Diffusion in Multicomponent Solids
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Lecture 27
Solution to Diffusion Equation: Periodic Boundary Conditions

Welcome to 27th lecture in the open course on Diffusion in Multicomponent Solids. In this lecture, we will go over one more boundary value problem with periodic boundary conditions. In this problem, initial concentration profile is represented by a square wave type of pattern, and we will solve the diffusion equation by separation of variables.

Last class we talked about homogenization problem. We solved the diffusion equation for periodic boundary condition pertaining to the homogenization. The initial condition there was that the concentration profile initially was sinusoidal type of wave. We just had one equation for C at x and t equal to 0.

Today, we will solve another problem in which we will solve the diffusion equation for periodic boundary condition. Here the initial profile is little different, we will deal with square wave type of profile to begin with.

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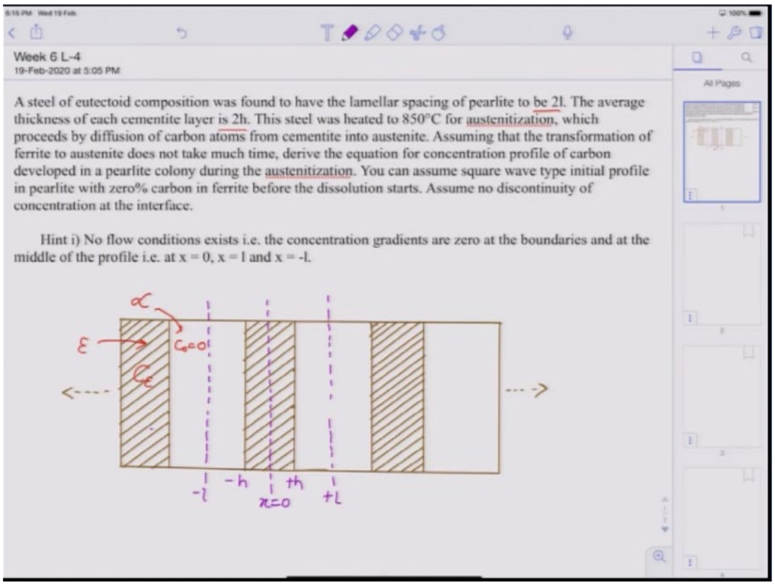

The problem is a steel of eutectoid composition was found to have the lamellar spacing of pearlite to be $2l$. So, the period here is $2l$, the average thickness of each cementite layer is

$2h$. This steel was heated to 850 °C for austenitization which proceeded by diffusion of carbon atoms from cementite into austenite.

Assuming that the transformation from ferrite to austenite does not take much time, derive the equation for concentration profile of carbon developed in a pearlite colony during the austenitization. You can assume square wave type initial profile in pearlite with 0 % carbon in ferrite before the dissolution starts. Assume no discontinuity of concentration at the interface.

So, we have a eutectoid steel here. The eutectoid microstructure basically is composed of alternate layers of ferrite and cementite, which is shown here in this figure. In this figure the hatched area is a cementite layer and the other layer is the ferrite layer. This is the profile to start with, the concentration of carbon in ferrite is 0. And the concentration in the cementite, let us denote it is as a C_{ε}.

Now we are dealing with pearlite spacing of $2l$, the period here is $2l$ and each cementite layer has a thickness of $2h$. If we consider our $x = 0$ at the center of any of the cementite layer, then the two edges of this cementite layer would be $x = -h$ and $x = +h$, and since the period is 2l, the center of the two adjacent ferrite layer will be $x = -l$, and $x = +l$.

Now this problem is little bit simplified here because this is actually a multiphase diffusion problem. We are having cementite and ferrite, two different phases. It is given that the ferrite quickly transforms to austenite, as soon as the steel is heated to the 850 °C temperature. So, we are dealing with austenite and cementite, and since the equilibrium concentrations of cementite and austenite are different, we expect that there should be a discontinuity at the interphase between cementite and austenite. But for the sake of solving this problem we are ignoring this discontinuity and we are treating the concentration profile as a continuous profile at any time $t > 0$,. At $t = 0$, it is a square wave type of profile, we are treating it just like a single phase diffusion condition. Also, we are assuming that diffusivity is constant.

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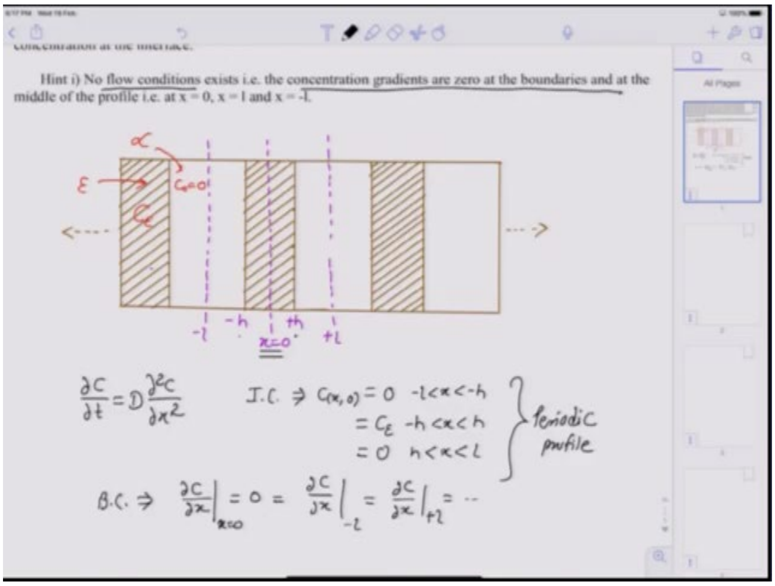

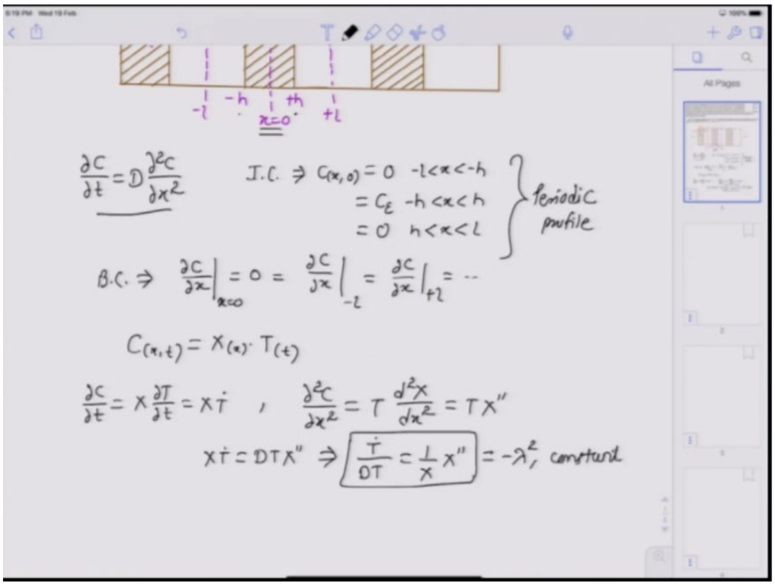

We are solving the diffusion equation which can be written as:

$$\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2}$$

The initial condition here is at $t = 0$ we know the concentration in any cementite layer is C_ε and in any ferrite which has been quickly transformed to austenite is 0:

$$I.C.: \quad C_{(x,0)} = 0 \qquad -l < x < -h$$

$$C_{(x,0)} = C_\varepsilon \qquad -h < x < h$$

$$C_{(x,0)} = 0 \qquad h < x < l$$

And the boundary conditions are a no flow condition which means the concentration gradients are zero at the boundaries and at the middle of the profile.

$$B.C.: \quad \left(\frac{\partial C}{\partial x}\right)_{x=0} = 0 = \left(\frac{\partial C}{\partial x}\right)_{-l} = \left(\frac{\partial C}{\partial x}\right)_{l} = \cdots$$

If you consider, middle of any layer, ferrite or cementite the concentration gradient is basically. And this is a periodic boundary condition, as we have a periodic profile here. We need to solve this equation, for periodic boundary condition, we can use separation of variable. Let us assume that $C_{(x,t)}$ can be expressed as an explicit function of x and t, we express it as:

$$C_{(x,t)} = X(x).T(t)$$

X is a function only of x, that is the distance coordinate, and T is function only of t, that is time. With this:

$$\frac{\partial C}{\partial t} = X\frac{\partial T}{\partial t}$$

and since T is only function of time t, we can replace this partial derivative with ordinary derivative, we can write:

$$\frac{\partial C}{\partial t} = X\frac{\partial T}{\partial t} = X\frac{dT}{dt} = X.\dot{T}$$

Similarly:

$$\frac{\partial^2 C}{\partial x^2} = T\frac{d^2 X}{dx^2} = TX''$$

If we substitute in the diffusion equation here, we get:

$$X\dot{T} = DTX''$$

which yields after rearranging:

$$\frac{\dot{T}}{DT} = \frac{1}{X}X''$$

Now if you look at this equation, the left hand side of this equation is only function of time t and the right hand side is only function of distance coordinate x. And x and t both are independent. This equality would be true, only if both the sides are equal to a constant, lets denote that constant as:

$$\frac{\dot{T}}{DT} = \frac{1}{X}X'' = -\lambda^2 = constant$$

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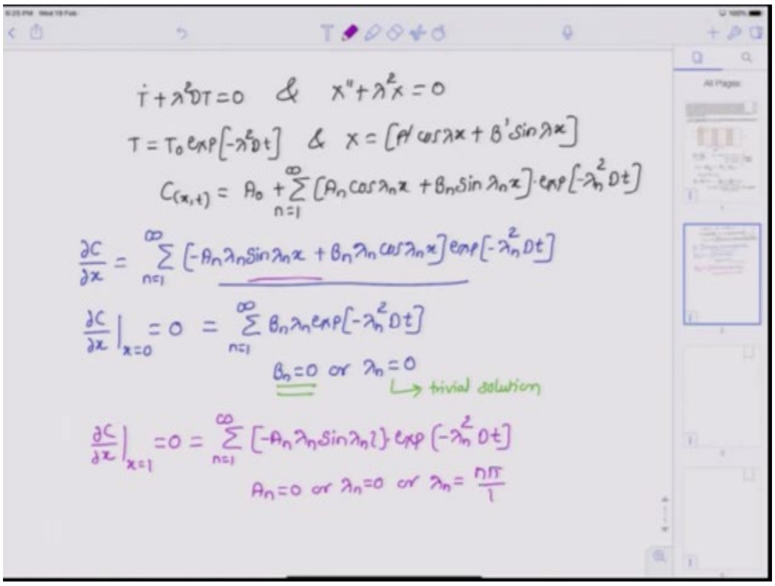

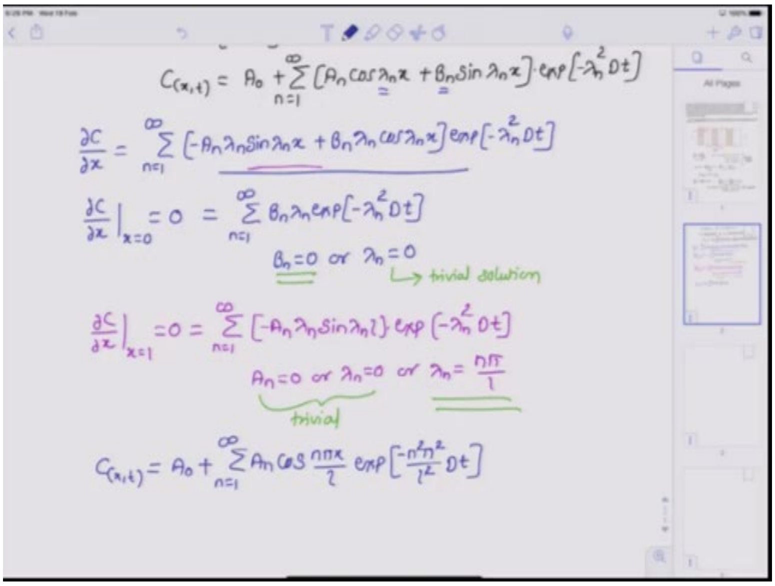

So, we get two individual differential equations one for T and one for X. We can write:

$$\dot{T} + \lambda^2 DT = 0 \qquad and \qquad X'' + \lambda^2 X = 0$$

The solutions for T and X are:

$$T = T_o \exp(-\lambda^2 Dt) \quad and \;\; X = A' cos\lambda x + B' sin\lambda x$$

Now the linear combination of the solutions will also be a solution (this will be true for large number of values of lambda) and we can express the function $C_{(x,t)}$ in the form of the series:

$$C_{(x,t)} = A_o + \sum_{n=1}^{\infty} (A_n cos\lambda_n x + B_n sin\lambda_n x) exp(-\lambda_n^2 Dt)$$

Where A_o is the value of $A_n$at $\lambda_n = 0$. Now we need to find out these constants, we use our initial and boundary conditions for this. First we will use the boundary condition. For this we need to evaluate derivative:

$$\frac{\partial C}{\partial x} = \sum_{n=1}^{\infty} (-A_n \lambda_n sin\lambda_n x + B_n \lambda_n cos\lambda_n x) exp(-\lambda_n^2 Dt)$$

Now:

$$\left(\frac{\partial C}{\partial x}\right)_{x=0} = 0 = \sum_{n=1}^{\infty} B_n \lambda_n exp(-\lambda_n^2 Dt)$$

as sin 0 is 0 and cos 0 is 1. Now for this to be true we should have either:

$$B_n = 0 \;\; or \quad \lambda_n = 0$$

But if we put $\lambda_n = 0$, then we get a trivial solution which will be independent of time here. So λ_n cannot be 0. All B_n have to be 0. Now at we have:

$$\left(\frac{\partial C}{\partial x}\right)_{x=l} = 0 = \sum_{n=1}^{\infty} [-A_n \lambda_n sin\lambda_n l] exp(-\lambda_n^2 Dt)$$

Now if this has to be 0 then either:

$$A_n = 0 \;\; or \quad \lambda_n = 0 \quad or \;\; \lambda_n = \frac{n\pi}{l}$$

Obviously, A_n and λ_n cannot be zero, otherwise we will get a trivial solution. So we have:

$$\lambda_n = \frac{n\pi}{l}$$

And we get:

$$C_{(x,t)} = A_o + \sum_{n=1}^{\infty} A_n cos\frac{n\pi x}{l} exp\left(-\frac{n^2\pi^2}{l^2}Dt\right) \quad (1)$$

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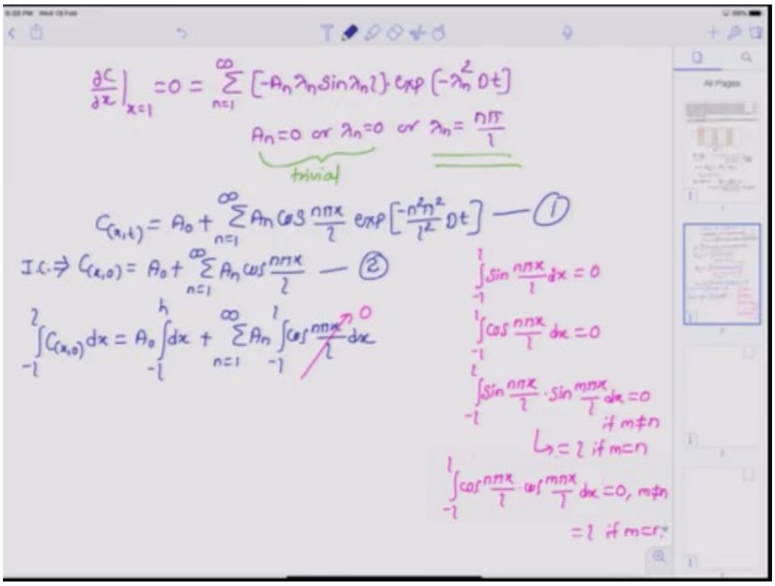

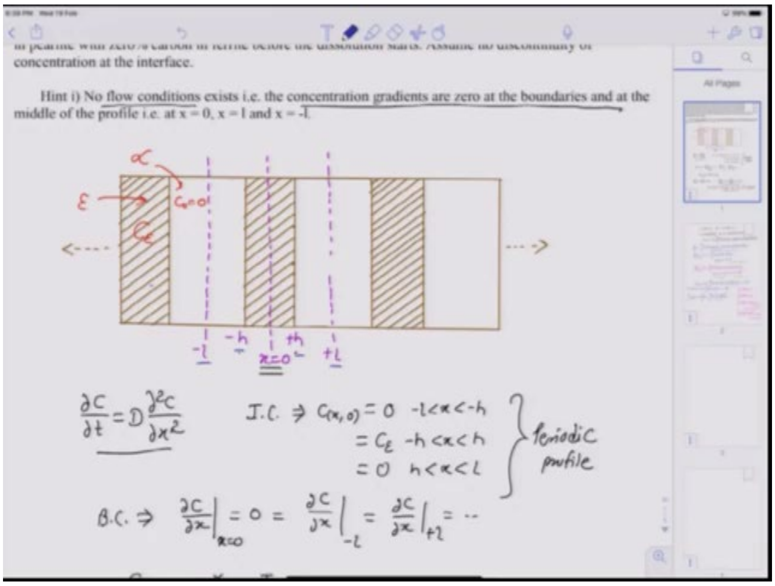

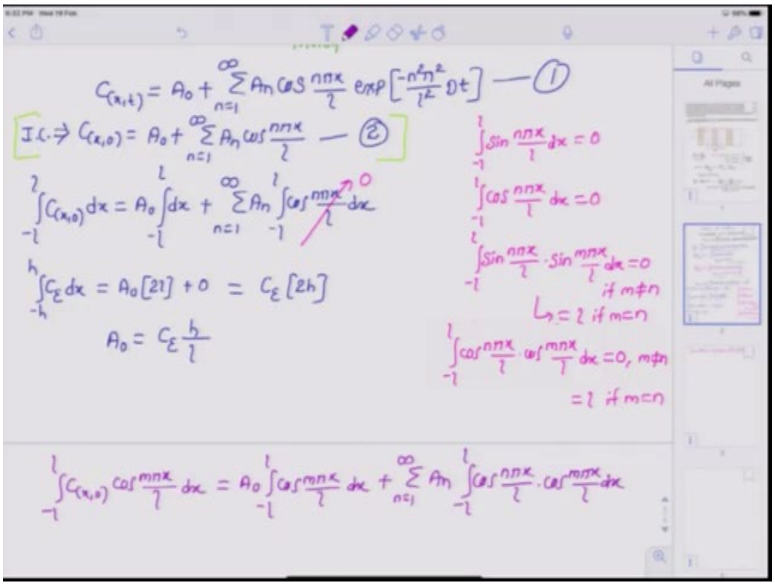

Now we need to find out, the values of A_o and A_n. In order to get values of this, we will use the properties of integral of periodic function. Sine n Pi x by l, cos n Pi x by l and their products. Let us quickly refresh these properties. We know:

$$\int_{-l}^{l} sin\frac{n\pi x}{l}dx = 0 \qquad , \qquad \int_{-l}^{l} cos\frac{n\pi x}{l}dx = 0$$

Then:

$$\int_{-l}^{l} sin\frac{n\pi x}{l}sin\frac{m\pi x}{l}dx = 0 \ \ , \ \ m \neq n$$

$$\int_{-l}^{l} sin\frac{n\pi x}{l}sin\frac{m\pi x}{l}dx = l \ \ , \ \ m = n$$

Both m and n here are integers. Similarly:

$$\int_{-l}^{l} cos\frac{n\pi x}{l}cos\frac{m\pi x}{l}dx = 0 \ \ , \ \ m \neq n$$

$$\int_{-l}^{l} cos\frac{n\pi x}{l}cos\frac{m\pi x}{l}dx = l \ \ , \ \ m = n$$

To make use of these, we will use the initial condition:

$$I.C.: \quad C_{(x,0)} = A_o + \sum_{n=1}^{\infty} A_n cos\frac{n\pi x}{l} \qquad (2)$$

Now to make use of the properties of the integrals, lets first take the integral on both side of equation 2. We get:

$$\int_{-l}^{l} C_{(x,0)} dx = A_o \int_{-l}^{l} dx + \sum_{n=1}^{\infty} A_n \int_{-l}^{l} cos\frac{n\pi x}{l} dx$$

$A_n's$ are constant so, we can take it outside the integral. We know between $-h$ to $-l$, and between h and l, $C_{(x,0)} = 0$. And between $-h$ to h, $C_{(x,0)}$ is C_ε. This should give:

$$\int_{-h}^{h} C_\varepsilon dx = A_o 2l + 0 = C_\varepsilon . 2h$$

As C_ε is constant, we get:

$$A_o = C_\varepsilon \frac{h}{l}$$

Now, we need the value of A_n. On multiplying both sides by $cos\frac{m\pi x}{l}$ we got:

$$\int_{-l}^{l} C_{(x,0)} cos\frac{m\pi x}{l} dx = A_o \int_{-l}^{l} cos\frac{m\pi x}{l} dx + \sum_{n=1}^{\infty} A_n \int_{-l}^{l} cos\frac{n\pi x}{l} cos\frac{m\pi x}{l} dx$$

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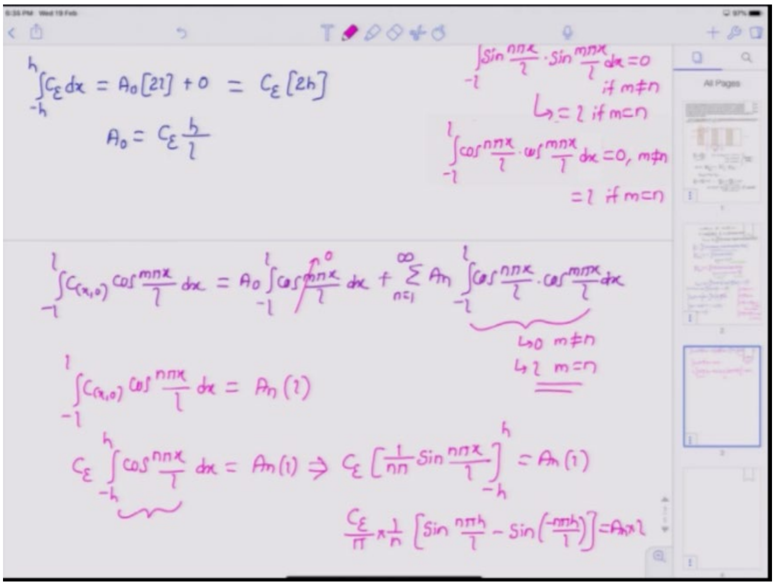

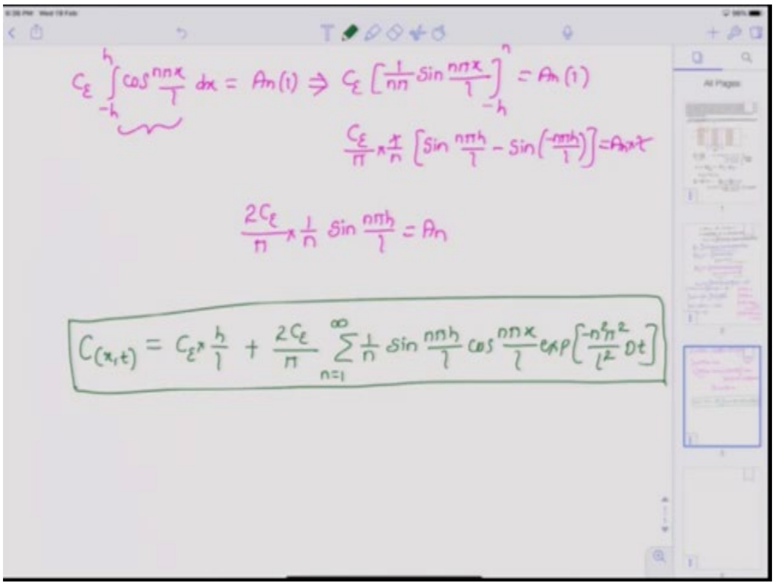

Now straight away, the first integral on the right hand side is 0. The second integral, we know this is 0 for all values of $m \neq n$ and this is equal to l for $m = n$. So $m = n$.

Because $m = n$ we will substitute m with n here. We can write:

$$\int_{-l}^{l} C_{(x,0)} cos \frac{n\pi x}{l} dx = A_n(l)$$

Again, $C_{(x,0)} = 0$ for the limits $-h$ to $-l$, and between h and l, and between $-h$ to h:

$$C_{(x,0)} = C_\varepsilon$$

We get:

$$C_\varepsilon \int_{-h}^{h} cos\frac{n\pi x}{l}dx = A_n(l)$$

If we evaluate this integral, you get:

$$C_\varepsilon \left[\frac{1}{n\pi} sin\frac{n\pi x}{l}\right]_{-h}^{h} = A_n(l)$$

$$\frac{C_\varepsilon}{n\pi}\left[sin\frac{n\pi h}{l} - sin\frac{-n\pi h}{l}\right] = A_n(l)$$

Following this we get the value of A_n as:

$$\frac{2C_\varepsilon}{n\pi} sin\frac{n\pi h}{l} = A_n$$

If we substitute for A_n and A_o, we get the solution for $C_{(x,t)}$ in the form of a series:

$$C_{(x,t)} = C_\varepsilon \frac{h}{l} + \frac{2C_\varepsilon}{\pi}\sum_{n=1}^{\infty}\frac{1}{n} sin\frac{n\pi h}{l} cos\frac{n\pi x}{l} exp\left(-\frac{n^2\pi^2}{l^2}Dt\right)$$

This is the solution that we have obtained and this is how we can work with periodic boundary conditions and solve the diffusion equation using first separation of variable and then using the series expansion. Again, we dealt here with the austenitization problem which actually is a multi-phase problem. The concentration profile will be little bit different because of the discontinuity in the concentration profile at the interphase at all times as long as the interphase is there.

We will see the more accurate type of profiles later when we study the multi-phase diffusion, but in order to understand how we solve the periodic boundary condition problem, I just over simplified it and just used it as a single phase diffusion problem. This gives us good flavor of solving the diffusion equation for periodic boundary conditions. We will stop here, thank you.