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Phase field modelling; The materials science, Mathematics and Computational aspects

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Module No.7
Lecture No.29
Non-dimensionalalisation
Of diffusion equation

Welcome we are using octave to look at some of the problems, of phase separation regular solution model and so on, and we are planning to use our care to solve the classical diffusion equation, and as part of this exercise the first thing that we want to do is to non dimensional, remember we had the free energy expression.

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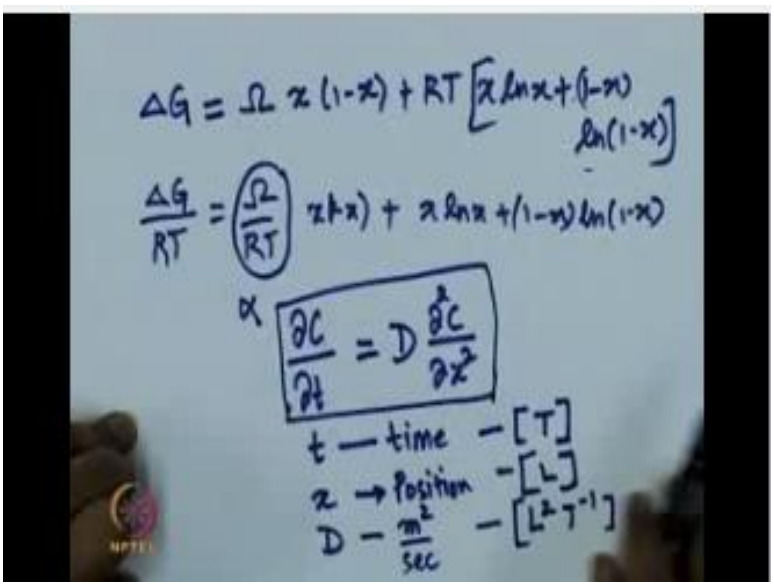

For example the free energy of mixing for the regular solution as, Ω x(1 – x) + RT x the RT[x + 1 x 1 – x] so what we did first was to non-dimensionalize this equation, because see this is free energy, and so every term then you know this is some high school physics probably you have learnt, that they should all have the same units our dimension, if this is energy this also has to be energy this also has to be energy.

And look at these terms so this is [xlm(x + 1) - x 1 (1- X)], where this is the fraction of B atoms X is a fraction of me atoms, so to the total number of atoms so that is just a number it does not have any units, which means all the unit is carried by RT in this case and Ω in this case, so what we did was to take RT as the parameter using which we will non dimensionalize this entire equation, and the which is what we did these call this as Δ G / RT as Ω / RT, for which we gave a short hand notation called α x ×1 - x + x ln (x + 1) – x(1-x), so all our computations for the free energy was done using such anon-dimensional expression.

Now we are going to do the next non-dimensionalisation which is for the partial differential equation, which is the so-called Fick's second law, ok we have derived this equation so I am going to write the 1 dimensional version of the equation and non dimensional zed certification ok, so the equation is something like that rate of change of concentration is equal to, D I have assumed the diffusivity to be a constant $\delta^2 C / \Delta X^2$.

Okay so what are the quantities which are dimensional here, so you can assume that the concentration to be a number, okay again like X so we will not worry too much about it, or even if you put some dimension like this is per mole say, and this per mole and this is also per mole so both sides it will be cancelled out so let us not bother about the dimension, for C, the other quantities that higher dimension is that T which is time has the dimension of time, and X which is position has the dimension of length, and then we have diffusivity which is generally given in m^2d / second, then that means it has a l^2d P^{-1} as its dimension.

What we are going to do? is that we are going to consider some characteristic time because time and, length are the only basic dimensional quantities that we have, D is basically a derived quantity, so all that I need to do is to choose two quantities one that refers to the characteristic time scale, the other one which refers to the characteristic length scale, that is sufficient for me to non-dimensionalize this equation okay. So that is what we are going to do so let us again take the equation, so this is the ficks second law.

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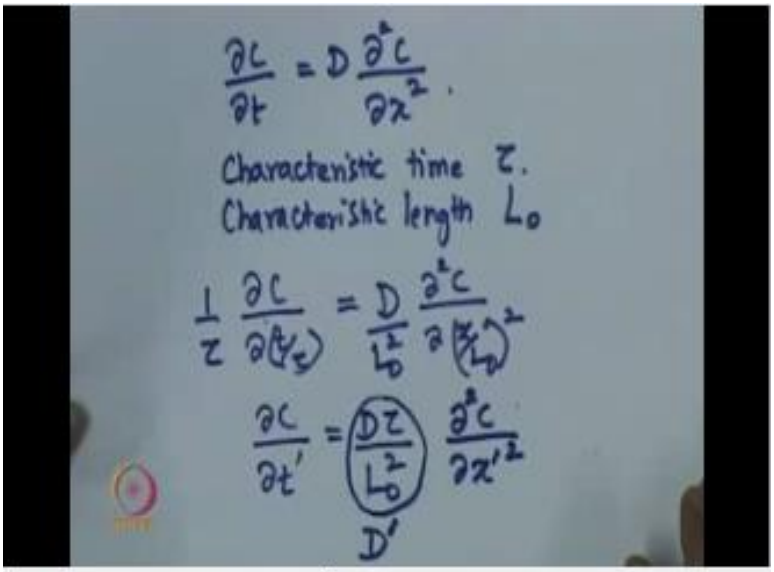

So that is ∂ c / ∂ t = d δ ^{2}d c / δ x^2, so I am going to take a characteristic time, now I am going to take a characteristic length, what are these quantities? we will discuss them so I am going to take this, and I am going to scale all the times by τ, and all the lengths by $L_{0,}$ so let us do that so if I take ∂c / ∂ T / τ, I have divided by τ so I will have 1 / τ = d δ ^{2} c / δ X / $L_0{}^2$, so which means $L_0{}^2$ okay.

So let us call the non-dimensional quantity T /τ now it is non-dimensional it is like a number right, it has seconds this has seconds so that got cancelled out so you will have ∂ C by ∂ T\` the \` two quantities are non-dimensional, is equal to D τ by $L_0{}^2$, notice that this quantity also now got non dimensionalize because D is m^2/second $l_0{}^2$d will have m^2 the τ will have second so everything will cancel, so you will have a deep prime to indicate that this is non-dimensional diffusivity that will be ∂^2 C / ∂ x $^{\grave{}2}$ okay. So let me write the non dimensional version of the equation once more, so what do we have?

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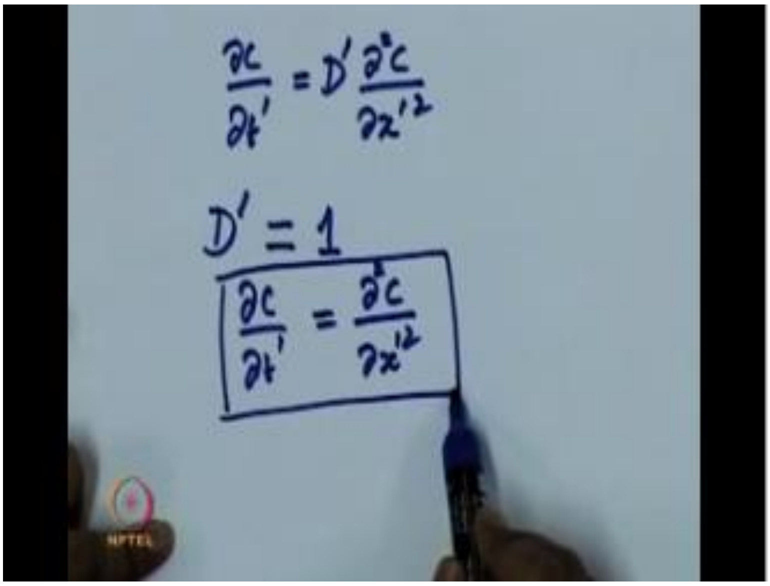

We have $\partial C / \partial T` = D` \delta^2 C / \Delta X`^2$, typically people choose sometimes the non dimensional diffusivity to be equal to unity, so sometimes the diffusion equation will be written without diffusivity as $\delta^2 C / \delta x^2$ okay, and as you will see later when we solve the phase field equations so typically we do this non-dimensionalisation, so all the parameters that go into the model become one.

Now you might be wondering what this characteristic time is and what is this characteristic length? Okay this is something that we do in our day to day life, non-dimensionalisation is something that we do all the time, for example if I ask you what is the price of this pen you will say okay 30 rupees, if I tell you what is the cost of this curve you are going to say 7 lacks.

So from the unit of rupees you have switched to the unit of lacks of rupees, simply because you want to say the number in some small rates typically the numbers that we want to tell is between somewhere between zero and say 100 right? Typically if you are asked okay what is the price of this Chuck piece? You will not give that an in rupee but you will say it in paisa maybe it is 50 paisa, if Chuck pieces are still being sold for 50 paisa.

And if you say what is the price of this house I mean somewhere the near IIT for example houses cost in corers, okay there you do not even use lacks for a car you might say seven likes but when you ask about the home you will say oh it is 1.2crores, so what we do is that we change the unit in which we refer, I mean there is nothing that stops you from giving the price of the home in pies, or the cost of the curve in rupees or pies okay, or the cost of the chalk piece in paisa right there is nothing wrong but we typically do it because we want to get the number say in some manageable range and that is between 0 and 100.

So typically this is the number and if you are very strict it should be between 0 and 1 or 0or 10 but up to 100 is okay, and beyond that if it goes you basically tend to change the unit and try to give the answer, so when we are saying the characteristic time and characteristic length that is what we mean, suppose you are looking at diffusion which is at some micron length scale right if you are looking at distances which are measured in microns, if you take the micron out of that by dividing everything by 10^{-6}, then the number is what you get.

On the other hand you might be looking at diffusion which happens over meters right, or centimetres so depending on what is the size of your material, over which you are looking at the distance, then you typically tend to take that as the characteristic length scale right. So you can think of the system size as the characteristic length for example, similarly suppose diffusion takes one day to happen then it is easier to use as time unit day.

Suppose if it happens over some 40,50 seconds then a day is not a proper unit seconds is the better unit, suppose some homogenisation requires diffusion to take place over 48days then days is better, and some might happen over minutes then it is better to use minutes, okay so the characteristic time scale again is a time scale associated with the problem with which you are dealing, and looking at the range of times that are involved typically you take that unit as the characteristic time scale and that is what we have done.

We have done this for two reasons, one is like I said that all the numbers lie between 0 and 100 and that is always preferable, because when we are doing calculations in the computer carrying numbers like 10^{-6} and you know if it is m^2 / sec and suppose your diffusion distances are in microns, and time scales are in seconds then you will have quantities like for diffusivity, 10^{-12}.

So we do not want to have such very small numbers coming up in calculations, that is one reason second reason mathematically speaking if you look at this equation, then it tells you that wherever for example, this d τ / $L_0{}^2$, right this $L_0{}^2$d could be in microns and that this could be in seconds, or this could be in meters and this could be in hours it does not matter as long as this D τ by $L_0{}^2$ becomes some number, equal to some K, the solution of the diffusion equation is going to remain the same right.

Which unit you are using does not matter you can always scale in that unit and you can plot your solutions, mathematically speaking there is one non dimensional equation which you have to solve, if you know the solution knowing the characteristic time and length scale associated with your problem, you can correspondingly scale and get the right solution for all the problems.

So this again is advantageous because when I am solving it numerically you want to solve it just once, for different D values and then corresponding to the actual values that I have for the, τ and L_0, then I will get the actual solution, so it is also much more you know economical to solve the non dimensional equation.

So no dimensionalization is an important process, we will non dimensionalize all the equations that we will solve and it is a better way of for doing computations, and the later I am also going to show that even free energies, sometimes we make them undergo some transformations, so that they become far more easier to deal with when we are using computers, okay so we will take a look at some of these things solving the non dimensional diffusion equation numerically and, solving the classical diffusion equation I mean using a couple of analytical tricks both we will discuss as part of the lectures that follow this than you

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