NPTEL
NATIONAL PROGRAMME ON
TECHNOLOGY ENHANCED LEARNING

IIT BOMBAY

CDEEP
IIT BOMBAY

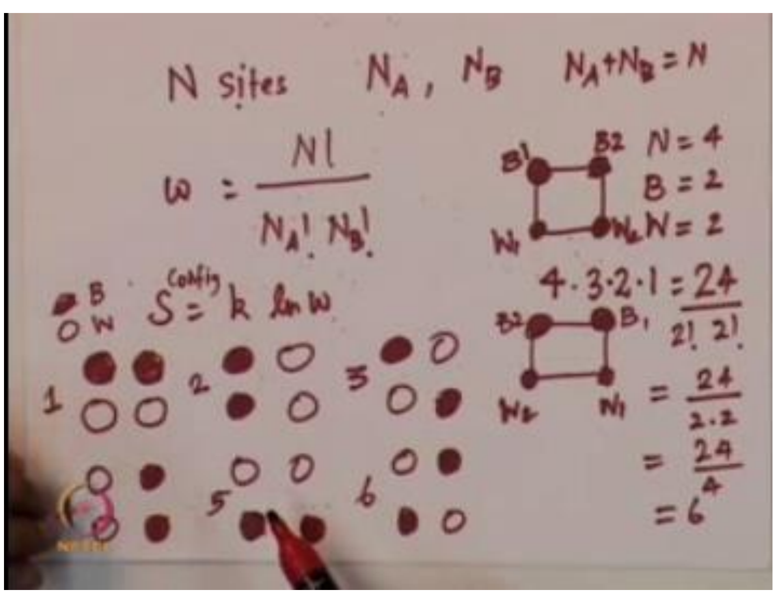
Phase field modeling; The materials science, Mathematics and Computational aspects

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

Module No.1
Lecture No.1
Tutorial – 2

Welcome to this tutorial in this tutorial we are trying to understand the expression that we write for configurationally entropy specifically we said that if you have N sites.

(Refer Slide Time: 00:29)



And so N is the number of sites and if you distribute N_A number of a atoms and N_B number of B atoms and N_A and N_B add up to N then we said that the total number of indistinguishable ways in which you can distribute this is given by N!/ N_A! N_B! So this is what we wrote ω and so s is k lane ω, so that is how the configurationally entropy was calculated and this is the number of microstates now why is this so.

So this is what we want to understand to do that I am going to take a very simple case I am going to take a lattice which has four points okay so N in this case is 4 and A I am going to take as black and B I am going to take as white let us say that I take two black balls and two white balls okay now you can think of the total number of ways in which you can distribute two black balls and two white balls on four sites and they can be calculated as follows.

Suppose I put the first blackball here B_1 then I will be left with one more black ball and two white balls so the one more black ball can go here or here or here so if one is given then there are three others and this one can go here or here or here or here so there are four sides for B_1 and now the next one B_2 that has one two three sides so there are 4 x 3 12 possibilities suppose if I also take the B_2 to be one of the sites then I am left with two sides.

So there are two items so they have to and the last one there is only one so there is 1 so 1x 2 x3 x 4 so that will be 24, so 24 is the actual number of ways in which you can distribute but we are going to assume that we are not going to distinguish between B_1 and B_2 suppose I put B_2 here this configuration looks indistinguishable from B_2 here and B_1 here okay so that means the this is not the total number of sites and similarly the w_1 and w_2.

So suppose W_1 was here and w_2 was here so I am not going to distinguish that between w_2 and W_1 here so that means the number of different ways in which similarly you know two of them can be distributed is given by 2! So it is 2! And another 2! So that is the total number of micro states that are available so 24 / 2 x 2 = 4 so 24 / 4 that is going to the 6 okay now what are these six indistinguishable ways in which the two black and two white atoms can be distributed.

So we can actually n miss them because this is a small number of things so let me take this so there are going to be 6 so let me do six of them okay so what are those six let me say black is filled and white is open so this is black and this is black so this is one configuration and it is possible that this is black and this is black so the other configuration is this is black and this is black right so there are only three in the other three of course.

So I am going to assume that this is black and this is black okay or this is black and this is black or I am going to assume that this is black this is black so these are the only six ways of course this is because of the indistinguishability so that is because we are not able to distinguish between these two and these two suppose if I am able to distinguish this as B_1 this as B_2 or this as B_2 to this as B_1.

So for everyone there will be two more right so there are so six and so into two that will be 12 and for the same with white also supposed I can distinguish this as w_1 w_2 and this as W_2 this as w_1 then for each one of these that will be two more so peril so we have now configuration one configuration two configuration three four five and six these are if the black and whites are indistinguishable if we can distinguish the blacks and whites then that will give for each four different ways the configuration will look the same.

But one will be called B_1 B_2 w_1 w_2 the other one will be called b_2 b_1 w_1 w_2 the other one will be called B_1 B_2 w_1 w_2 and the other one will be called $b_2b_1w_2w_1$ so like that so then 6 x 4 that is the total number of so if you have N sides and N_a and N_B number of A and B atoms or black and white items that you can distribute and if you are going to assume that among themselves A and B are indistinguishable then you have to divide by this $N_A! \, N_B!$ Otherwise the total number of ways in which you can distribute is just given by N! Okay.

So this is the basis of writing this ω expression once you have written that of course you can write the configurationally entropy which is what we did in the lecture okay so this is again a solved problem from Porter and easterly so this is the same example that is given taking a site with for taking a lattice with four sides and putting two black and two white there of course you can make it a little bit more complicated or slightly different.

Suppose you take three blacks and one white for example or three whites and one black for example so how many are the number of sides you can do in a similar fashion and you can use the formula and you can compare and see that they always match so, so this is this is how the counting of the configurations is done. 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

NATIONAL PROGRAMME ON TECHNOLOGY

ENHANCED LEARNING

(NPTEL)