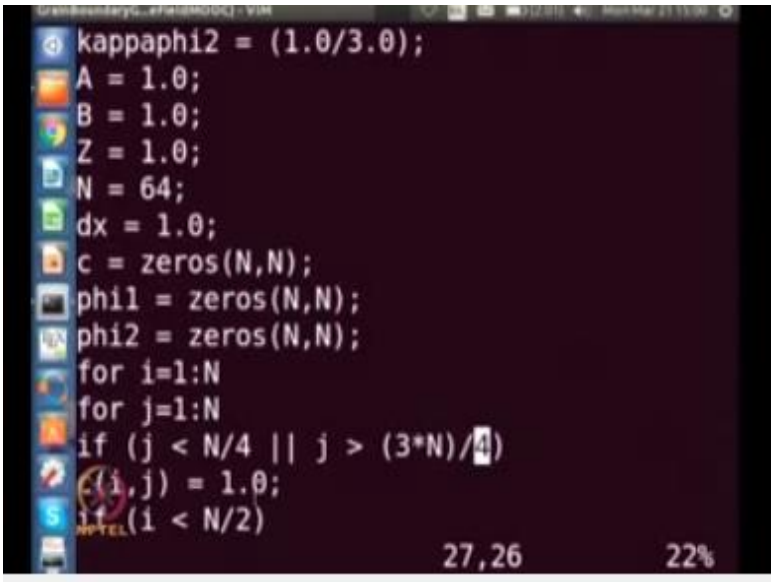

The central half is basically the vapor where C will continue to be 0, phi 1 phi 2 will continue to be 0, so wherever this C is one now half of it I will assume phi 1 is 1 and the other half I will assume phi 2 to be one okay, so if you end all these if conditions and at the for loop you basically have micro structure in which the central half is vapor and the first quarter and the last quarter or basically the solid.

In the solid that there are two grains one half is grain one the other half is grain to with periodic boundary condition then you have three grain boundaries that are available okay, so this is the initial condition of course we are going to plot it using mesh command it is sufficient just to look at the composition profile, because wherever composition profile is one the phi is going to be one either phi 1 or phi 2, wherever it is zero phi' are also going to be zero.

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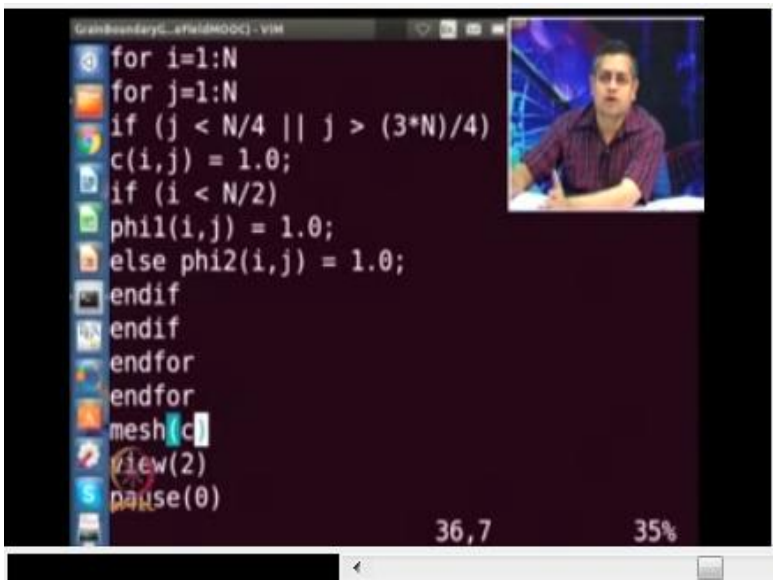

So if you just can plot composition you can look at the structure so that is what we are going to do and view 2 is to look down upon the microstructure so it is perpendicular or the projection of the surface of composition onto the plane and the past zero is to make sure that it goes to the next figure when the plotting happens, okay. So of course we have to define the periodic boundary condition because we are you going to use the spectral technique so half n and del K all those have to be defined.

I have not defined the l1 l2 and the m the mobility and the relaxation parameters because they are all one so I haven't explicitly introduced them here but one can introduce them and make them equal to one and you will get the same results. So these are the time loops or so first time loop runs from 1 to 50 the inner loop is to make sure that after every two time steps we plot the microstructure.

So that is why that is there and then we start the j, k loop which is for every mesh point and I have to define a gc and you can see gc is nothing but 2* A*C (1-c)*(1-2) + plus 2*B*c times this is I function minus 2 times that times 1-T times the Xi function and then you have I think I have

made a mistake here, this should be Xi function sorry there is no Xi function so 2 z(1-T) times because it is phi 1^2 phi2^2 + phi2^2 so it is phi2^2 + phi2^2.

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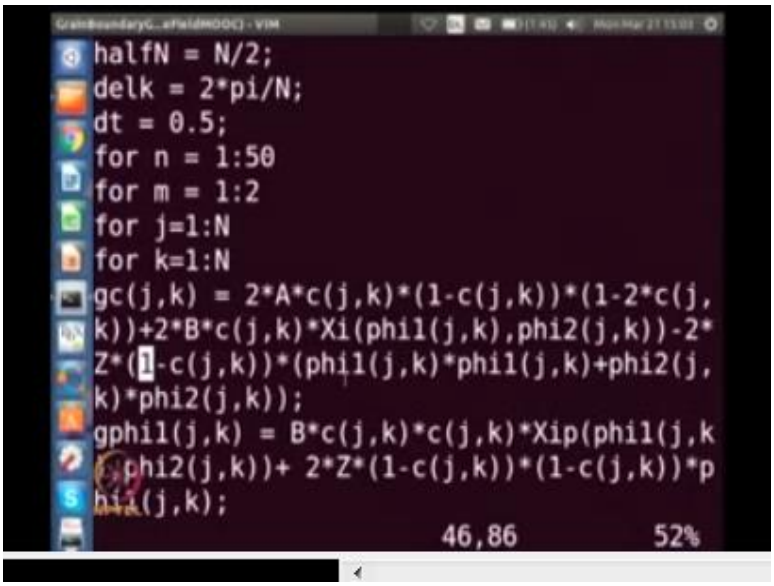

So that is the Gf c and G phi 1 and G phi 2 you can see, so the first one $Ac^2(1-c)^2$ does not have any phi term, so that does not appear Bc^2 and then Xi Prime this is differentiation with respect to phi 1, So phi 1 is first and phi 2 is next + $2Z(1-c)^2$ times of phi 1 similarly phi 2 will be Bc^2 Xi prime but with respect to phi 2 So phi 2 is first and phi 1 is next and 2 $z(1-c^2)$times of phi 2,so this is the basically the G functions, once I have the g function I Fourier transform composition and the phi 1 phi 2 to the Fourier space and the other parameters are also fully transformed and then we implement the periodic boundary condition here.

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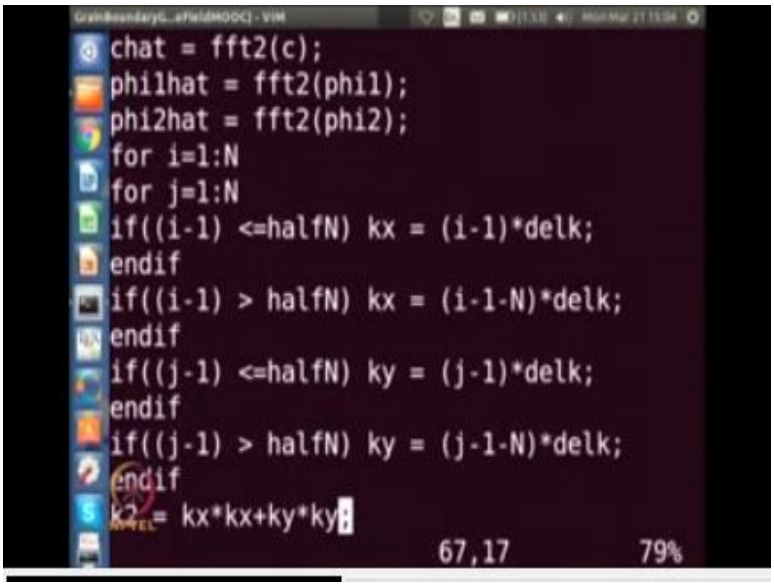

And we evolve so the c evolution is by the carnelian equation so that is why there is a k4 and k2 here and the phi 1 phi 2 to evolution is Alarcon so there is no k 2 here and there is a k 2 in the denominator instead of k 4. So once you do this of course after every time this is done you need to take c phi 1 phi2 to the real space so that the G's can be calculated in real space and then they can be Fourier transform for the next step.

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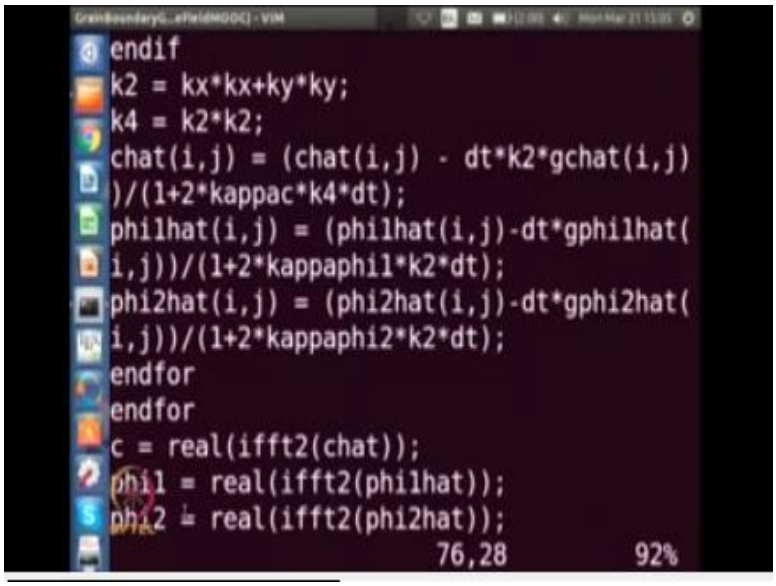

And after every one of these two steps it is going to plot the composition profile and then the final end for is for the complete time loop, so this is a code in which we have now implemented the equation that we have seen so we have a free energy in terms of c phi 1 phi2 and we have written down the evolution equation for them and we have taken the appropriate boundary condition.

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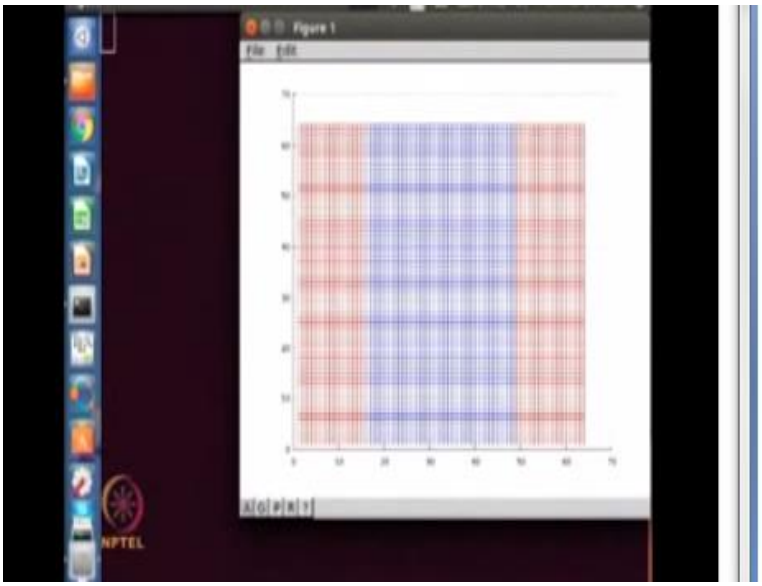

So now if we run this code we will get the microstructure to grow okay, so I octave and then I say source grain boundary grooving dot Oct okay, so you can see that this microstructure has this red which is 1 this red is 1 and this is the vapor and initially there was no this colored portion, because there was no interface but now an interface has formed and because this is the half portion it has to start grooving here and you can already see some hint of grooving here of course it is also going to groove at these two points because that is another boundary that we have.

So slowly this is going to develop a groove, so it is going to have a groove here it will come it will have a groove here it will go and then it will have a groove here, so that is what this structure is going to be you can see already that it is developing the grooves and here also you can see an hint of a groove. In this projection it does not look very clearly but after this 100 time steps are run when the groove is big enough of course we will change the projection and look at the grooving, but one can see that what was very flat developed these kind of curved regions to make sure that the grain boundary energy here balances the resolved boundary energies in this direction.

Okay so that is the primary reason why grain boundary growing happens and you can see that the grooves are developing here okay. So as you can see I think now it is much clearer, so we had a straight boundary and that boundary now has so in 3d suppose if you had the structure so this would have been in the third dimension so it will be like a channel, that that would have run through so we can see that we will see that channel structure by rotating it and looking at the channel structure.

So there are analytical solutions about the shape of the groove and what Rajdeep had shown in his thesis is that this profile that you generate using the faithful model, actually matches with the analytical group profile or group structure that has been formed by Mullins so, so all these details are available in Rajdeep thesis so we are basically trying to do the calculation from his thesis so now that the calculation is done let us take the structure and look at how it looks okay.

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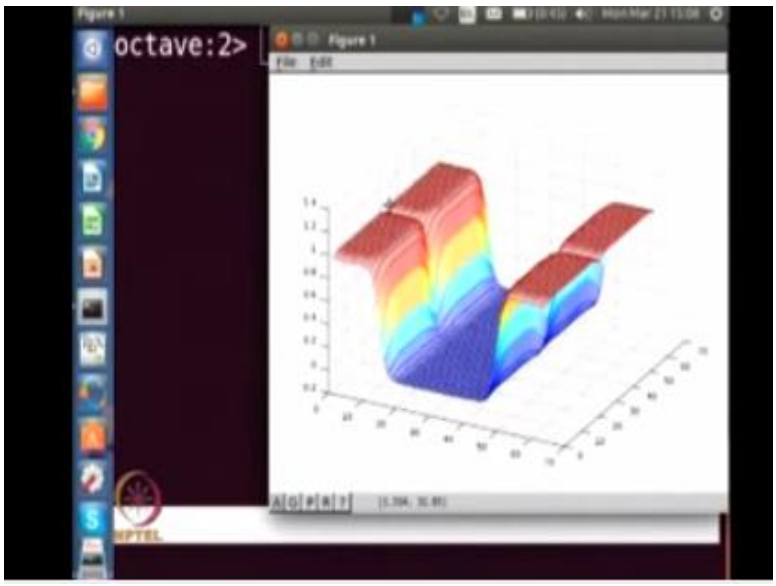

So as you can see this is the rule okay and this is the other group and the decomposition profile contours clearly show how the group structure looks like, so in color it's very nicely visible so one can see that this is the red line and this is the yellow line and this is the blue line etcetera. So this is basically the grain boundary go, so you have a solid this is vapor this is basically a

reflection of the same thing for periodic boundary condition and in this solid because this is one grain and this is another grain the region between the grain as you can see develops a group so, so for example from here it is very clear what the groove is? So it is a groove like that and here also it is a groove like that, so there is a small dip in the structure and that is basically the grain boundary.

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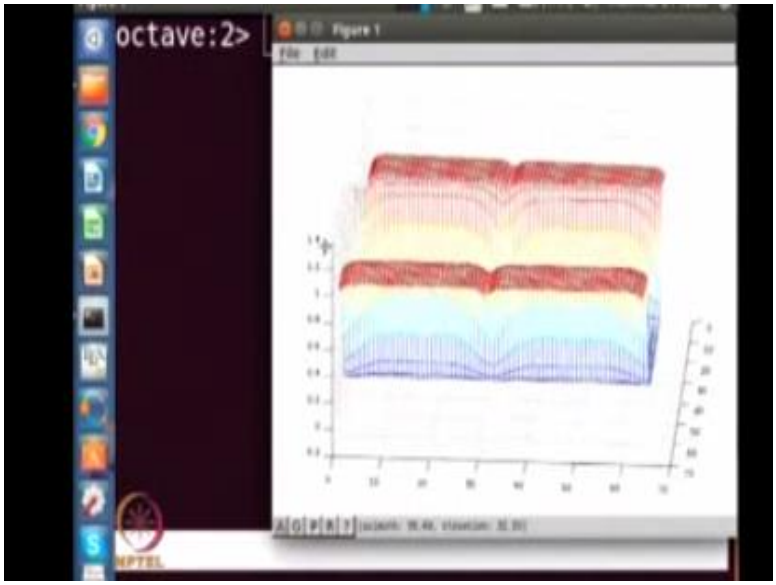

So by using such a simple model and rather simple implementation one can generate structures like this. So to summarize any given problem which is related to microstructures one can describe using order parameters and in terms of those order parameters and their gradients if we can write the free energy we can also look at their time evolution. So, and that time evolution of microstructures is very important and interesting because this is what helps us to study many many phenomena that happens in materials.

But there is one more code of this type that can be written which is for example for the solidification scenario when solidification happens when the boundary breaks up as a dendritic solid that comes about in an under cooled melt when the solid is growing so it also involves to order parameters one is related to energy so that is like a corn Hilliard equation but typically the

evolution equation is written in terms of temperature and that is not conserved, so that is one equation the other equation is of course solid liquid conversion.

So if you can write this phase transformation, if you can describe this phase transformation microstructure using an order parameter phi and if you can use the temperature order parameter and then you can couple them appropriately then you can actually get the solidification problem also studied, so we will use this gratification problem as one of the tutorials to look at how the microstructure evolves during dendritic solidification and we haven't done that as part of this course, because we have been looking at solid phase transformations primarily.

The phase field models that are related to solidification or slightly different in their philosophy or in their flavor as we will see in the next part in the next lecture but, but in terms of numerical implementation and in terms of the way the equations look they are not very different so one can do that also but the theoretical underpinnings are very different. So I am not going to go into those details that are the reason why I am not doing that problem as part of this course.

But as an extra tutorial or exercise it is a good idea to do that problem also so, so this brings us sort of to the end of the application section of the course so we have looked at many many different micro structural features and how they can be modeled using phase field models and what are the steps involved in developing the model and in doing a numerical implementation. With a very small computational power laptop which runs octave we are able to get lots of interesting microstructures plot them and see them and get a feel for what is happening.

So that brings us to the end of this problem namely grain boundary grooving modeling so there are lots of tutorials that are possible in this part of the code so, for example the free energy structure plotting the free energies and looking at it and plotting the profile of the interface and looking at it and comparing it with the analytical profile so there are plenty of things that one can do and we will do some of it as part of the tutorial and which will bring us to the end of the course on the applications of phase field modeling. Thank you.

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