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

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Module No.22
Lecture No.80

Overview of phase field modeling

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Phase field modelling

The viewpoints, the challenges and way forward

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Welcome we have come to the end of this four-part course on phase field modeling so this is a good time to try to understand phase field models at a slightly broader perspective so this lecture is to give the idea about what phase field modeling is now that we have done everything starting from classical diffusion equation their failure writing continuity equation writing Allen Cahn equation and using them by themselves or in combination to solve many of the problems that one can see that are related to micro structural evolution so it is a good time to step back and look at what these phase field models are and how to understand them.

So this presentation is a very short presentation it is a sort of summary presentation and a little bit abstract in its tone so now that we have gone through the course and we have looked at several examples so many of these things should make sense to you so let us go through this thing so this is about the viewpoints the challenges and what can one do beyond what we have done in this course or that is what this short module is about.

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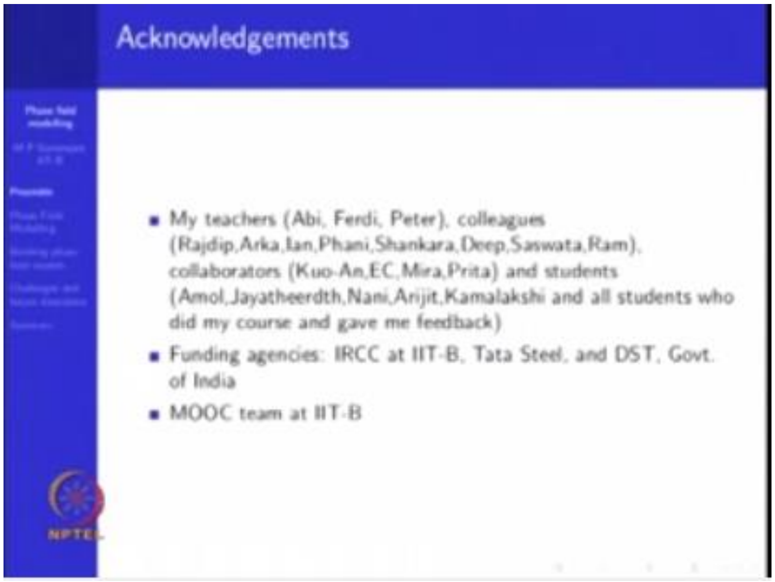

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- MOOC team at IIT-B

Before I do that I have to thank several people I have learnt phase field modeling from my thes is advisor Prof. Abinandanan and I have spent some time in Germany and in us with Prof. Ferdinand Haider and Prof. Peter would his so they are my teachers in phase field models and while I was doing PhD and while I was doing my work with peter in US for example so I had several colleagues from whom I have learnt lots about phase field modeling so this includes

Rajdeep whose grain boundary grooving work we discussed Kuo and An who did the grain growth problem with me and Panier Shankar deep.

Deep is the one who wrote the first phase field thesis in this country and Shahaado and Ram those where my colleagues in indifferent places and then I had several collaborators Kuo with whom we had done some work related to grain boundary grooving and Prof. Chandrasekhar and Prof. Mira Mitra here at IIT Bombay with whom we worked on implementing numerically solving phase field equations using wave lets and Prof. Peeta and who is my colleague with whom we are trying to now do problems like plasticity induced micro structural evolution using the phase field modules.

And of course all of this is not possible unless you have students so I have a whole bunch of students Amol is the first student to do phase field models in the lab then Jayateerdth then Nani and Arijit kamalakshi because they are the current PhD students who are doing the do phase field modeling related work now in the group and they are also the TS for this course so they are there and I have taught this course on micro structural evolution modeling so several batches of students took the course they gave me their feedback and most of the teaching material is based on my interaction with them.

So that helped me understand what works what does not work which is a good starting point and how to go about doing the course so I would like to thank them and at various stages I have been funded from DST government of India and from industry Tata steel for example and from IIT Bombay the industrial research and consultancy center for example so I would like to thank them and all this recording and lectures and the course would also have not been possible but for the help for the mook team that we have here at IIT Bombay so I would like to thank them also.

So this as far as the acknowledgments are so lots of people are involved even though it is just that I who come and give lectures but all their involvement is very important in making the course useful interesting and worthwhile so at this point I want to make a disclaimer so I am going to talk about what is the phase field model and how to look at it and things like that so this is the overview of different points of view.

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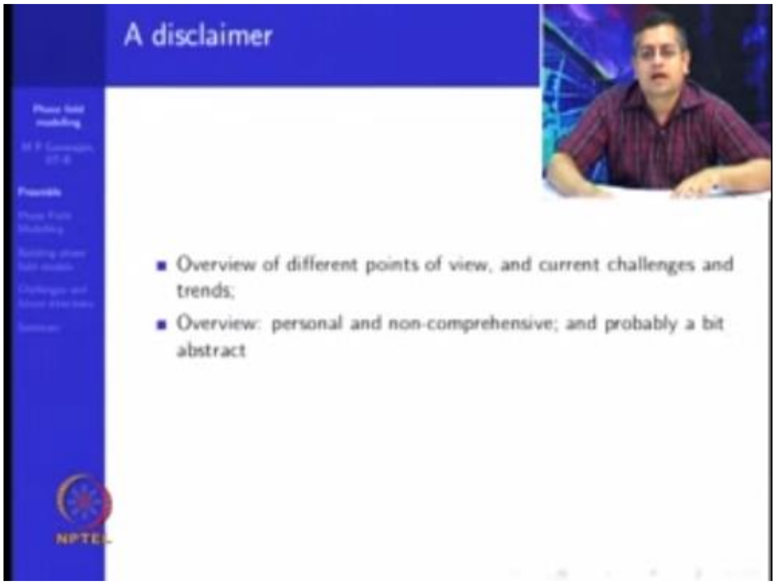

A disclaimer

- Overview of different points of view, and current challenges and trends;
- Overview: personal and non-comprehensive; and probably a bit abstract

Okay some of the points of view is what I have some of it is not what I think but those are existing viewpoints so I would like to give the complete picture not just what I think what other people think and how they look at it because some of you might find that interesting who might be interested in that part so I am going to give a overview of different points of view and I also want to talk about the current challenges and trends a little bit because the reason why one might want to do this course is to go beyond what is taught in this course and look at new problems and use the phase field modeling as a technique to solve problems that might come about in academic or industrial research or practical application problems.

So that is what we are going to do and this overview is however very personal so this is what I think and it is so it is biased by what I know and what I have not done obviously and it is also not very comprehensive this is not like a review where I have taken into account everything that has been done using phase field models for example we never had a chance to talk about phase field models of fracture okay so there are huge bunch of problems for which phase field models are being applied and models are being developed but we have not talked about them so.

So there are lots of things that I am not going to talk as part of this so it is not complete in that sense and it is going to be a little bit abstract that is because we have looked at lots of phase field information so now we should be able to step back and look at things not in great detail but as overview so that is what we want to do in this part of the lecture okay so if you ask what is phase field modeling there are many different answers that you would get so I have listed four representative answers and I have also given what kind of researchers are having this kind of viewpoint.

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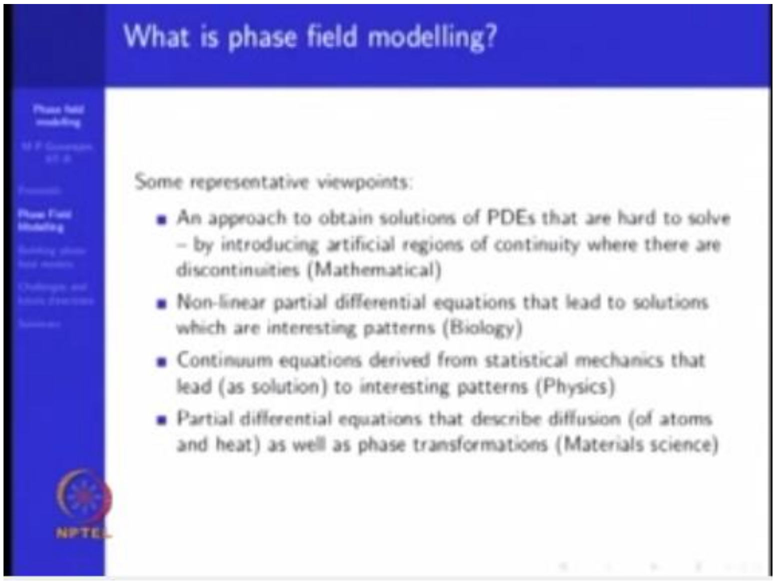

What is phase field modelling?

Some representative viewpoints:

- An approach to obtain solutions of PDEs that are hard to solve – by introducing artificial regions of continuity where there are discontinuities (Mathematical)
- Non-linear partial differential equations that lead to solutions which are interesting patterns (Biology)
- Continuum equations derived from statistical mechanics that lead (as solution) to interesting patterns (Physics)
- Partial differential equations that describe diffusion (of atoms and heat) as well as phase transformations (Materials science)

For example mathematicians think that phase field modeling is an approach to obtain solutions for partial differential equations that are hard to solve we have seen that you can look at the Cahn Hilliard Allen Cahn kind of equations as some nonlinear partial differential equations and when you put them together you have this highly nonlinear coupled partial differential equations and now are priori we need to know if there is a solution and so if move so what is the type of solution and so on.

So it becomes very difficult to solve such ODE if you post them in the classical setting as sharp interface models but because diffuse interface approach can give us equations which we can solve so more mathematically oriented researchers think that phase field modeling is basically an approach for solving PDS okay they think that there is an introduction of artificial region of continuity so given that there is discontinuity like a shockwave.

For example you replace that region of discontinuity by a continuous part and then you ask what is the functional for which the Euler-Lagrange equation will give me this evolution equation in which if I make the interface with go toward 0 I will get the classical evolution equation so this is how it is post and so phase field modeling is just looked at as a technique or strategy to solve partial differential equations but this is very mathematical view point right so you think that actually there are discontinuity and replacing them with continuous functions is just a an artifact to make the calculations simpler or easier the second one is of course very interesting.

So this is from biology and the most important paper in this field was written by Alan Turing who is a great computer scientists he called it as chemical morphogenesis so it is available if you Google you might be able to find this paper so some of you might have seen that some of these structures that we develop for example during spinodal decomposition so we get his black regions and white regions in our representation or blue regions and red regions right so Alan Turing thought that Allen Cahn kind of equations which are reaction diffusion equations because they are deficient equations and there is a source term.

And source term can be thought of as some chemical reaction giving rise to some species so these reaction diffusion equations can give rise to this kind of interesting patterns okay alternating black and white so if you look at some of the patterns on some animals like zebras for example so Alan Turing thinks that these equations can now explain how these patterns are formed okay here again the emphasis is on the patterns that form so PDS are just thought of as tools to get such interesting patterns.

So this is another viewpoint on phase field modeling and comes from the field of biology the third viewpoint is that you can think of statistical mechanics and you can think of problems in statistical mechanics that lead to interesting patterns and what kind of coarse-grained the free energy that you can derive from the statistical models and then their minimization and during minimization how it evolves and things like that so this is a viewpoint this is a much more closer to the kind of viewpoint that we have but this is more physics based view point.

Here again the importance is on the patterns and on statistical models so what kind of models lead to what kind of patterns to the extent that we are talking about statistical models statistical mechanics based models we are talking about the physics of course the approach that we took in this course is the last one I have called it as the material science or you can call it the metallurgy approach this is the approach where we think that these are partial differential equations that describe diffusion except that the constitutive law is no longer fixed law because we also want to describe phase transformations or deformation induced microstructures okay.

So if you depending on who what is the back ground or the person that you are asking this question what phase field modeling or what is the kind of problems that they look at you will get many different answers so these are the only representative answers these are not exhaustive there could be other view points about phase field models but we have taken the approach that phase field models are just some nonlinear diffusion equations and that is a good view point to take if you are looking at solid phase transformations okay. Now having said that so what are phase field models so here is an answer.

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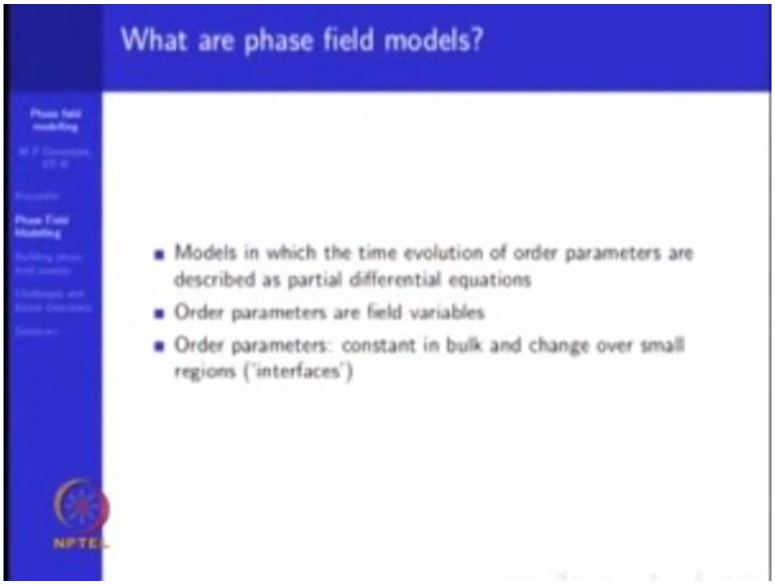

What are phase field models?

- Models in which the time evolution of order parameters are described as partial differential equations
- Order parameters are field variables
- Order parameters: constant in bulk and change over small regions ('interfaces')

So models in which the time evolution of order parameters are described as partial differential equations so that is a definition of phase field model that you can use because that is what we have been doing we have been looking at the time evolution of the order parameters and what do the order parameters do they describe the microstructure so in this viewpoint.

Now order parameters are field variables that means they have value for all positions in the domain for all times okay and the typical characteristic of such a model is that the order parameter is constant in the bulk and wherever changes we say that there is an interface okay. So this is a slightly more detailed answer to the question what is phase field modeling and from a materials point of view okay.

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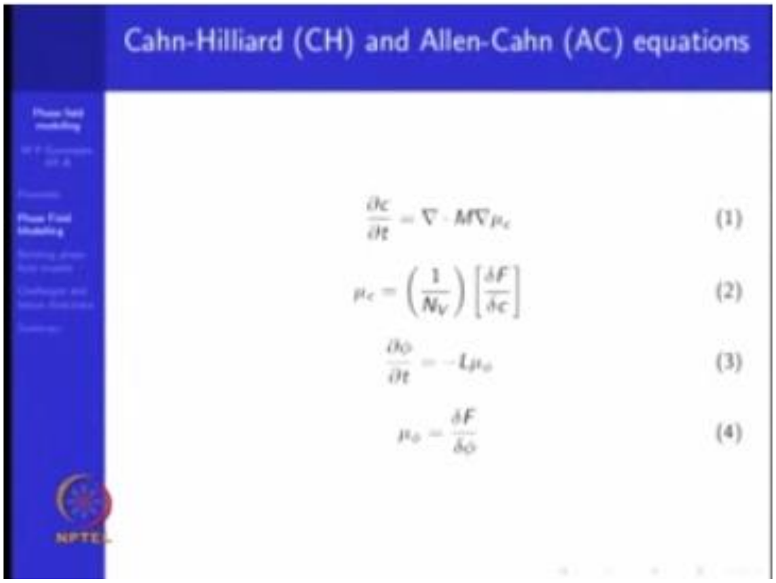

Cahn-Hilliard (CH) and Allen-Cahn (AC) equations

$$\frac{\partial c}{\partial t} = \nabla \cdot M \nabla \mu_c \quad (1)$$

$$\mu_c = \left(\frac{1}{N_V}\right)\left[\frac{\delta F}{\delta c}\right] \quad (2)$$

$$\frac{\partial \phi}{\partial t} = -L \mu_\phi \quad (3)$$

$$\mu_\phi = \frac{\delta F}{\delta \phi} \quad (4)$$

Now there are two canonical phase field models that one looks at what is called the Cahn Hilliard equation which is the equation one here and the chemical potential is what is defined in the equation 2 and this is basically because the concentration is a conserved order parameter that is if you take an integral of the concentration field over the entire domain and if you differentiate it with respect to time that is going to be zero because the integral is going to be a constant C_0 so d / dt (C_0) is going to be 0.

So that wherever such a condition is obeyed then we have to write the Cahn Hilliard equation on the other hand the Allen Cahn equation is non-local it does not worry about the conservation because the order parameter is such that it does not have to be confirmed conserved for example you can have an order parameter which describes whether the system is solid or melt but there could be situations where the domain is completely melt and after awhile it can become completely solid which is what happens in solidification setting for example so such physics is described using the Allen Cahn equation so equation 3 is Allen Cahn and the chemical potential definition is what is given in equation 4.

These two Cahn Hilliard and Allen Cahn are basically can be thought of as the prototype phase field equations and you can think of any other phase field model to be a combination of these two so you can write this generic phase field model which will basically be a combination of these two and which is what we have been doing for many different interesting micro structural phenomena now you can compare the Cahn Hilliard and Allen Cahn equation with the classical diffusion equation.

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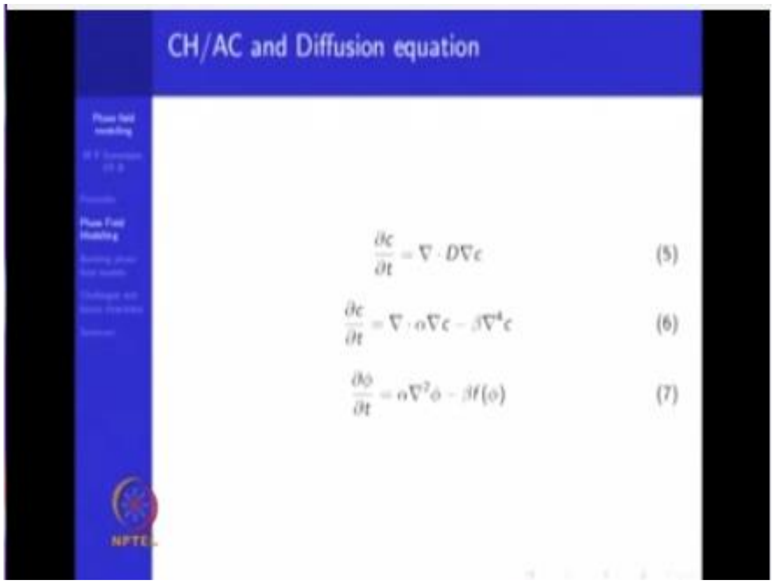

CH/AC and Diffusion equation

$$\frac{\partial c}{\partial t} = \nabla \cdot D \nabla c \quad (5)$$

$$\frac{\partial c}{\partial t} = \nabla \cdot \alpha \nabla c - \beta \nabla^4 c \quad (6)$$

$$\frac{\partial \phi}{\partial t} = \alpha \nabla^2 \phi - \beta f(\phi) \quad (7)$$

And here you can see that equation 5 is the classical diffusion equation, equation 6 is the Allen Cahn equation 7 is the Allen Cahn equation so in terms of the structure of the equation they look like nonlinear diffusion equations the physics is very different but in terms of the equations they look like diffusion equation nonlinear diffusion equations okay classical diffusion equation is just linear but this look like diffusion equations with some non-linearity thrown in one case there is a higher order derivative or gradient term on composition in the other case there is just a source term in the order parameter F(e).

So because they look like this that also gives us an idea that the solution methodologies could be the similar to what is used for solving the diffusion equation and specifically in this course we have actually used the spectral technique for solving the phase field equations okay now here is the recipe which we have been following for every problem.

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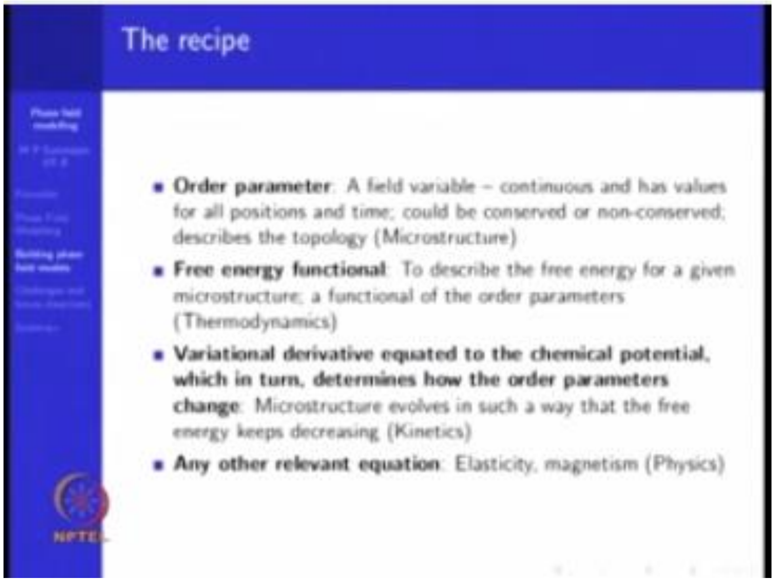

The recipe

- **Order parameter**: A field variable – continuous and has values for all positions and time; could be conserved or non-conserved; describes the topology (Microstructure)
- **Free energy functional**: To describe the free energy for a given microstructure; a functional of the order parameters (Thermodynamics)
- **Variational derivative equated to the chemical potential, which in turn, determines how the order parameters change**: Microstructure evolves in such a way that the free energy keeps decreasing (Kinetics)
- **Any other relevant equation**: Elasticity, magnetism (Physics)

So it consists of about four steps in all the things that we did in this course we actually saw three of them and the fourth one we did not have a chance to look at the first is to describe the microstructure using a field variable so that could be conserved or non-conserved the purpose of this order parameter description is to describe the geometry of the microstructure once you have defined the geometry for the given geometry you have to describe the thermodynamics that is done by giving the free energy or entropy in some cases but we have been sticking to free energy functional because in solid phase transformations.

Where most of the times we are assuming that temperature is a constant so isothermal problems this is a very good thermodynamic description and then we take the variation derivative of the free energy and we write this constitutive law which says that rate of change of the order parameter is proportional to the gradient in the chemical potential or proportional to the chemical potential itself and this some part of it we have done for example when we write the Cahn Hilliard equation that there is mass conservation is also incorporated into the equation.

It could be more complicated than that for example you might be looking at stressed system then you have to solve the equation of mechanical equilibrium right or you might be looking at some magnetic or electric or electromagnetic system then the Maxwell's equations have to be solved and those field variables have to be incorporated into the free energy the magnetic free energy or the electric free energy or the elastic free energy so sometimes the phase field models will be coupled with these other physics that is involved and then it becomes more complicated.

So one of the very common problems that people use extensively is to look at the effect of elastic stress effects on microstructures there we have to solve the equation of mechanical equilibrium and you have to get the stresses and strains you have to calculate the free energy contribution from these stresses and strains and you have to put it back into the free energy calculate the corresponding chemical potential then the evolution will be very different from when you neglect these stresses because stresses play a key role in the micro structural evolution.

So that is the four-step we did not have much of a chance to look at it but if you want to do anything which is complicated sometimes you might end up with having to incorporate the fourth step also.

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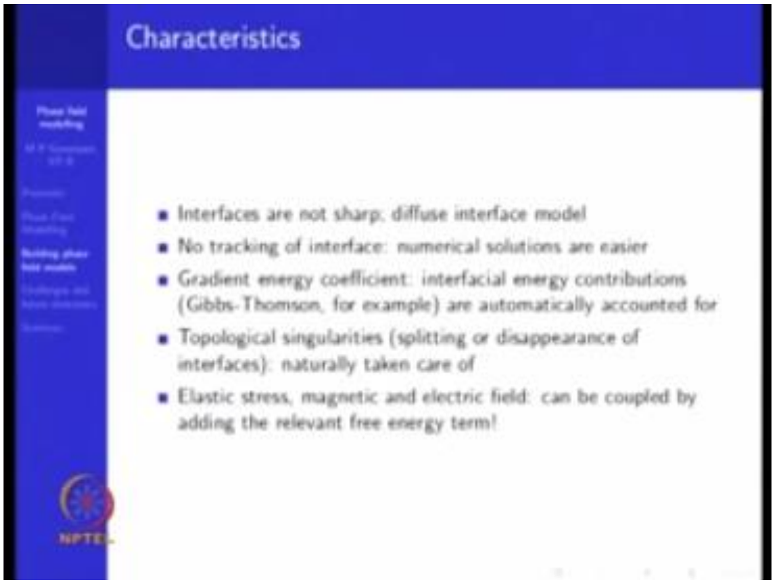

Characteristics

- Interfaces are not sharp: diffuse interface model
- No tracking of interface: numerical solutions are easier
- Gradient energy coefficient: interfacial energy contributions (Gibbs-Thomson, for example) are automatically accounted for
- Topological singularities (splitting or disappearance of interfaces): naturally taken care of
- Elastic stress, magnetic and electric field: can be coupled by adding the relevant free energy term!

Now what are the characteristics of the phase field model solutions we see that the interfaces are not sharp okay so you always have a very diffuse interface and we can also track the interface which are without having to look at where the interfaces that is because you can say that wherever the order parameter half between the two bulk then that is my interface for example if my order parameter goes from 1 to 0 wherever 0.5 value is reached for the order parameter I will call that as an interface.

So there is a operative definition for the interface which you can use and so when you are doing the calculation you do not have to keep track you also do not have to keep track because it is not a sharp interface which has discontinuities in which case you have to incorporate some jump condition at the boundary but because we are assuming everything to be smooth continuous we do not have to incorporate any jump condition which is all automatically incorporated.

Now we have also discussed the relationship of the higher order terms the gradient terms in the free energy to the interfacial free energy okay that means any interfacial free energy related effect will automatically come into play in the phase field models gives Thompson an example we looked at how the composition changes for example for a curved interface.

So they are automatically accounted for you do not have to do it manually and because we do not track interfaces if there are interfaces which are merging or splitting all that is automatically accounted for in this models of course like I mentioned you if you have elastic fields or magnetic fields electric fields they all can be correspondingly included into the model by incorporating their energy contribution to the free energy so that way I have been phase field models have some advantages over other models that one can use. For looking at the same physical phenomena.

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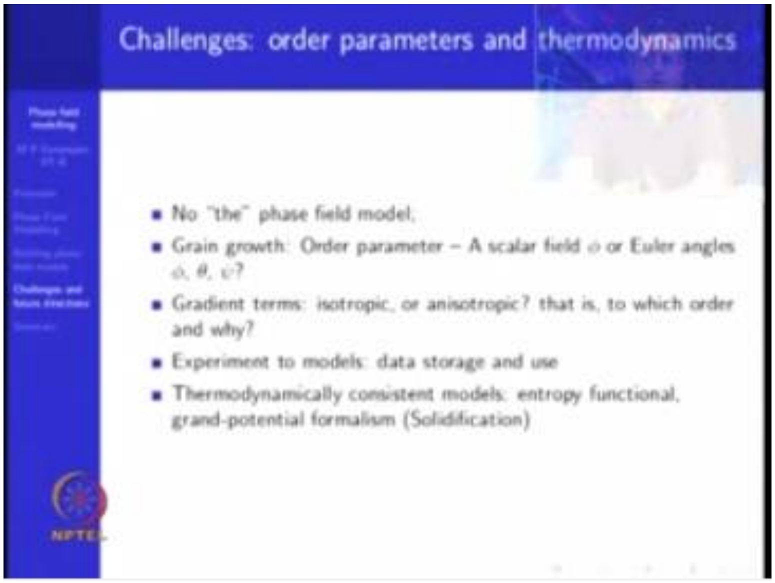

Challenges: order parameters and thermodynamics

- No "the" phase field model,
- Grain growth: Order parameter – A scalar field ϕ or Euler angles ϕ, θ, ψ?
- Gradient terms: isotropic, or anisotropic? that is, to which order and why?
- Experiment to models: data storage and use
- Thermodynamically consistent models: entropy functional, grand-potential formalism (Solidification)

Now what are the challenges of course you have noticed that there is no the phase field model for example we have looked at order parameter based grain growth model where we use the scalar field the fee but we know that different grains are described by their orientation so you can use the Euler angles as the order parameters and their variation can for example describe the microstructure yes it is possible as long as you can use these order parameters and write the free energy in terms of order parameters and their gradients you should be able to do and similarly this is something that we have not discussed in great detail but becomes important if you look at the literature is that we have assumed everything to be isotropic.

You know even the grain growth case interfacial energy was assumed to be isotropic it need not necessarily be so okay so inter facial energies could be an isotropic and an isotropic and play a key role in the micro structure in which case how do you incorporate the an isotropy is one of the important problems and there are methodologies that are being developed including in our group here so there are many different ways in which you can incorporate the anisotropy into the model and there is also the problem of making connection between the phase field models and experiments one of the reasons why phase field models are being studied in this great detail is because they look at micro structures and from an application point of view microstructure is the bridge between the processing and the property.

So if I have to get some property I need to know what processing does to my microstructure so I know whether I will get the property or not and phase field models are the models to do this microstructure part so which means we need to at some point connect our models with experiments in that case of course there is a connection at the thermodynamic level so there are programs like Cal fat which is for calculation of phase diagrams can we take those thermodynamic information and incorporate in our models and where do I get information about the gradient energy coefficient is there a way to get it from some other models or some other information and the motilities.

So there are lots of parameters in addition the microstructure it says the geometric information itself can also be used as an input are as a benchmark for the phase field output in which case you know the experimental microstructure information could be quite complicated could be quite costly in terms of storage so how do you make this connection is one of the problems on which there is lots of effort that is being spent at the moment of course there is also the question of thermodynamic consistency in the case of solid phase transformations we demand free energy and its minimization in cases like solidification where temperature is not a constant one may have to look at entropy functional and there are formulations like grand potential formalism which becomes important in such cases to look at.

So these are some of the challenges associated with order parameters and thermodynamics there are also.

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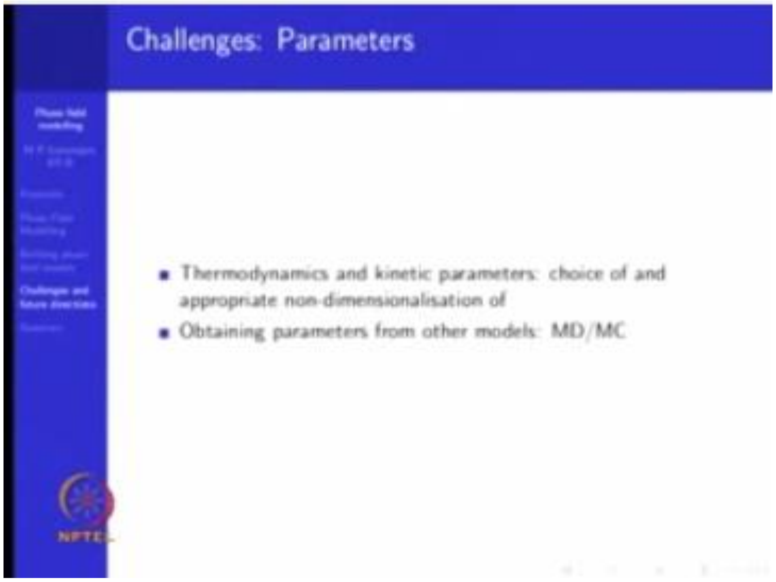

Challenges: Parameters

- Thermodynamics and kinetic parameters: choice of and appropriate non-dimensionalisation of
- Obtaining parameters from other models: MD/MC

Other challenges in terms of what parameters go into the phase field model and why and how do we obtain them from if not from experiments from other modeling techniques like atomistic models can we do get the parameters put it in the phase field model do the microstructure get the micro structural information put it in a finite element model so these are the type of questions which become important especially if we have some application in mind so in those cases then how to get these parameters and how to make different models talk to each other becomes an important problem.

So there are lots of effort that is being done at this moment to answer some of these questions or to make progress on some of these questions of course the lost problem about which I want to talk about is that we have been looking at solid phase transformations one of the other important ways in which the microstructure changes is by mechanical deformation okay so deformation induced micro structures and their modeling is very important that means like we have done phase transformation part using the phase field model can we do plasticity part in the phase field model. So that becomes an important question the difficulty with plasticity is that it is very complicated.

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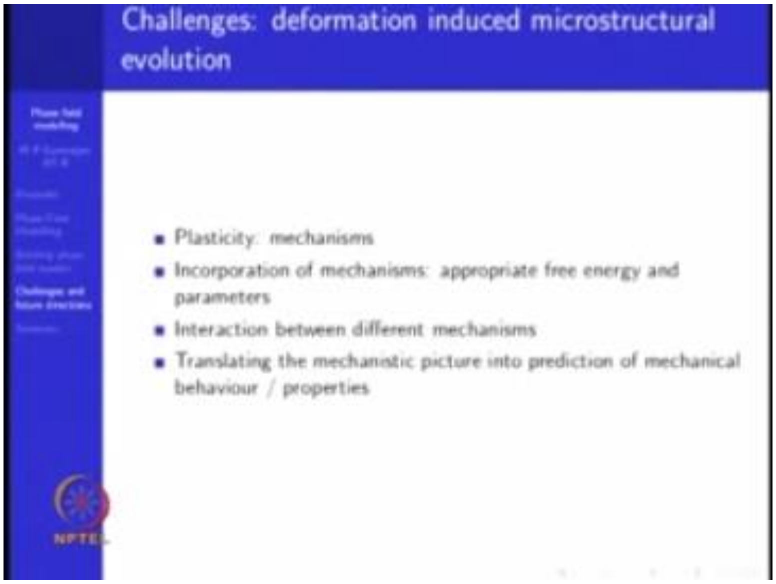

Challenges: deformation induced microstructural evolution

- Plasticity: mechanisms
- Incorporation of mechanisms: appropriate free energy and parameters
- Interaction between different mechanisms
- Translating the mechanistic picture into prediction of mechanical behaviour / properties

There has more than one mechanism and they might all be competing or they might all be interacting with each other so this how to bring it into a phase field model is a very crucial question and it is also a very challenging question and of course apart from this there are other challenges like large calculations we want to do or parallel calculations we want to do for example in some scenarios spectral techniques are not very good for scaling in terms of parallel computation then we need to do finite-difference kind of models.

How accurate are they and how better can we do this so this kind of other computational issues are also things about which we have to think about if you want to do large-scale or application oriented phase field models so that brings us to the summary so one can think of phase field models.

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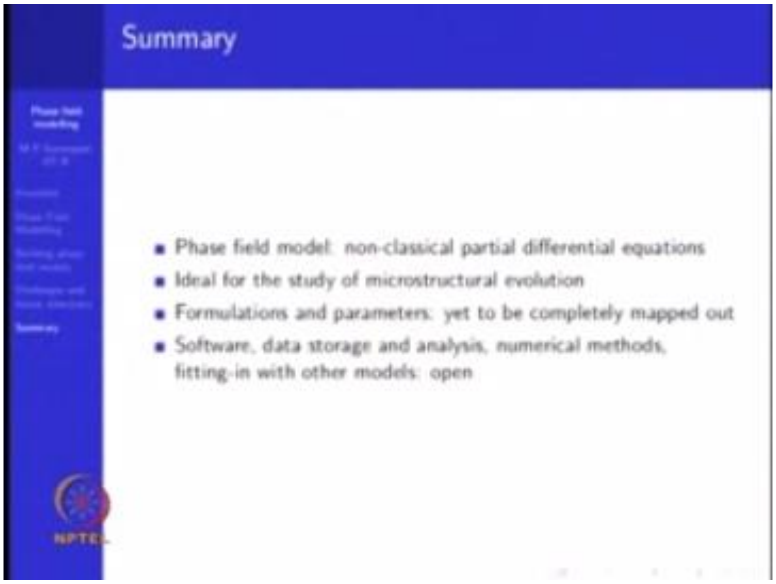

Summary

- Phase field model: non-classical partial differential equations
- Ideal for the study of microstructural evolution
- Formulations and parameters: yet to be completely mapped out
- Software, data storage and analysis, numerical methods, fitting-in with other models: open

As some non classical partial differential equations their ideals for the study of micro structural evolution we have seen several examples but the formulations and parameters is not it mapped out completely there are many problems that are not yet solved and one can solve if one can formulate it properly and there are issues related to the formulation which is basically the math associated with the problem the material science associated with the problem and the numerical methods associated problem.

So there are lots of open problems which means that it is a field which is growing alive and kicking and anybody who wants to do and especially because there is a wide variety of problems that one can tackle more mathematical problems modem materials oriented problems more physics oriented problems and more computational oriented problems so say they all have their relevance and they are all interesting and so I hope that in this course helps you to start in this direction I hope that this course is a starting point for you in this journey thank you

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