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

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Module No.20
Lecture No.76
Grain growth:
Fan-Chen mode I

Welcome we are looking at the examples of how phase field models can be used to study micro structural evolution, we have looked at several cases in this lecture I want to go back to a problem that we looked at earlier for simplicity sake when we looked at the grain growth problem earlier we use the same Allen Cahn model with the same free energy and we looked at how a grain embedded inside another grain actually shrinks.

Now in most of the grain growth problems that is not the kind of microstructure that one encounters in the case of grain growth if you go take a look at a typical grain growth problem for example so, you will see lots of grains right, so if you if you look at the micro structure you will see lots of grains and so in our way of doing phase field modeling we need to describe this microstructure, now what does these grains represent? Each grain represents the orientation of the unit cell in that region with respect to some reference frame.

So you can take that reference frame to be the laboratory coordinate frame for example, so I have a reference frame and in this reference frame so i have a unit cells right, now this unit cell is

rotated in three dimensions so it requires some Euler angles or something like that to describe its orientation there are many different ways in which you can describe the orientation and suppose this is oriented this way right, so that is one of the grains and maybe so let us call that as orientation one.

Maybe there is another one which is oriented this way okay, so that is orientation to maybe another one which is oriented this way okay, so let us call it as orientation three so, like this if you have n different grain orientations you have to denote each one by a different number. So this is a micro structure in which we have about 12 different grain orientations now the order parameter that we use to describe this has to be then it can be thought of in two ways, one way is to think of η_i where i goes from 1 to 12 okay.

Now how do we define these order parameters in the i'th grain suppose if I am looking at the sixth the grain then $\eta_6 = 1$ the other η_i not equal to 6 are all zero okay, so similarly now η_7 will have in this region η_i7will be one the all the other η which is not equal to 7will be 0 and the interface between 6 and 7 is a region where η_7 will go from 1 to 0 and η_6 will go from 0 to 1, so this region is what is given by this so, in the bulk the corresponding order parameter will be unity rest of the order parameters will be 0 in the boundary depending on what the boundaries.

Suppose if it is a triple junction between 10, 7 and 6 so all $\eta_{10,}$ $\eta_{7,}$ η_6 are going to have non zero values at this point between10 and 7 only η10 and η_7 will be non zero the rest all will be zero. So the region where these order parameters take a value between 0 & 1 are the interface regions where they take value of unity is basically that particular orientation where they become 0 is a region where some other orientation exists. So we can think of these order parameters as representing the orientation of the crystallites with respect to some external frame of reference and that is how we describe.

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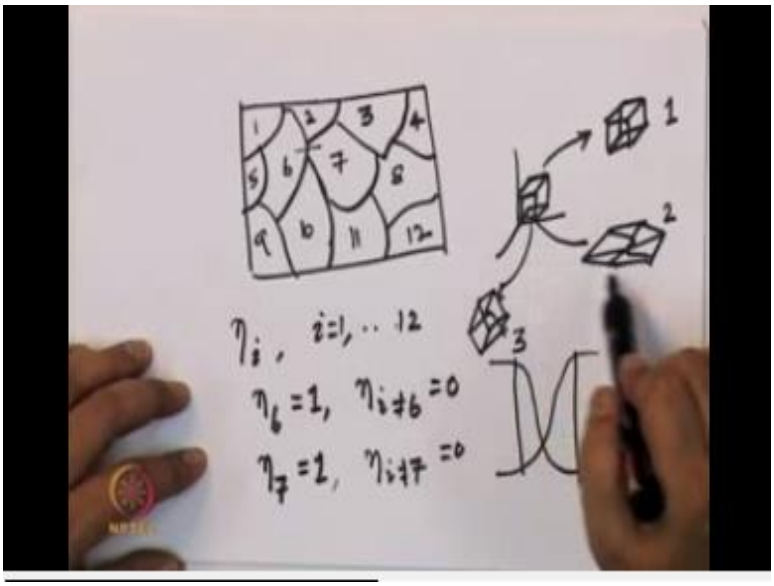

We can also think of vector order parameters I can think of a vector η which has 12 components 0 0 1 0 0 0etcetera 12 zeros if it has that would then corresponds to orientation η =3 okay, so we can consider this η_i as the order parameter which describes a microstructure as usual wherever there are gradients in η_i will be the reason where there is a grain boundary. Now we have to write a free energy that describes such a polycrystalline or grain microstructure.

We know that at the end for example out of all these 12 any one of the grains can actually eat up all the others and become a single orientation, all the 12 have the same energy in the single crystalline state because with respect to some external frame of reference we are describing them as η_1, η_2, η_3 etcetera, it can so happen that η_3 will survive or η_8 will survive or η_{12} will survive or η_{11} will survive which ever crystals that survive, finally if you go to a single crystalline state all of them should have the same energy.

It should not matter with respect to some arbitrary frame of reference how I am describing its orientation should not determine it's free energy, which means we need a free energy such that all the there should minima corresponding to each η okay, so we need minima for each η_i and the

free energy this is the bulk free energy density right, the bulk free energy density that is f_0 that you define should be the same for all we $\eta_{i.}$

So this is what will make sure that at the end suppose you end up with only one single grain it will have the same energy it does not matter which i survives, so we need to write this bulk free energy density so this becomes the first problem, so that there is the particular bulk free energy density which is given by Fan and Chen okay, this model was written sometime in 1996 or1997 so nearly about 20 years ago.

So Fan and Chen give a free energy bulk free energy density f_0 η_1 and $\eta 2$ etcetera up to $\eta_{p,}$ so if you have P orientations then their bulk free energy density looks like this $-\alpha$ so it is a sum over i $-\alpha \eta_i^2/2 + \beta \eta_i^4/4$ some runs from i equal to 1 to P and this alone is not sufficient you also need cross terms that is because we want to make sure that any one of the $\eta_,$ takes a value of 1 or -1 then the rest of them should be 0 for the minima, if we if you just leave with this then all these order parameters taking a value of 1will also be a minima, so we don't want that okay.

So we have this γ summation i = 1 to p; j not equal to i to p , η_i^2 $\eta j2$,so this is a bulk free energy density for appropriate choice of α, β and γ, we make sure that there are 2p minima and they are at η_i = +/-I, η_j not equal I = 0 okay, now we are going to restrict our η to be only on the positive side from 0 to 1 for example so that then we are going to get for a system with p order parameters P minima that is how we are going to achieve this okay.

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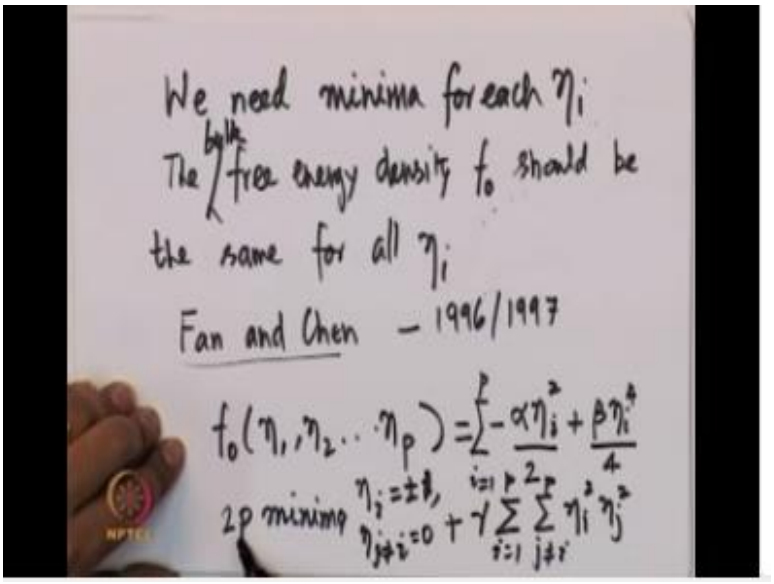

So these are 2 P minima are right for example if I take η_1 whether it is plus 1 or minus 1 rest of them 0 is a minima η_2 either plus 1or minus 1 with rest 0 is a minima and so on so that is how we get 2p minima and this is achieved for this function provided so there is a condition on the α, β and γ, provided that $\gamma > \beta/2$ so that is the constraint okay. Now the total free energy density of course once you have the required minima with the required property you can write the free energy density, because that is nothing but this f_0 which is a function of η_1, η_2 etcetera up to ηp + summation i $\kappa_i |\Delta \eta_i|^{2}$* dv.

So this is the free energy density so we have achieved the first aim namely to describe the thermodynamics of the system using the order parameters we have chosen and their gradients but this is a very very simple-minded model, because we are assuming that these η's represent of the order parameter it is not necessary that if you have two orientations the grain boundary energy between them and if you have two other orientations the grain boundary energy that you would have in that case need to be the same.

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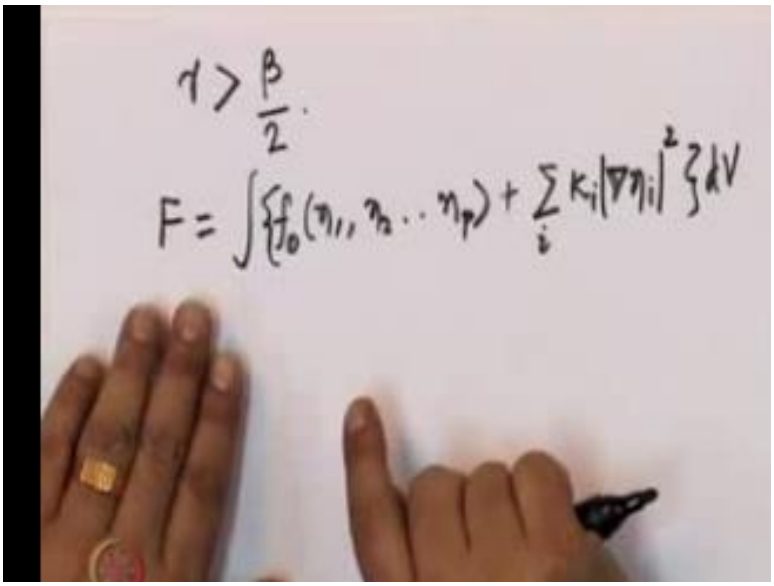

In other words this κ_i that we are assuming for the gradient coefficient actually might depend on what is so, so it here we have assumed that it just depends on the gradient for the particular order parameter it need not necessarily be so if suppose you have a grain boundary which is given like this let us say this is η_8 and so this is η_{11} for example, and so κ the might actually depend on eight and nine as compared to this suppose this is η_8 and this is η say 2 this κ 8, 2 need not be the same that is because if you go to a textbook like Porter register link you will see that the grain boundaries can be classified into many different types okay, one of them for classification for example describes grain boundaries as small angle grain boundaries and high angle grain boundaries okay.

But actually a grain boundary has five macroscopic degrees of freedom and there could be special orientations in which the grain boundary region will have perfect matching across planes so it will have very low energy those are known as CSL or coincidence site lattices at the boundary and so on and so forth so, if you actually look at the grain boundary energy for low angle boundaries it varies with the miss orientation as it is defined linearly and for higher angles there could be special places where it dips otherwise ,it just keeps as a constant .

So typical grain boundary energy as a function of the miss orientation θ is some function which looks like that okay, now this also should be consistent with the crystalline symmetry and all that so, we are going to make a very very simple-minded grain boundary a grain growth model in which we are going to assume that this coefficient depends only on the $\Delta \eta_i$ and in fact we are going to further assume that this κ is independent of five for any orientation, we are going to use the same κ.

Now that means that we are looking at something like a soap bubble captions not really a grain growth scenario okay so add the towards the end of this lecture we will discuss what kind of modifications need to be done for but for now we are going to assume that all κi are going to be the same and as usual we are going to use non dimensional values and, we are going to use unity for all κi.

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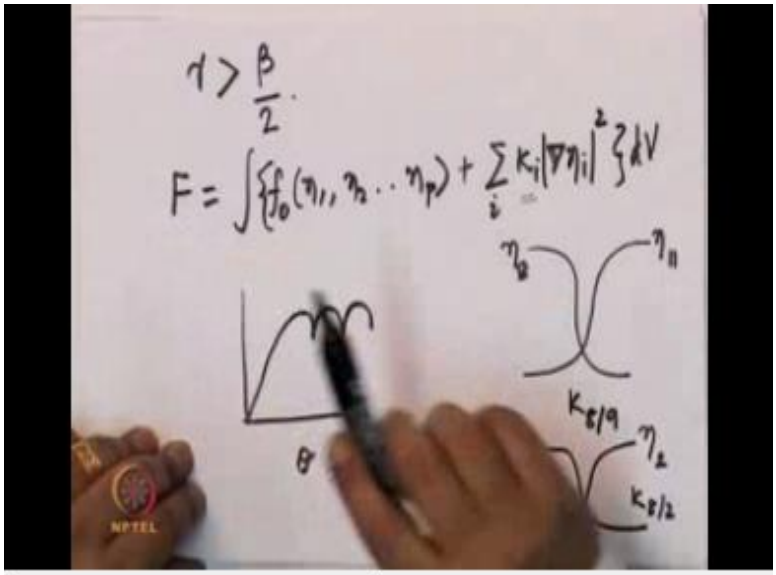

So we have described the microstructure in terms of order parameters and dev gradients, we have written a free energy in terms of the order parameters and their gradient sand so we can actually write the evolution equation so for each η we need to write an evolution equation and the evolution equation is something like this $\delta\eta_i/\delta t$ = -Li the growth rate of the different boundaries

could be different again this might depend on the other order parameter across which this grain boundary is formed again, we are going to assume a very simple minded all L irrespective I is the same and it has a value of 1,that I am going to assume $\delta f_0/\delta\eta_i$ because this equation is for $-\kappa_i\Delta^2\eta_i$ so it's $-2\ \kappa_i\Delta^2\eta_i$ so, this is what the equation is so i is equal to 1,2 etcetera to p.

So there are P equations and coupled equations because this term has all the η's in it is what is to be solved, so let us call this as g(i) and we are going to solve using periodic boundary conditions so $\delta\eta_i/\delta t = -Li$ g tilt i and $-2k^2$ this minus and this minus is going to be plus and so, Liκi so with and from the δ^2 we are going to get a $-k^2$ so, this remains as $-\eta_i\Delta$ and let us take this at time T plus delta T this being a non linear term I want to take it at time T this is gi at time T and so here we are going to say η_i tilt $t + \Delta t - \eta_i$ t/ $\Delta t = -$Ligi tilt t-2 Liκik^2 η_i tilt t+ Δt, so we are going to take this here and we are going to write η_i d tilt t + Δt is going to be η_i tilt t –Li Δt gi tilt t/1+2 Liκik^2 Δt right so, this is the evolution equation.

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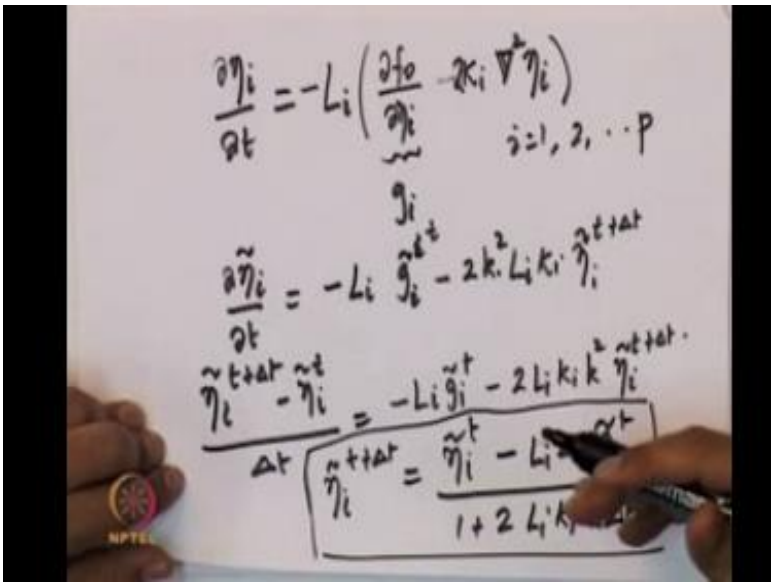

So we need to write an evolution equation for each one of the order parameters and then that code will then do the grain growth so to show how this works in the numerical implementation scenario i am going to assume that there are six different orientations and because, I am using

periodic boundary condition i also have to make sure that my initial profile is having this periodicity so, to make things easier so i am going to actually start with an initial profile which is something like this so i am going to take a domain we are going to do it in 2d and I am going to randomly pick these points and I am going to give a value between 1 and 6 so this could be it is like a six-sided die the time costing so, if it turns out to be 3 I'll call this as 3.

And next random so that turns out to be 5 i will call this as fine and the next grid point i will go and I will roll this die and then if I get to I will call this as 2 and so on so, I am going to take the initial domain to be given randomly any of these order parameters and that is the microstructure that i am going to evolve and see how this grain growth scenario works out okay, for doing this i have written the code as you will see that like the model that we have assumed the code is also very, very simple minded and there is lots of brute force used in solving this okay, so it is not very elegantly written but it is written in a very transparent manner okay.

So it is very easy to see what is happening in the code so that you can understand how the code works and we will discuss some of the issues that one might come across in solving a problem like this, now there is should also be a way to look at these micro structures that we are developing, of course if there are six orientations then I can look at okay orientation one where or where it is there so in someplace it will be nonzero it will be unity rest of the places that will be zero.

So that is grain one and then I need to go look at where $\eta 2$ is nonzero that will be the second grain and the rest of the region where it is 0 will be the other grain and so on so there is an easier way to actually look at the grain boundary which is what I used in the code and that depends on this idea right so we said that let us look at this grain structure suppose if I have a grain like.

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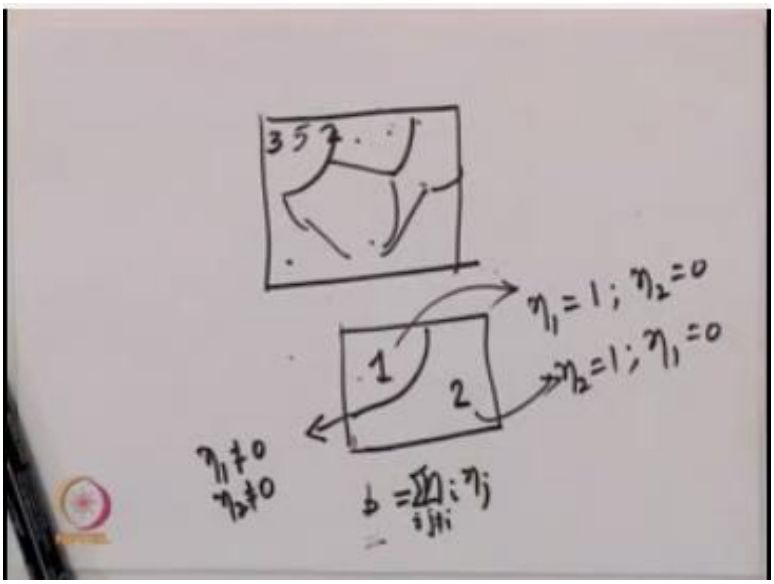

This and a grain like this I said that η 1 will be = 1 η2 will be 0 in this region and in this region η2 will be 1 η1 will be 0 and in the boundary region is where this boundary is where both η1 is not equal to 0η to not equal to 0 so what I am going to do is that I am going to define a function called the boundary function and this function is basically η_i η_j it is double summation i and another summation over j not equal to i now as you can see in the bulk all the other η are 0 so that is always going to give 0 and in this also.

For example in this region η2 will be 0 in this region η1 will be 0 so when you multiply ηj that quantity is going to give you 0 here but in this region where both are non zero it is going to give a non-zero value so if we plot this function then we will see that it becomes 0 in many places those are actually the grains and wherever it is non zero then those are the grain boundaries so this is a easier way to visualize the boundary structure of course it does not tell again the case for example that we are considering there are six different grains.

So it will it will give you something like this but it will not tell what is this grain what is this grain what is this grain what is this grain okay so that is not going to happen that is because this information does not worry about what is the grain it just lights up only the grain boundary so we

can see the grain boundary structure which means whatever is away from these boundaries are basically the grains. So to look at actually what this grain is then we have to start plotting η1 η2 η3 and see when this region becomes 1 rest of them become 0 so that will correspond to that particular grain okay so this is just a trick to visualize the grain boundary structure that I am going to use so as usual we go to the code so let me show you the code.

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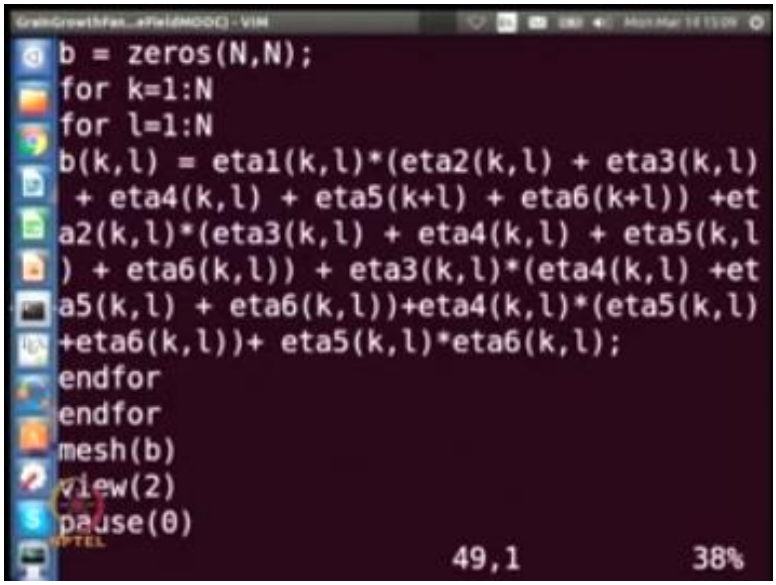

It is called grain growth function.oct after fan Chen who wrote this model so as usual we first say clear all the variables the figures everything and more off because I want to plot the microstructure as it is evolving and P is six because I have assumed that there are going to be six different orientations and so Kappa 1:6 I am assuming they are all 1 and L1:6 I am going to assume all of them to be one alpha is 1 beta is one gamma is one C gamma should be greater than half beta is one so half beta 0.5.

So gamma should be greater than that I have taken gamma to be one so this will have the required number of minimum and so I am going to do this on a 64 x 64 system again for simplicity shake I'm not distinguishing between x and y direction everything along x and y directions to be the same dx is the same as dy Nx is the same as NY and the first thing so this is a

new command probably that you have not seen till now so I am going to define a random number generator called unidrnd stands for discreet and uni stands for uniforms so it is going to generate a uniform discrete random number between 1 and 6.

That is what six stands for on a N by N matrix okay so which means so I have N by N points and for each point I have generated a random number that random number is going to be 1 or 2 or 3 or 4 or 5 or 6 okay now I have defined the six order parameters η1 η2 E η 3 etcetera to be 0 to start with then I go look at the Ø at a particular point if it is equal to 1 then I make eta1 to be 1 at that point that rest remains 0, if it is 2 then eta2 is 1 the rest are 0 and so on and so forth.

So this is basically the initial structure that I showed you this is how I generate the initial structure and the advantage with this initial structure is now I do not have to really worry about periodic boundary condition automatically as it evolves the system will make sure that there is periodic boundary condition, because the Fourier transform automatically implicitly assumes periodic boundary condition, okay.

Now this is the boundary function I said, so I define be to be 0 at all points initially and then I define so eta1 multiplied by 2,3,4,5,6 plus eta2 multiplying 3,4,5,6 right and then eta3 multiplying 4,5,6 then eta2 multiplied 5 and 6 and eta 5 multiplying eta 6 this is because when I am multiplying a eta2 for example I do not have to put eta1 because eta1 eta2 is already here okay, so boundary is defined as summation, double summation i and j not equal to i, okay so our j greater than i, in this case because we are going in order so you can do it like that so that is the B.

So now I plot the b and I save view2 so that I am looking down on this and pause(0) means it will pass for 0 seconds at that point and then it will plot the next one because we want to see a movie of how this evolution is happening, okay.

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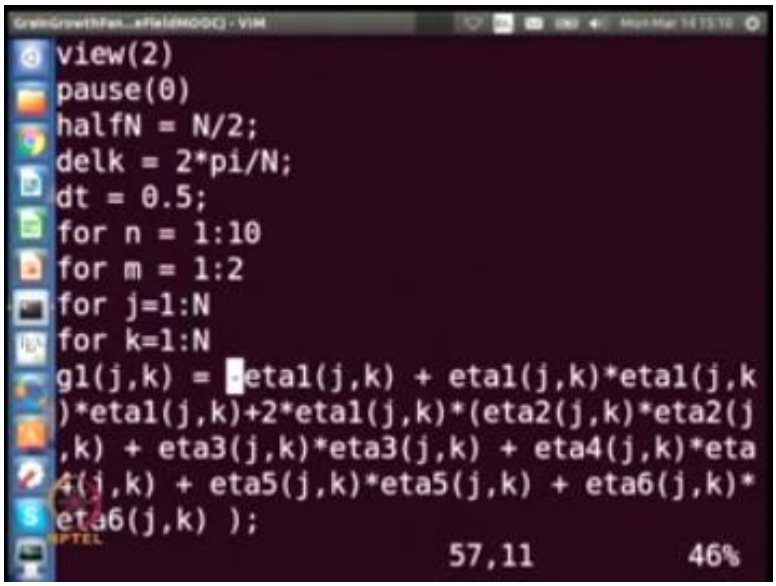

So of course halfN I have to define to define periodic boundary conditions halfN is N/2 and I have to define the grid spacing in the reciprocal space which is 2pi/N and I have to define the deltat and now so I am going to make this a little bit simpler so for n=1:10 m=1:2 let us say okay, so we are going to so the first and the second both our time loops but this time loop is there because after every two time steps which is after every time unit because dt is 0.5 so two time steps will make it two in 2*0.5 so one time unit I want to look at how the microstructure looks like okay.

So for i,j and k running from 1 to N I now have to generate this gi, gi $\delta(0)/\delta\text{eta}$ so what is that quantity we know what the free energy expression is a free energy expression is.

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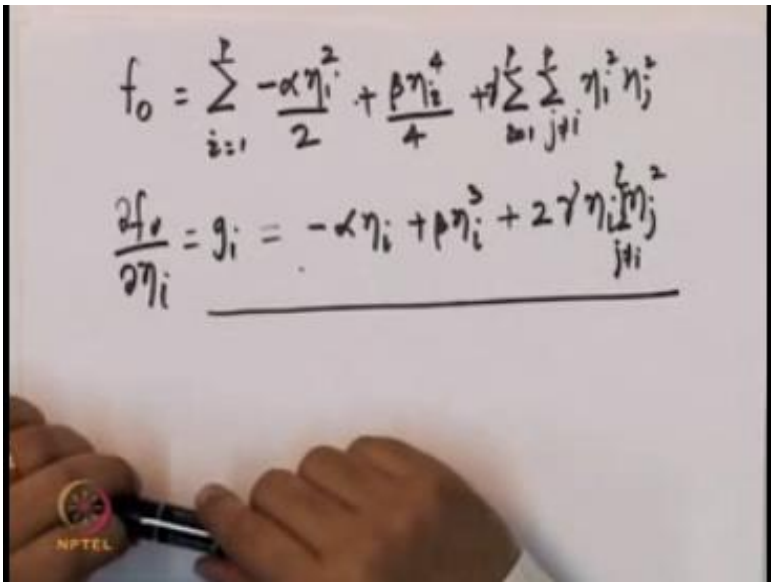

f_0 is nothing but Σi-$\alpha \eta i^2/2+\beta \eta i^4/4$+double Σ with γi 1 to P this is also 1 to P and j not equal to I to P ηi^2 ηj^2 so$\delta f_0/\delta \eta i$ which is called gi is to be now defined as you know 2 times $\alpha \eta i$ 2 and 2 will get cancelled so i will get -$\alpha \eta i$ and then 4 times $\beta \eta i^3$ 4 and 4 will get cancelled +$\beta \eta i^3$ and then in this because iI is the only one j is not equal to i so that I do not have to worry so it will become +$2\gamma \eta i \eta j^2$ whereas there is a summation over j not equal to i to P on ηj^2 so this is the gi, so that is what is implemented in this code, so we will take a break at this point and then we will go back and see how this implementation and the evolution implementation is done in the code, thank you.

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