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

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Module No.2
Lecture No.8
Fick's laws

Welcome we will start with the discussion of classical laws of diffusion, these are known as Fick's laws, Fick's first law and Fick's second law. As you will see later it is really not Fick's second law, Fick's first law is a law it is a constitutive law.

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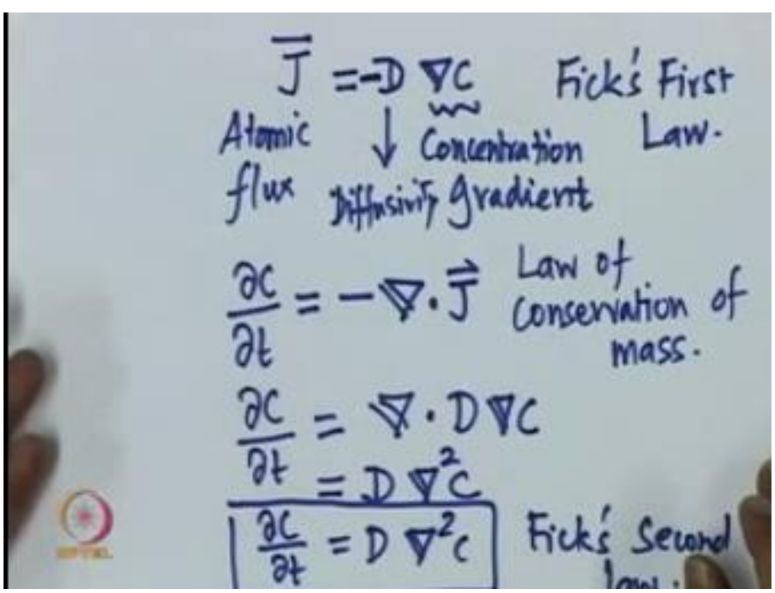

It says that the flux of atoms is proportional to the concentration gradients and the proportionality constant is known as diffusivity and Fick's first law states that the atomic flux in will be in such a way as to minimize the concentration gradient so that is indicated by a negative sign okay. So this is atomic flux, this is concentration gradient, this is a proportionality constant which is known as the diffusivity okay.

In terms of cause and effect you can think of concentration gradient as the cost for the effect namely atomic force if you have concentration gradients and then atomic flux will happen in such a way that this concentration gradients are evened out and how fast or slow it will happen is the decided by the constant which is a material property which is known as diffusivity, negative sign basically is telling you that the ΔC is getting reduced because of the atomic flux.

So this is known as Fick's first law okay. And if you are we are talking about atoms and there is a law of conservation of mass and you can show that law of conservation of mass indicates that if you have a particular composition at any point the rate of change of composition at that point is equal to negative of divergence of the atomic class okay, this we will do as a tutorial. So we will do a simple mass balance to derive this expression okay.

Now if you then substitute this J from here into this expression what do you get, you get $\partial C/ \partial t$=- , - sign goes away it is $\nabla.D \nabla C$. Now typically assumes that this diffusivity is a constant if so you can pull out d out of this ∇ and then you can write it as $d \nabla^2 C$. So this is sometimes known as Fick's second law $\partial C/ \partial t$ is $d\nabla^2 C$, this is called Fick's second law like I said this is really not a law, this is a constitutive law this tells about the material behavior okay.

This tells about what is the effect of concentration gradient and atomic plus in your given system and the system dependent information is there in the diffusivity. However, this so called a second law is nothing but that this constitutive law combined the width so this is nothing but law of conservation of mass. Remember this is a universal law right mass should always be conserved. So you have a constitutive law which is specific for different materials you combine it with a universal law which is a conservation of mass you get to this second law of diffusion okay.

So this is called the Fick's second law or the equation for concentration, time dependent diffusion equation okay. So it basically describes the rate of change of concentration at any point how it evolves is what this one describes okay. Now let us take this second equation and find out what does it mean physically, to do that I am going to write the diffusion equation in 1d.

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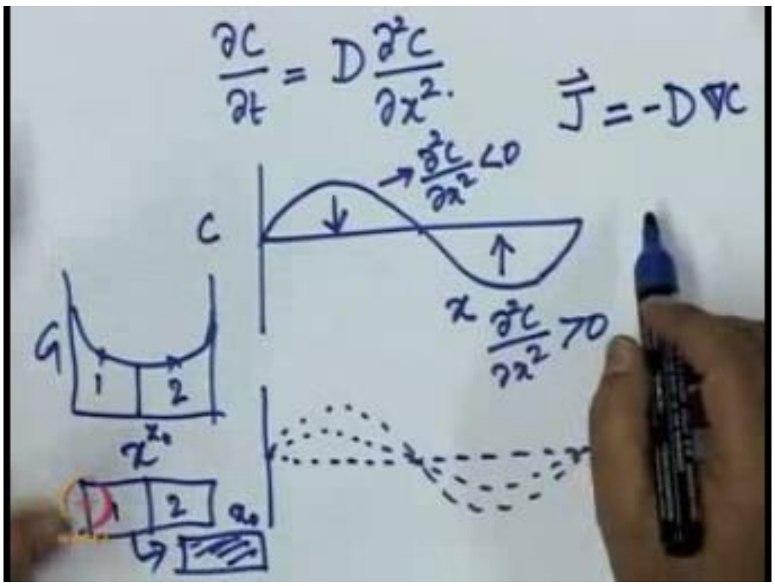

So let me write $\partial C/\partial t=D\nabla^2C/\nabla x^2$ okay. Now what is the physical meaning of $\nabla^2C/\nabla x^2$ let us say that I take a composition profile, composition as a function of position some sort of sinusoidal wave okay, you can show that $\nabla^2C/\nabla x^2$ is nothing but the curvature of this curve okay. Now this curvature you can show is negative, this curvature is positive. What so $\nabla^2C/\nabla x^2$ is basically the curvature of the composition profile.

And what Fick's law is telling you is that diffusivity is a constant and a positive constant okay, what Fick's law is then telling you is that in regions where the curvature is negative, the rate of change of concentration is going to be negative which means the concentration is going to reduce. If it is zero at some point then the concentration is not going to change at that point. If it is positive then the concentration at that point is going to increase.

So what is the effect of this, so after some time you will see that you had this as the concentration profile, but as time goes by it becomes like that because you remember any where it is zero it will remain that point no, it will not change. So after a while you get a concentration profile which is like this. In other words this equation is telling that if you have any compositional heterogeneities they are all going to get evened out and the system is going to become more homogenized okay.

So this is the physical meaning of the, so called a second law of diffusion it says that compositional changes if they exist they will get evened out, they will get evened out to provided your diffusivity is a positive constant, because if it changes sign then the solution will change and assuming that diffusivity is a positive constant, then this diffusion equation is actually telling you that compositional fluctuations if you have they will all get evened out.

Remember in the earlier case when we discussed that there is only one case namely when you have free energy versus composition curve which is like this, when you take two different compositions so one and two and you have a weld of these two compositions it is going to become homogeneous of some overall alloy composition okay. So this is the only case where you see homogenization which means this equation describes cases like this.

On the other hand when we had a double well potential then we see that this equation does not describe the case of a mechanical mixture forming from an alloy like this you take two different compositions A rich and B rich and then A rich becomes rich in A, B rich becomes rich in B that is not explained by this because the very first step where we started with said that J is proportional to concentration gradient.

And the concentration gradient decreases with atomic flux okay, that is what the negative sign said assuming that diffusivity is a positive constant okay. So that is the case that we want to discuss a little bit more in detail which will bring us to the end of this module okay, we will discuss this in the next part. Thank you.

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