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

Prof. M P Gururajan
Department of Metallurgical Engineering
And materials Science, IIT Bombay

Module No.4
Lecture No.18
Diffusion & mobility I

Welcome in the last section that we were discussing we took the classical diffusion equation and we substituted a solution which was sinusoidal for composition and the amplitude of the sinusoidal waves was time dependent we substituted this solution into the equation and from there we tried to see what happens to the amplitudes with the different wavelengths so that was the derivation I did and towards the end of that derivation I introduce the relationship between mobility and diffusivity I showed that they are connected through the second derivative of the free energy with respect to composition okay.

Today I want to start by deriving how that relationship comes about in the first place we will do that first and then we will go back to the expression that we derived and we will discuss it and see where classical diffusion equation fails to capture what happens during spin order decomposition and that will automatically lead us to the first phase field equation which is known as the Cahn Hilliard equation.

And so when I introduce that equation that will be the sort of logical conclusion to this set of discussions lectures that we have been happy so let us start by deriving the relationship between

the diffusivity under mobility to do that let me start with a different expression for the flux we have seen that the Fick's first law which gives a relationship between flux at the concentration gradient it is something like this.

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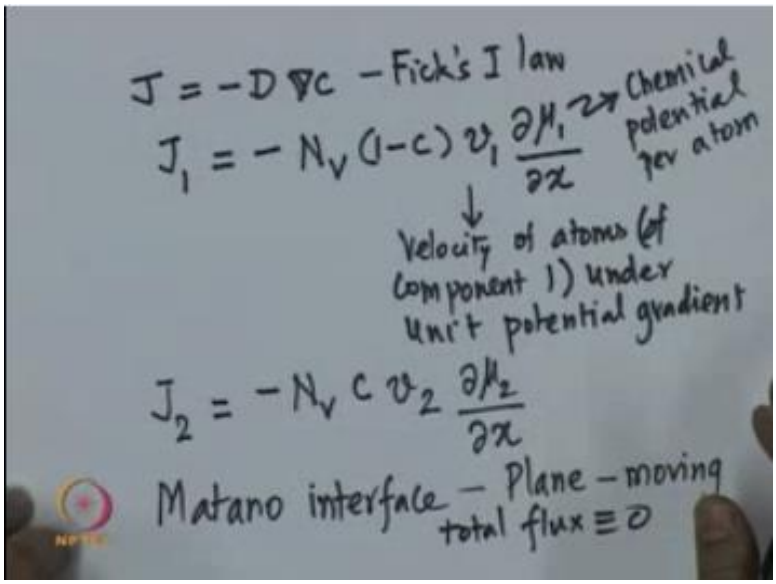

So j = -D ∇ C, so this is the so-called Fick's first law but now I am going to write a flux expression for atoms of component J_1 = - N_B at the number of atoms per mole1 - C which is the composition of atoms obviously V_1 and $\partial\ \mu_1/\ \partial_x$ where V_1 is the velocity of atoms of component one that is at velocity of a atoms under unit potential gradient right so per unit potential gradient what is the velocity of type 1 atoms that is $V_1\ \partial\ \mu_1/\ \partial_x$ is obviously gradient on the chemical potential $\mu_{1,}$ μ_1 is the chemical potential per atom.

So it might be a good exercise always to do a dimensional analysis to see that the dimensions on both sides are in agreement I will leave that as an exercise to you so it will be a tutorial at some point for you to take an expression like this and put the dimensions for each one of the quantities and see what is the dimension or units of this quantity $j_1$which is the flux of component 1 atoms of component 1 in a similar fashion we can write J_2 which is nothing but -N_V total number of items per mole.

C because we are looking at the 2 component 2 and the composition is typically the fraction of atoms of type 2 to the total number of atoms so composition C is always representing the fraction of B atoms so that is why it is C $V_2 \partial \mu_2 / \partial_{x,}$ so this are the flux remember here also it is actually J_2 and when we set the see that is basically corresponding to the B atoms okay so this is the Fick's first law.

Now we are trying to write different type of expression the reason being that we have argued and we have shown also graphically that connecting the atomic flux to concentration gradient is not always correct because spontaneously diffusion happens to reduce free energy to minimize free energy and the correct quantity which represents that minimization is basically the chemical potential so the right way of representing atomic flux is to connect them to the chemical potential gradient.

And we have also seen that when you connect the flux to chemical potential gradients the constant that comes is the mobility whereas the constant that connects the flux to concentration gradient is known as diffusivity we are trying to find out the relationship between diffusivity and mobility I have not introduced mobility yet I am going to define mobility at the end of this derivation.

But for now I am going to say that the flux of atoms of type 1is given by of course it is going against the gradient for the chemical potential so that is why a minus sign is there and the chemical potential gradient is there and the chemical potential gradient is multiplied by the total number of atoms and the composition and the velocity of that type of atoms under unit potential gradient so that is going to define the flux, and similarly you can define a flux for V atoms so you have a lattice in which V atoms are moving V atoms are moving.

So you have found out the flux for these two we are going to define the flux with respect to a particular frame of reference okay, so that is the next step that particular frame of reference is known as a reference plane it is called Matano interface so let me okay so this Matano interface

is a plane and it is a moving plane okay and this plane is defined in such a way that the net flux across this plane is zero okay for which the total flux okay.

So if you can identify a plane which is a moving plane with respect to which the total atomic flux is zero such an interface is called Matano interface, so I want to define the fluxes with respect to such an interface okay this again is probably a tutorial that we can do at some point is to show that if you want to define the flux of say for the B type of atoms or b or to type of atoms let me call that as J.

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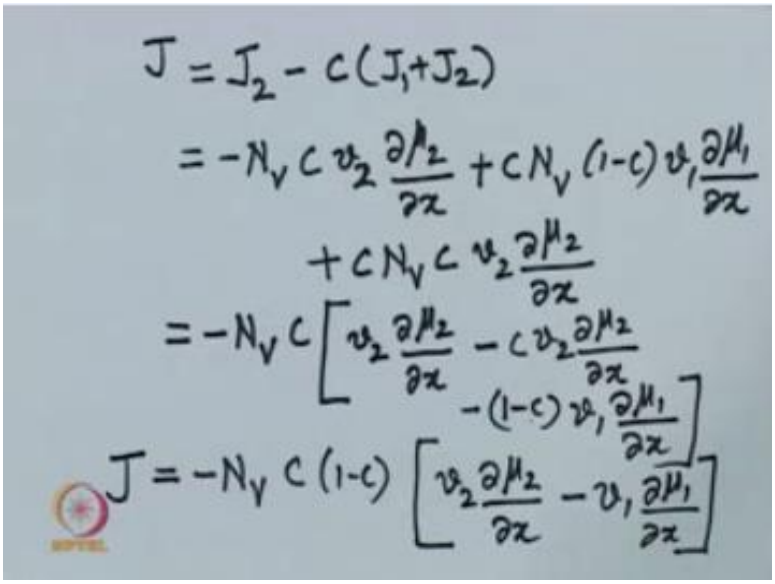

Because that is what is part of the classical Fick's law so that J is nothing but $J_2 - C(J_1+J_2)$, now why is this flux is this because we are trying to define the flux for atoms of type 2 with respect to Matano interface with respect to Matano interface if you do this is the flux expression this is what you can derive and show, so we will do it probably as a tutorial but for now you can accept that this is the plus if so then I can substitute.

Let me substitute for J_2, J_2 I said this - N_V CV_2 because this is J_2 ∂ μ_2/ ∂_x, and the similarly J_1 and J_2we have so let me also do that there is a minus sign and there is a minus sign in the flux J_1 and

J_2 so I am going to pull that minus sign I am going to put it with this so that is going to become C so CN_V 1 - C times V_1 times $\partial \mu_2 / \partial_x$, so that is this part J_1 and for J_2 we are going to have C N_V times another C V_2 times $\partial \mu_2 / \partial_x$ right so this is the expression J_2 - C times J_1 +J_2.

Is this expression okay so now let me do a little bit of algebra let me pull $-N_V$ C out common to all of it so then what do I get I get $V_2 \partial \mu_2 / \partial_x$ minus okay, so there is this N_V C which I have pulled so I will have C times V_2 times $\partial \mu_2 / \partial_x$, so from here if I pull C N_V, so I will get the minus 1 - c times v_1 times $\partial \mu_2 / \partial_x$ right, so as you can see $V_2 \partial \mu_2 / \partial_x$ minus C times we do $\partial \mu_2 / \partial_x$, so you can pull $v_2 \partial \mu_2 / \partial_x$ together so that will be 1 - C there is 1 - C here.

So let us pull all that together $-N_V$ C times 1 - c right so then what do you get because1 - c is gone so this is $v_2 \partial \mu_2 / \partial_x$ - 1 - C is full $V_1 \partial \mu_2 / \partial_x$ okay, so this is the flux so to remind ourselves again what did we do we took the we know the Fick's law which is written for atoms of type B the flux for atoms of type B is related to its concentration gradient that is Fick's first law but our interest is to correct the diffusivity which is relating the flux to the concentration gradient with mobility.

Which connects the flux with chemical potential gradient because that is the thermodynamically consistent way of doing this a fixed law works in some cases but this law this new type of Fick's law that you can think of always works because this always is saying that the system will spontaneously evolved in such a way that free energy is getting minimized right that is from where we got this.

So we did all those free energy curves and we tried to show that even though it looks like a pill diffusion if you look at chemical potentials chemical potential gradient is are in the right way for that diffusion to take this so keeping that in mind so we are trying to define the flux for type 1 atoms or type A atoms which is given by $-N_V$ 1 -C which is a composition of the A type of atoms V_1 which is the velocity of a type of atoms under unit potential gradient times the chemical potential gradient.

And the chemical potential is defined parrot okay so that is the reason why there is this N_V because remember the chemical potential was defined as the free energy the derivative with respect to adding some number of A atoms or number of B atoms that is what define the chemical potential so and then if you want to make it a concentration gradient if you want to relate it to concentration then there is this total number of atoms that you need to multiply in the same fashion for the flux of atoms of type 2 then it is N_V times C which is the concentration of B type of atoms.

V_2which is the velocity of atoms of component 2 or B type of atoms under unit potential gradient and $\partial \mu_2 / \partial_x$ okay, now these are the individual fluxes of a and B type of atoms but I want to define the flux of B type of atoms okay this is what my interest is this J is nothing but a quantity a flux which is defined with respect to what is known as a Matano interface what is a Matano interface Matano interface is a moving plane and that plane is defined by this condition namely that net flux across that plane is zero.

If you try to define the flux for B type of atoms with respect to Matano interface then that expression is given by this equation which is that the flux is equal to J_2- C J_1 +J_2t so all that we did is to substitute the expression we wrote for J_2 and J_1 and J_2 and I did a little bit of algebraic manipulation so I pull the N_VC first and then I realized that the first term inside has1 - C common if you pull 1 – C then it becomes J =-N_VC 1-C $V_2 \partial \mu_2 / \partial_x$ - $V_1 \partial \mu_2 / \partial_x$ okay.

So I am going to again do a little bit of manipulation on this you will understand the why and how I do the manipulation and that is what I will do in the next part of this lecture okay, so we are going to take this expression for the flux and we are going to do a little bit of algebraic manipulation a small manipulation to get to a place where we get an equation which looks similar to the Fick's law and then compared to identify how the diffusivity is connected to the mobility. Thank you.

NPTEL
Principal Investigator
IIT Bombay

Prof. R.K Shevgaonkar

Head CDEEP

Prof. V.M Gadre

Producer

Arun Kalwankar

Digital Video Cameraman

&Graphics Designer

Amin B Shaikh

Online Editor

&Digital Video Editor

Tushar Deshpande

Jr. Technical Assistant

Vijay Kedare

Teaching Assistants

Arijit Roy

G Kamalakshi

Sr. Web Designer

Bharati Sakpal

Research Assistant

Riya Surange

Sr. Web Designer

Bharati M. Sarang

Web Designer

Nisha Thakur

Project Attendant

Ravi Paswan

Vinayak Raut

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