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

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Module No.21
Lecture No.78
Grain boundary grooving I

Welcome we are looking at the applications and we are looking at how to use phase field models to model some of the micro structural features that one typically sees we have looked at spinodal we have looked at order domain growth we have looked at grain growth and so on, so the problem that we want to discuss today is what is known as grain boundary grooving. Now what is the grain boundary grooving, let us assume that I have a grain structure which means there are two grains and let us also suppose that this grain boundary separating these two phases is cutting the surface. But in a perpendicular manner it so it is like this.

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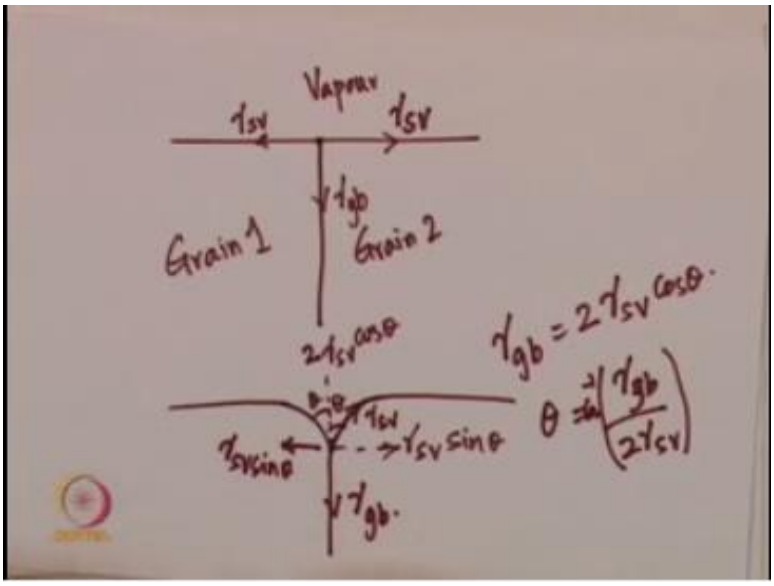

So I have surface and I have a grain boundary, so this is Grain1 and this is Grain2 and let us say that this is vapor, okay so there is no grain so we have a surface and that surface consists of two grains so this is a grain boundary and obviously this surface has an interfacial energy let me call that as γ_{sv} and similarly this has a γ_{sv} and this has γ_{gd}, now as one can see at this point there is an imbalance of forces because this γ_{sv} and this γ_{sv} can cancel out each other but this γgd is unbalanced, right so these interfacial energies can be thought of like surface tensions. Let us assume that they are they are all isotropic and no dependence on different grain boundaries for example the surface vapor energy and this grain boundary energy is also like some surface attention let us assume.

If you assume that then these forces need to balance, so to balance the forces the system is going to produce what is known as a grain boundary grew. So this is the perpendicular, so the grain boundary near this point is going to take a shape let us say that this angle is θ now this γ_{sv} will get split into two parts so it will be $\gamma_{sv} \cos\theta$ and there will be a $\gamma_{sv} \sin\theta$ component and so there will be another γ_{sv} suppose let us assume that this is a symmetric group then you will have $2\gamma_{sv} \cos\theta$ in the perpendicular direction and this is $\gamma_{sv} \sin\theta$.

Now this $2\gamma_{sv}\cos\theta$ can actually balance γ_{gb}, okay so γ_{gb} is $2\gamma_{sv}\cos\theta$ so the group angle θ is going to be $\gamma_{gb}/2\gamma_{sv}$ cos inverse, so it is going to go towards this structure and such a groove is known as a grain boundary groove. Now there are many different physical scenarios and many different reasons for grain boundary grooving for example, if the other phase is not vapor but it is a liquid what happens to the boundary group so they are also there will be grooving except that the energy that it will balance will be the liquid melt and the solid the surface energy, so γ_{sl} so $2\gamma_{sl}$ will what be balanced by the γ_{gb} so there will be a groove angle and grain boundaries also happen to be regions of fast diffusion so sometimes if there are liquids, liquids can go through the grain boundary and lead to other interesting effects.

The subtypes grain boundary grooving is also useful for example, if you put a sample which has a flat surface in the furnace for a while then all the grain boundary regions get grooved then it is easier to look at the grain structure and where the grain boundaries are because there are grooves where the grain boundary is so you can take it to a microscope and easily look at the micro structure using grain boundary group.

So typically we have to take a sample and you have to polish it after polishing you have to etch it so that the grain boundary regions are preferentially removed so you can see under a microscope easily the grain structure, so some samples typically some ceramics samples where it is very difficult to polish and things like that so grain boundary grooving could be a mechanism which is like equivalent of etching for metals and alloys to look at the grain boundary structure.

Now this is the system that we want to model a grain structure so you have two grains meeting at a flat surface with vapor at that point they are going to groove, so this is the structure that we want to model. So obviously, for the phase field model first we need to decide on how to describe this microstructure and we want to use Fourier transform technique to solve this problem so we are going to use the periodic boundary conditions so we need to come up with an initial profile which is periodic and then we are going to write the free energy from there we are going to derive the evolution equations and then we have got to solve the problems.

So that is what we want to do in this lecture, so now that this is the given geometry so let us find out how to model this using the phase field model. So for doing the phase field modeling I am going to assume that the microstructure that I am going to look at is looking like this.

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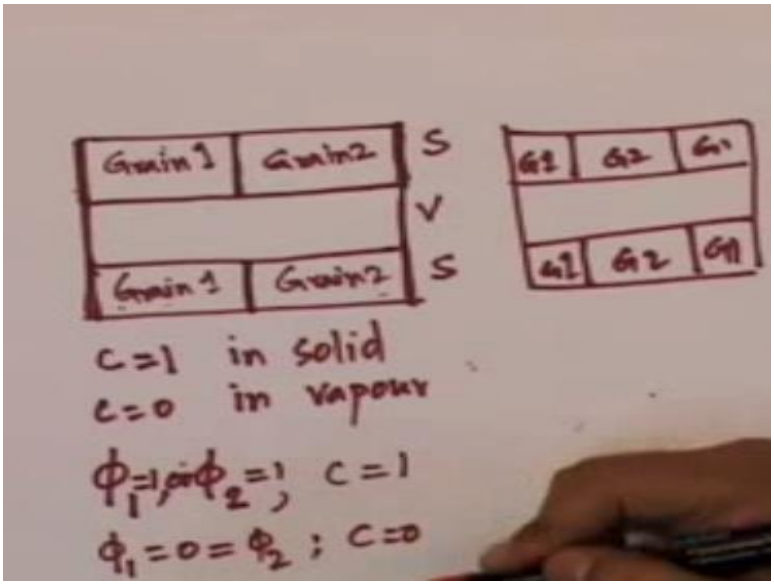

Remember that I need periodic boundary condition, so I am going to assume that this is solid and this is vapor and this is solid so I have solid here I have solid here by periodic boundary condition that is satisfied, okay. Now I am going to put a perpendicular boundary, I am going to put up a perpendicular boundary, now typically one might tend to think that there is only one grain boundary, right so I have Grain1 here I have Grain1 here and Grain2 here, so the periodic boundary condition here also satisfied Grain2 continues to Grain2, Grain1 continues to Grain1 so there is a grain boundary between them.

But this is not the only grain boundary because of periodic boundary condition because this is going to repeat here, so there is a grain boundary here because by periodic boundary condition Grain1 is sitting here so Grain1 and Grain2 so there is a boundary here there is another grain boundary here, okay. So there are in all three grain boundaries, okay this is the case for which we are going to write the code and solve the problem.

Of course as a tutorial for example, you can take the other geometry and try to solve the problem, so in terms of solid vapor solid it has the same structure and then we say that this is Grain1 and then this is Grain2 and this is Grain1 again. In this case you can manage with only two grain boundaries instead of three grain boundaries like we have here but effectively this is also only two grain boundaries because this and this is the same boundary by periodic boundary condition so we are dealing with two grain boundary case except that one of the boundary is split apart because of our periodic boundary condition.

Now if this is the structure, the initial structure that we are going to take now how do we describe this microstructure of course to describe this microstructure we need at least three order parameters so what are they I need a order parameter which is conserved order parameter, which is like C normalized in such a way that you know vapor will have very little of this material so C=1 in solid and C=0 in vapor this is the first order parameter.

The second and third order parameter of course all the ones which represent the grain structure so that means they will be ϕ_1 and ϕ_2. Now wherever ϕ_1 and ϕ_2 are there because they represent grain structures the minima should be such that ϕ_1 and ϕ_2 C=1, okay so that is either ϕ_1=1 and ϕ_2=1 means C=1 only ϕ1=0= ϕ_2 C=0 that is in vapor there is no grain orientation 1, there is no grain orientation 2 there is no composition, right so let me assume that this is like your copper for example there is very little of copper.

So i can say that 0 copper and no orientation 1, no orientation 2 that will be vapor and in Grain1 ϕ_1 will be 1 and because it is a solid C will be one but grain ϕ_2 will be 0 in grain two on the other hand Ø1 will be 0 Ø2 will be 1 C will be 1, so this is the order parameter that describes the microstructure, so if we say that this is the description then the job is to write a free energy functional which will have all these properties. This has been done this has been done in the group where I was doing my PhD more than once.

In fact the first thesis master's thesis on this on phase fill modeling in this country was written by one processor Breda Chatterjee he wrote it for the grain growth the grain boundary grooving

problem and later preserved Raj deep has solved this problem so we are going to use the free energy functional that is given by Raj deep by his PhD thesis they have taken into account all these minima and how the free energy should behave everything so our job becomes easier.

So what is the free energy functional that was used interms of the free energy structure what Sudip used and what Raja used they are not very different but we will go with what Raja used.

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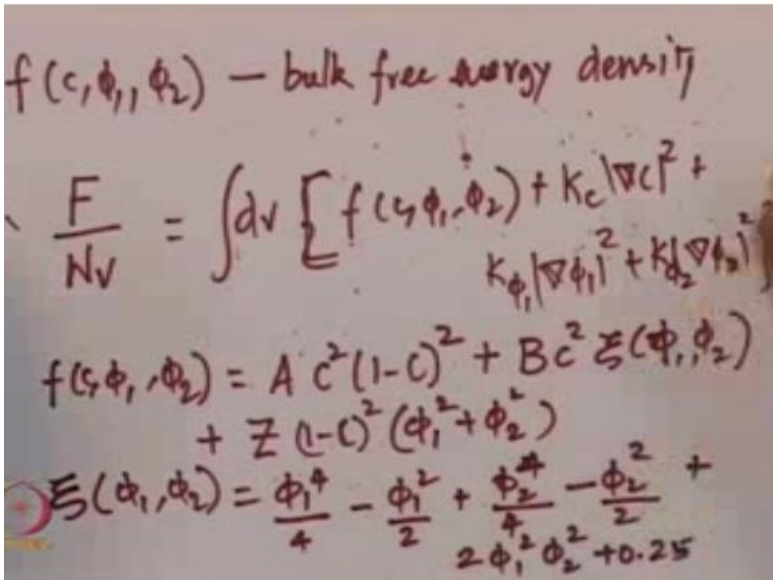

So the free energy now is a function of C Ø1 and Ø2 so this is the bulk free energy density right so we have this part which is the bulk free energy density and we need to give this F in such a way that it will obey all these conditions and the total free energy will be actually an integral over volume of f(C, Ø1, Ø2) + $k_C |\nabla_C|^2$ + K Ø1 $|\nabla$ Ø1$|^2$ + K $|$Ø2$|^2$ right so this is the total free energy for which we are going to write the eleven Allen Cahn equation.

Now what is the form of this F(C, Ø1 , Ø2) so that is what I want to describe now, has this structure $AC^2 (1-C)^2$ so this is going to make sure that there is a minima for c = 0 and there is a minimum for c = 1this we have been using for quite some time now to couple to make sure that

when C equal to 0 the minima also has Ø 1 and Ø 2 to be equal to 0 we are going to write the next part that is B C^2 and some functions I of Ø 1 and Ø 2, okay.

I will write down what this functions is plus some z times $1 – C^2$ so when c = 1 we want both Ø 1 and Ø 2 to have their value as one either Ø 1 or Ø2 to have their value as 1 so that that solid c = 1 will correspond to some orientation, so that coupling is taken care of by this $Ø 1^2 + Ø2^2$ okay, so now the only thing we need to describe is this function of Ø1, Ø2 of course this will have the required double well potential in terms of Ø1 and Ø4.

Ø2 so it is $Ø1^4/4 – Ø1^2/2 + Ø2^4/4 – Ø2^2/2 + 2\,Ø1^2\,Ø2^2 + 0.25$, okay and so now why is this the free energy that has all the required properties of course you can do the plotting of this free energy at the different cases and you can look at what happens to this free energy so that also we will do as a tutorial but for now we now have a free energy functional so once we have the free energy functional it is possible to develop the evolution equation. So to do that so let me write down the free energy expression incomplete.

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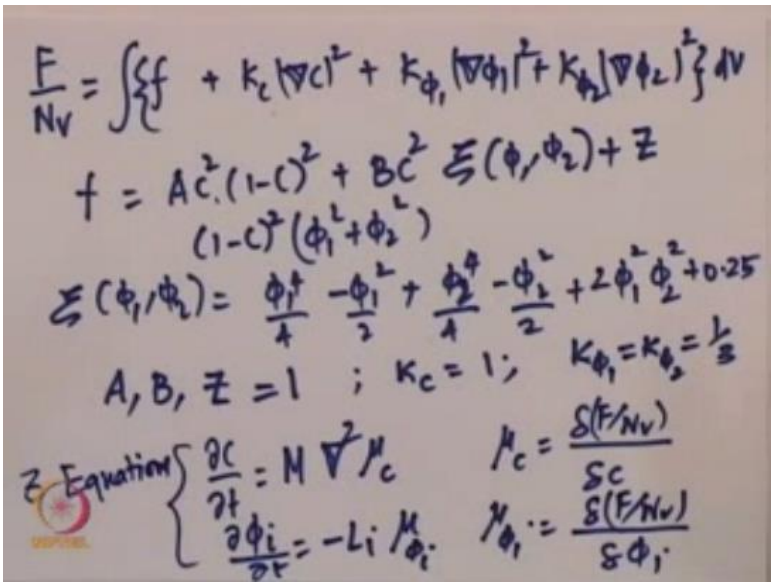

So now I have f/Nv as nothing but $f + K_c \nabla_c^2 + K_{\emptyset 1} \nabla_{\emptyset 1}^2 + K_{\emptyset 2} \nabla_{\emptyset 2}^2 dv$ and this f is nothing but $AC^2 (1-C)^2 + BC^2$ sum function of Ø1 Ø2 plus z $(1-C)^2 \emptyset 1^2 + \emptyset 2^2$ where this function is has this $\emptyset 1^4/4 - \emptyset 1^2/2 + \emptyset 2^4/4 - \emptyset 2^2/2 + 2\emptyset 1^2 \emptyset 2^2 + 0.25$, now we need to know all this ABZ, k Ø1, K Ø2 etc and again they have been chosen appropriately we are going to sign they are non dimensionalize.

So ABZ all are taken to be equal to 1 and kappa c is taken to be equal to 1 and kappa Ø1 = kappa Ø2 = 1/3 so this is the values that we are assuming, now we need to look at the evolution equation of course because there is one concerned order parameter you have to write the continuity equation for that so $\partial c/\partial t$ we would assume that the mobility is constant and it is unity so $m \nabla^2$ acting on μc.

Where μc is nothing but $\partial / \partial c$ and as you can see this variational derivative is going to give me $Kc \nabla^2 c$ with the negative sign of course and this is going to give me $\partial f0/\partial c$ right so that $\partial f0/c$ then is has to be differentiated, so this will give 2AC(1-C)(1-2C) when you differentiate this will give me 2BC this will give me -2z times 1-c multiplied by this corresponding quantity, similarly for $\partial \emptyset_i/\partial t$ we are going to use $-Li\mu\emptyset i$.

What is the $\mu\emptyset i$ that is nothing but $\delta F/Nv\, \delta\emptyset i$ okay, so I is equal to 1 and 2 so there are going to be two equations so totally there are three equations one can he lead and the other two are Allen Cohn equations and of course we know how to deal with these equations in the Fourier space so all that is key to this model is this free energy functional if you choose the free energy functional correct and if you use the correct parameter values that the minima has a required property namely when C equal to 0 both Ø1 Ø2 will be equal to 0 that is the minimum .

And C = 1 either Ø1 or Ø2 has to be one the other one has to be zero so that is the minimum invest in which case you will have three minima corresponding to the vapor phase grain one and grain two and we know what is the initial structure that is consistent with periodic boundary condition so now knowing the evolution equation knowing the parameters that go into the evolution equation we can then implement it in octave.

And look at whether the grain boundary start screwing if we start with a flat solid vapor surface which has a grain boundary cutting to it in a perpendicular fashion, okay so that is what we will do so we will try to model this problem in octave and see what happens to the evolution of the microstructure, thank you.

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