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

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Module No.20
Lecture No.77
Grain growth:
Fan-Chen model II

Welcome back we are looking at Fan-Chen grain growth model we are looking at the octave script for implementing this in a case where there are six different orientations we have had an initial random orientation for each side given and now we are into the evolution part of the code so there we had to define this partial derivative of the bulk free energy density with respect to H and that was called G so with respect to the I there is GI so because there are six variants are six different orientations we have six G so g1 for example.

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Is $-\eta 1 + \eta 1^3 + 2\eta 1$ times $\eta 2^2\ \eta 3^2\ \eta 4^2\ \eta 5^2\ \eta 6^2$ so it looks very complicated but it is very simple so when I say g2 then I have $-\eta 2 + \eta 2^3 + 2\ \eta\ 2 \times \eta\ 1^2\ \eta\ 2^2$ will be not there $3^2\ 4^2\ 5^2$ and 6^2 and so on so similarly we have G3 which is $-\ \eta\ 3 + \eta\ 3^3 + \eta\ 3^{3+}\ \eta\ 4^2\ \eta\ 5^2\ \eta 6^2$ and $-\eta 4 + \eta\ 4^{3+2}\ \eta\ 4\ \eta\ 1^2\ \eta\ 2^2\ \eta\ 3^2\ \eta\ 4^2\ \eta\ 5^2$ and $\eta\ 6^2$ and so on and so on so for 4 also and 5 also and for 6 also, so just to make sure that we have written the expression correctly it is $\eta\ 5 - \eta\ 5 + H\ 5^3 + \eta\ 5 \times 1^2\ 2^2\ 3^2 4^2 6^2$ + $-\ \eta\ 6 + \eta\ 6^3 + 2\ \eta 6 x 1^2 3^2 4^2 5^2$.

So now we have all the g's that we require of course we need to take them to the Fourier space so g 1 hat g2 hat etcetera up to g6 hat it is a 2d Fourier transform so we take this g’s and we take the you toss to the Fourier space η 123456 as soon a transform and we know the evolution equation so to implement it we first have to implement the periodic boundary condition.

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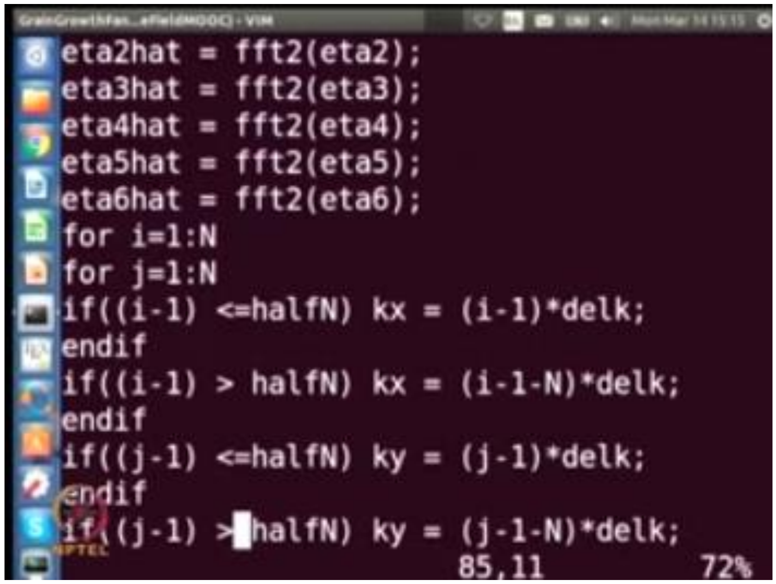

And calculate the k squared and now η1 and Fourier space is nothing but η 1- g δ T / 1 + 2κK ^{2} and L is one in both cases so I have not put it here but we can put It so we can make it L1 xDT /L 1 1into Cup our and it is the same in all cases so we are going to assume that l1l2 they are all the same but let us put it okay.

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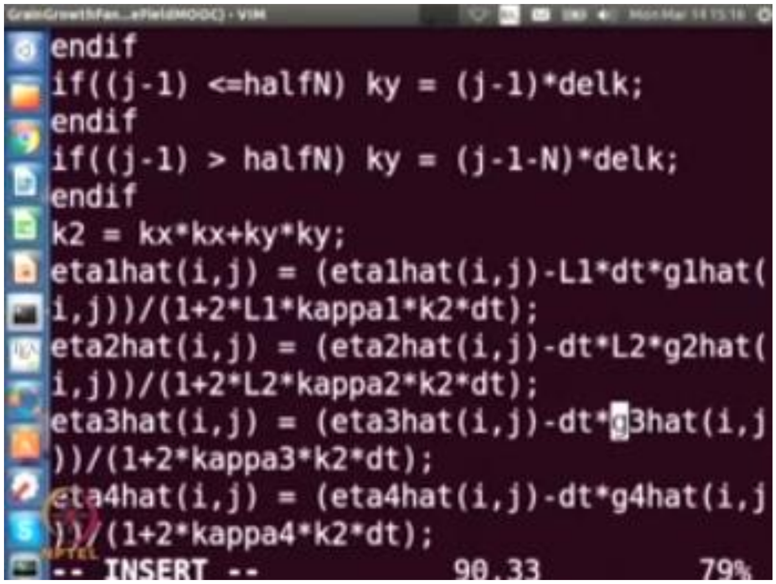

So this will become l3 into G hat / l 3 x κ this is l4 x κ 4 and this is l4 and this is l5xG hat / l5 xκ5 and finally this is l 6 okay, so this L is the only thing that is missing so we have put so this is consistent with whatever expression we have assumed and after that of course we have to take them all back.

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Into real space because the G start to be calculated in real space so after every two time steps again I am going to calculate this B and I am going to plot and then the outer loop is for the the other time unit so this will plot it so many times so this is the code.

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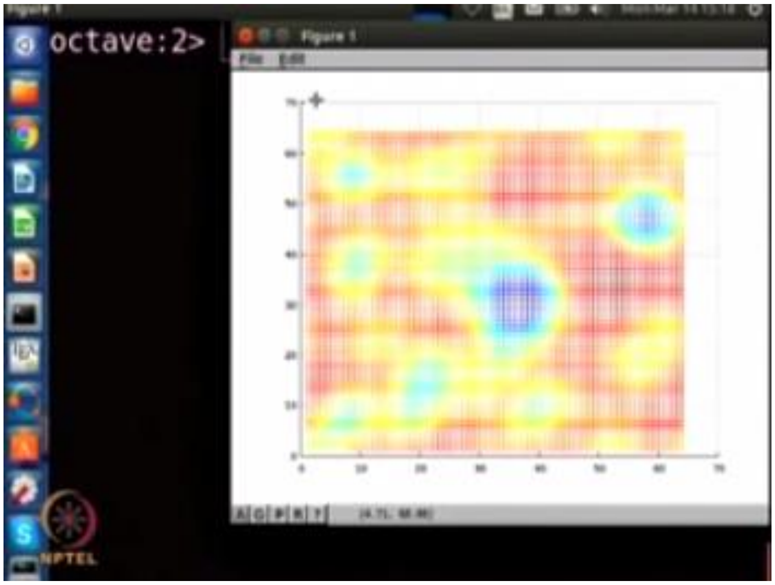

So let us go to octave and let us source this grain growth function dot Oct ok so of course initially everything is 0 because at every point except for one grain that star0 then it starts forming these grain structures the blue actually represents regions where the value of B has become zero which means that in these regions some grain is going to get one the rest are becoming zero so that is what the boundary structure that is developing so as far as I remember all these yellow and red or regions where you have the nonzero values.

So you can see that there is one grain that is developing here another one developing here probably one or two or developing here also okay so this is what is evolving so it was a very short amount of time in which we have gotten this.

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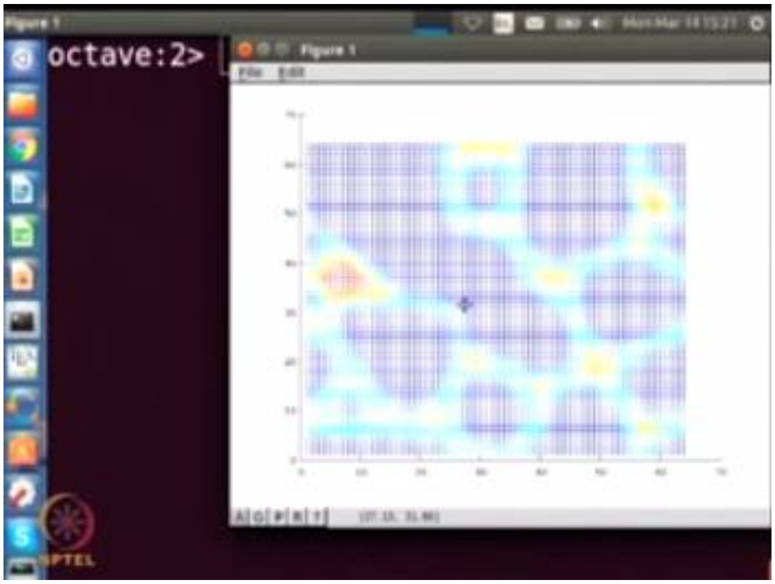

So we can run this code with a slightly longer time steps so that we can clearly see what is the kind of microstructure that is developing so let us make it five instead of two so every 2 and a half of time units once suppose we start plotting then what happens to the structure okay so it will take slightly longer than the previous code but it will start developing the structure initially everything is 0 so everything is almost like an interface and then there are regions where it starts becoming 0 and you can see that it is already consistent with periodic boundary condition this and this is the same this and this is the same and this and this is the same.

So it is doing that the evolution implicitly because of Fourier transform assumes periodic boundary condition and starts developing this kind of structure okay so this and this reminds the same grain and this is one more grain probably there is another grain that is coming up and between them okay, so this grain that came up now it is growing and because of periodic boundary conditions you know here also it is showing up okay and so that now is evolving so you can see lots of grains.

And between the blues if you see a boundary that means this is a different orientation this is a different orientation okay if not it will just become one single blue patch if it does not become that means that it actually shares grain boundary with the other region okay so that is what we are seeing so all this is one grain but this and this are different grains both are blue because some order parameter is one here rest are 0 summer order parameter is one here rest are 0 and the reason in between them is basically the boundary.

So we will actually look at which grain is one here and which grain is one here etcetera after this calculation completes but you can see the grain structure okay so this is a grain and because of periodic boundary condition this is part of this grain and these two are basically part of this grain and there is a grain boundary here so this is a grain this and this is a grain and this is a different grain and this is a different grain and this grade is different from this and this is basically part of this rate so one grain is becoming really big so this is here, here, here, and here okay and by periodic boundary condition actually this is also part of the same grain okay.

So this is the grain structure that now I have got now if you want to know what is the grain that is there in different parts of course you can say mesh η1 and view 2 okay so if you now go look at.

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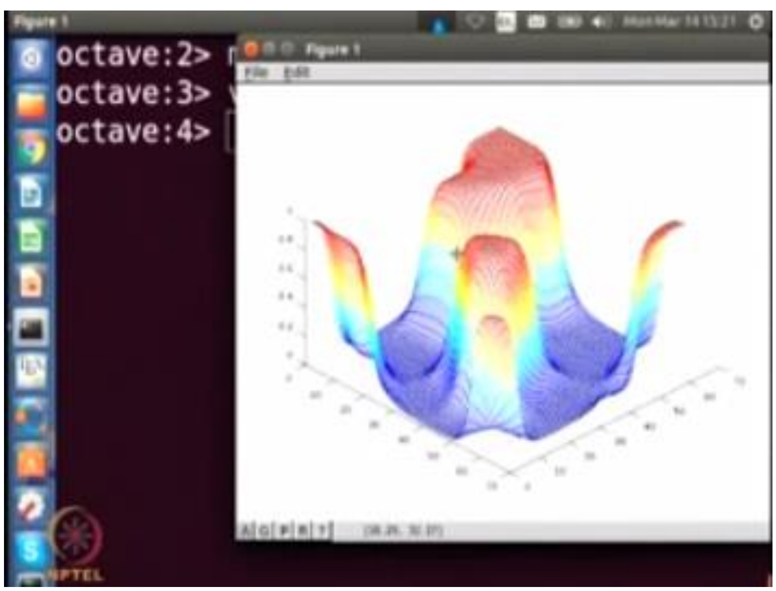

So now it is only η1 that is printed and you can rotate and zoom and you can see this structure so the grain one is there so this is all part of periodic boundary condition so it is the same rain and then there is another one oriented grain in the middle let us look at grain to where it is.

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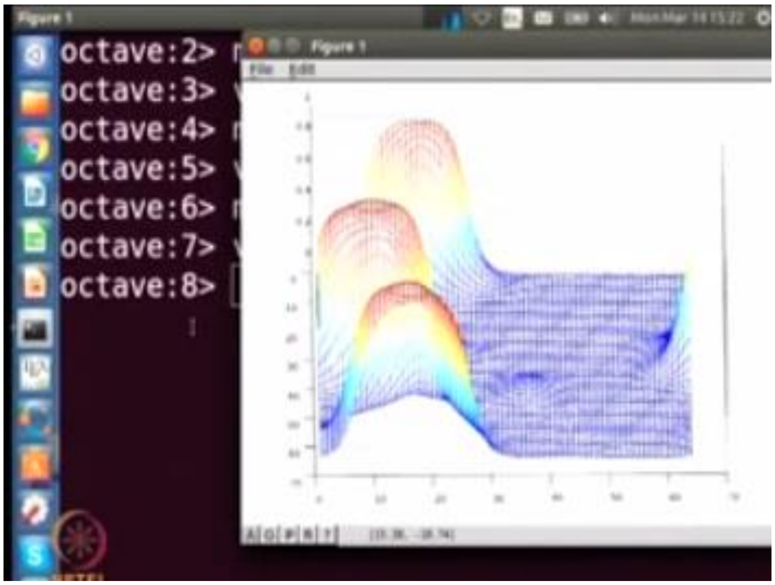

So Green two is this okay by periodic boundary condition this is the same but it has in two other places also okay so we can see that if you go to the 3d so you can see so these are the places where it is one rest of the places the η two is zero so that represents the regions where it is grain to so you can put η 3 and vo2 so to look at where it is grain three so these two grains are basically two three grain η equal to three grains and you can see this is already I mean consistent with periodic boundary condition this is slightly here and half of it is here and half of it is here.

So that you can see very neatly if you if you do go to the 3d right very beautifully seen here all right so now we can look at where it is η 4 and again this is very nice so this is one single grain for where the 4 is nonzero rest of the places 4 zero, so you can see this again is consistent with periodic boundary condition.

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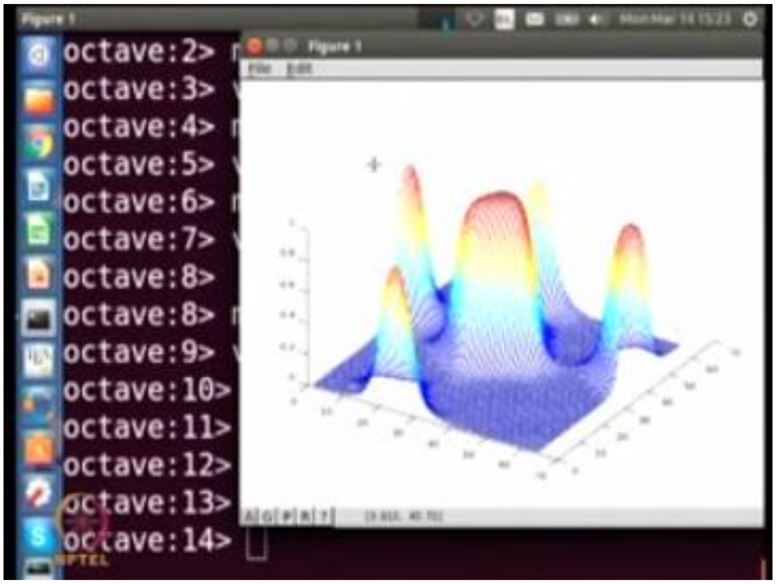

So let us plot η 5 and this is the grain with η = 5 and let us plot the last one I = 6 so η = 6 actually has one two three grains are there with η=6 okay, so now yeah so those are the this one this is basically the same this is basically same so those are the three places where this beat i equal to six is set so basically this entire region now we split up into it grains of orientation 1 2 3 4 5 6 etcetera which is what is seen when you plot this B.

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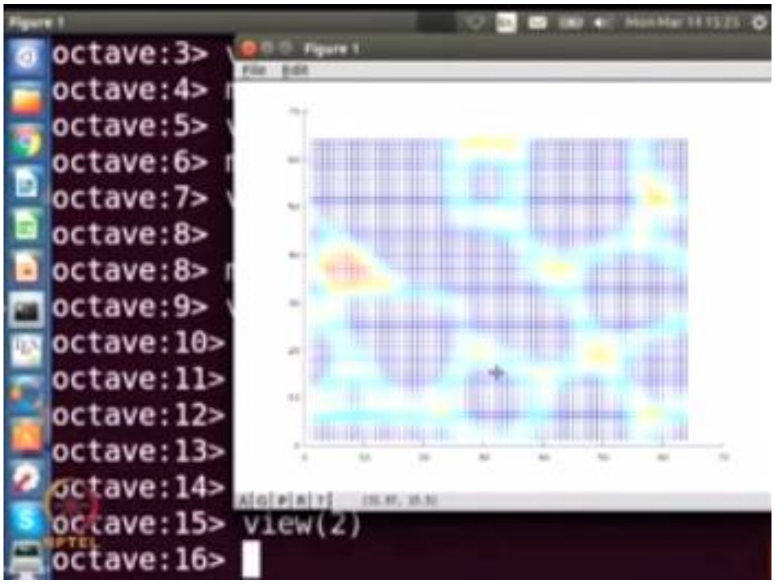

And let me make it view okay so it is very easy to see so there are these grains and each one is different orientation so there are many different ways in which you can plot these for example you can give a different color for example you can split this 0 2 256 into six parts and you can start giving colors to one as some say shade of red and 2 as some shade of blue and 3 as some shade of green and so on and so forth so you will also get microstructure which looks similar to this so called the orientation maps that one gets from EBSD.

That that you can get from plotting also but in this case I am interested in showing where the grain boundaries so these are all the boundary regions and this is again a region which has not completely become an to a single grain so either this or this is going to eat this up so that is what is going to happen after a while okay so these are regions which are like triple junctions so this is a different orientation this is a different orientation this is a different orientation so there is a region in between so this is a triple Junction.

Or maybe more than three there are about four of them meeting here and this is a triple Junction because there are three of them meeting here and so on and so forth so this is a model which describes the grain growth now this model is also nice in the sense that there are lots of things that are possible using this model, the first thing to notice is that we have assumed a very simple-minded model so from the material sides point of view one can say that different grain boundaries will have different growth kinetics different grain boundaries will have different interfacial energies or grain boundary energies and what type of interfacial energy they will have and what type of growth kinetics they will have will depend on not just that grains orientation but the orientation of the adjacent grain or adjacent grains.

So you can try to put that physics by try to come up with a free energy which will incorporate all this information okay so from a material science point of view this is a very simple-minded model there is things there are things that one can do to improve it and there are several models which have been there in the literature to do it this is nearly 20 years old model, the second thing is you see that whenever there is a grain one order parameter is unity rest of the order parameters are zero right so in that case there is not any evolution that is going to happen in that particular region.

So there are things that are possible to do numerically so you can write a code which will do calculations only wear more than one η is there or η is having a value between zero and one wherever the η is our one or zero in those regions you do not have to evolve the evolution equation this becomes very important because see we have just looked at to 6 orientations if you want to do proper statistics and if you want to evolve ending if you want to do it in three dimensions then you should be looking at large number of grains if you have large number of grains suppose you say thousand rains.

Then you are solving thousand equations and solving thousand equations and all the domain points suppose you are in 3ds like 512 cube and thousand equations is too costly but if suppose you say that this is bulk of the grain there is nothing that is going to happen here only the boundary is where I have to concentrate and then correspondingly your computational effort can be brought down so there are models or implementations which concentrate on this aspect okay so and the third one is of course related to the coding aspect because you want to write a code to which you want to say okay.

Let us take a case where there are now 12 orientation or 15 orientations now my code is written by assuming that there are six orientations and everything find accordingly so if you want to write a generic code which will generate a script which is meant for this particular case so then there are programming languages like Python for example or scripting languages like Coker said for example so it is possible to write a script to which you can say okay generate octave script which is meant for some 15 grains or 15orientations.

And then that code will actually generate the octave script which you can then run and do the calculation, so this is also true of most of the faithful models face while modeling when you are working with them and you are developing new phase field models there are mathematical aspects there are material science aspects there are programming aspects and there are numerical aspects and whatever we is your interest there is something to that interest that is relevant to faithful modeling.

So this is one of the reasons why I like phase fill modeling a lot because there is lots of things that can be done depending on your interest and your inclinations and grain growth problem is actually an ideal problem and in my opinion this is a problem which is still not solved that satisfactorily in the literature both from an experimental point of view are from a modeling point of view because we have some nice results in the ideal scenario in two dimensions and things like that but in actual 3d and in real solids there are lots of things that are happening which are eight to be captured in terms of grain growth models.

So this is in that way a nice model and as you can see six equations on a 64 / 64grid is not difficult so probably you can take the model and run it on a larger system and see or modify it to do maybe 10 or 12 orientations for example and look at microstructure so you can really generate nice-looking microstructures the other thing to do is to actually put different colors to different grain orientation so that involves figuring out how to give coloring scheme in octave it is possible to split the given color range into the number of grains.

And each orientation then is colored in a particular fashion if you do that then without all this boundary you can just look at the microstructure and say okay all these blues are one grain one orientation all these are second orientation and so on and so forth it is also possible and the ideal case should be that you take an experiment or microstructure read that information into the phase field model and evolve in the model and the wall the experimental microstructure and compare.

This is something that is attempted but not done satisfactorily as it so it is a more open-ended problem which is a kind of problem which is ideal to look at towards the end of this course so we are coming towards the end of this course and so it is a nice problem from that point of view to look at because there is so much that needs to be done using these models, so I will stop it at this point so we will look at a different problem which incorporates some elements of grain microstructure with two phase coexistence that we will do in the next lecture. Thank you.

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