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

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Module No.2
Lecture No.8
Tutorial – 7

Welcome in this tutorial we want to look at the mass conservation and understand what that means in terms of diffusion equation okay so what we are considering.

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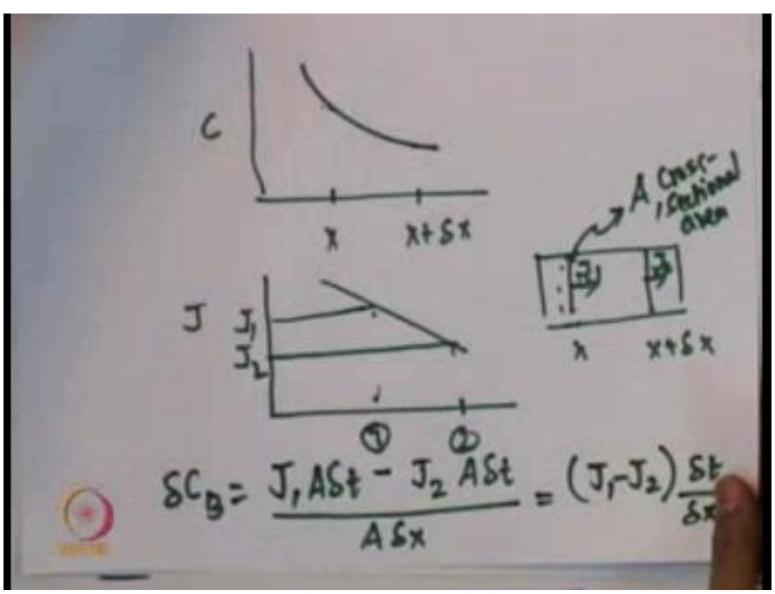

Is a composition versus position suppose we have some composition profile like this okay so let us consider a point X let us consider a point X +δ X okay so we want to look at the system which has a composition profile like that and then you can write the flux okay now the flux is going to be like this so this is J_1 at the point 1 and you are going to get flux J_2 at the point 2 okay so you have these two points right X and X +δX and you have a flux $J_1$and you have a flux J_2 okay now how much is the change in the concentration because of the fluxes okay let us assume that this cross-sectional area is A which is the cross-sectional area.

Now if you take this δ C_B that is the change in composition because of this flux is J_1 Aδt will give how much is the flux here – J_2 A δt that will give how much is the flux here / Aδ_X is basically going to give you the flux so that is nothing but J_1 – J_2 okay so the A & A are going to go away and you will get δt/ δX so that is the δC_B okay so let us rewrite this expression so we have.

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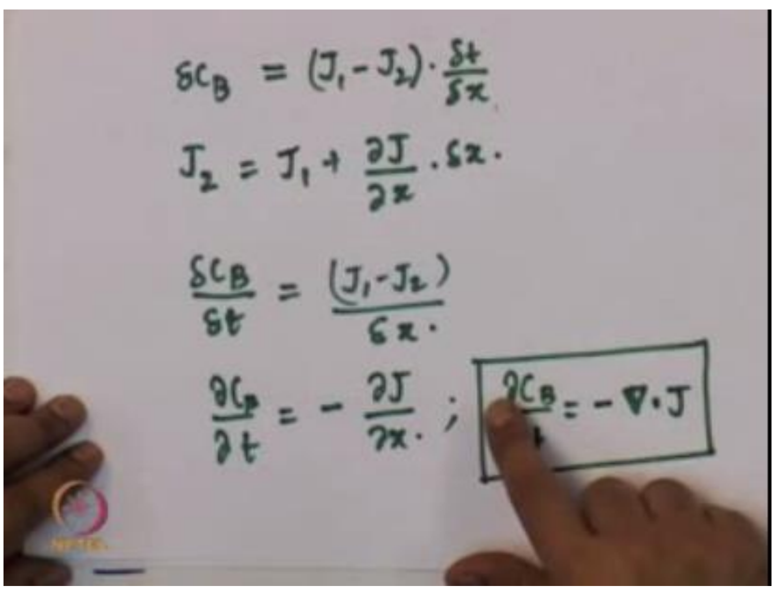

δC_B / δ C_B = J_1 – J_2. δt / δx okay but you can say that J_2 is nothing but J_1+ J_2 / ∂ x δx so we are assuming that the two points x and δx are quite x +δx are quite close to each other so you can say that the flux J_2 will be related to J_1 by expanding about J_1 through our Taylor series expansion you will get something like this so let us put this back so $J_1 – J_2$ will be - $\partial J \partial x \delta x$ so in other words $\delta C_B / \delta t$ will be = $J_1 – J_2 / \delta x$ and in the limit this δx going towards sub-zero one can show that $\partial C_B / \partial t$ is equal to minus $\partial J / \partial x$.

Now if you generalize it in three dimensions then you get doe $\partial C_B / \partial t$ is nothing but $\Delta. J$ in other words the rate of change of composition at any given point Is nothing but the negative of the δJ, J is the flux so you are taking the divergence and that basically gives you the rate of change of it in other words if you have more B atoms coming in then what is leaving at that point the composition is going to increase if you have less atoms coming in then what they are leaving at that point the composition is going to decrease and if the whatever number of B atoms are coming in that is what is going out that is δJ is 0 then the composition at that point is not going to change so this is basically related to the physical meaning of divergence also so basically this shows that mass conservation.

If you use then you get the so called the second law of Fick's law of diffusion so rate of change of concentration is basically -δJ and J is related to concentration through the Fick's first law if you put it together then you will get the so called a second law okay so this is what we wanted to prove that by looking at mass conservation you can derive this relationship between rate of change of concentration and the flux rather the divergence of the flux okay so that is what we have derived thank you.

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