Defects in Materials
Prof. M Sundararaman
Department of Metallurgical and Materials Engineering
Indian Institute of Technology, Madras

Lecture - 11
Point defect-Interstitial

So far we talked about different experimental techniques with which vacancy concentration formation energy as well as the migration energy of vacancies could be determined. Similarly for the interstitials also we require that same information interstitials what we require is only the concentration of the interstitials which are going to be there, and their migration energy. Because understand until the self interstitials because most of the time interstitials are elements which are added as impurities to the sample.

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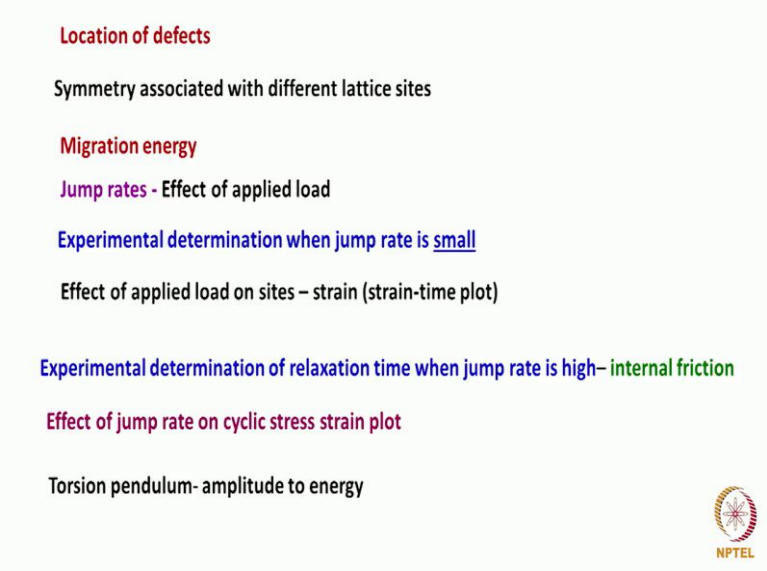

So, what are to get this information what we should know is that as I mentioned earlier like vacancies it is only removal of an atom from a lattice site, where as in the case of an interstitial what is essentially is going to happen is that there are many equivalent sites to which the interstitial can go and occupy. So, what we should know is, what is the site at which the interstitial is occupying, and as we had seen also that even if one interstitial is self interstitial is a generated in a lattice, it moves an adjacent atom and occupies a position which does not correspond to an interstitial site which is dictated by

crystallography right. So, it generates a distortion that also will have an effect on the mobility of this defect, now it is something like a complex which it forms.

So, just even if it occupies position a interstitial position intestacies position in the material, the symmetry associated with that site itself will give a lot of information about how the interstitial is going to behave. The other information which you require is the migration energy of the interstitial, how can we get this information. Generally we mentioned that the interstitial moves much faster compared to that of vacancies, so that the jump rate the rate at which interstitial jump from one site to another site is very high; this can be measured using 2 types of experiments one is an experiment which is like a tensile stress, you apply some load and try to find out how in response to that load the strain is a function of time develops.

That is another type of an experiment which we can perform, generally this type of an experiment is extremely useful when the jump rate is small; that means, that slowly it is taking place. The other type of an experiment is when the jump rate is rather very fast; in that case the type of experiment is being done is that instead of a static loading system we can do a cyclic loading that type of an experiment is what we call it as an internal friction experiment. This is what the other ways it is called as a torsion pendulum; this can be used to get information about the migration energy as well as the concentration of interstitial defect which are present in that material.

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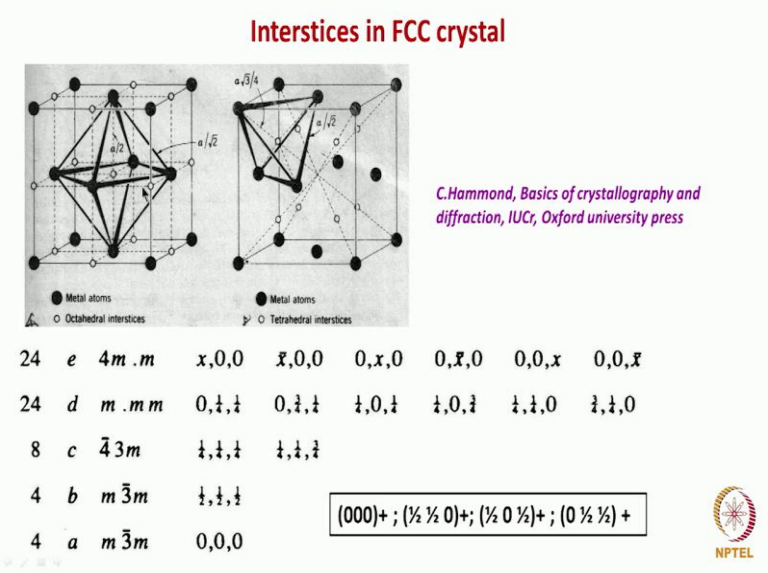

These are all the. So, before we go into these experiments let us just try to understand about the relationship between the symmetry of the sites which are mentioned where the interstitials can go and the distances of which adjacent atoms are there are located with respect to the interstices.

If you look at here this a vacancy we can have a octahedral as well as a tetrahedral sites right, the same information we get it this is from the relevant portion of the Wyckoff position table which is given in the international crystallography table I had given, from this we can notice that there are once atoms occupy these positions corresponding to 4 a, near position Wyckoff position; the b Wyckoff position we can have 4 positions are there; that means, that at the center are at the phase the corner edge phase middle; these are all the places where the impurity atom which is a small interstitial can come and occupy it.

The distance from this position to all the adjacent positions where the atoms are there or equal correct; so there is a symmetry which is being maintained and the same symmetry is reflected here also it is m three bar m it is cube symmetry. If you look here that tetrahedral interstices which are there here also around each of this center of this at the atoms are with respect to interstitial impurity, atoms are located at distance which are the same distance right. So, this also has got the symmetry which is a cubic symmetry. In fact, that we can see that there are other positions are like that where mirror symmetry is there this symmetry position if these two are not possible or if these two positions in allowing some elements have occupied it, then maybe the next element which we add will come into this position or this will be the interstices square to which suppose we add a third element which are verifying we whose size is very small they will try to occupy these positions.

So, essentially what is important here is that, it is quite symmetric in these; it does not matter suppose I apply a note to this sample, then what will happen? Take a sample fly a load which is essentially the elastic region, this sample will get elongated correct. So, when that gets elongated since it is a slightly symmetric all the sites are going to get elongated in the same way. There is no asymmetry which is involved this one. So, same energy is spent on irrespective of where that interstices whether it is at the center or if this edge or this particular edge it does not make any difference.

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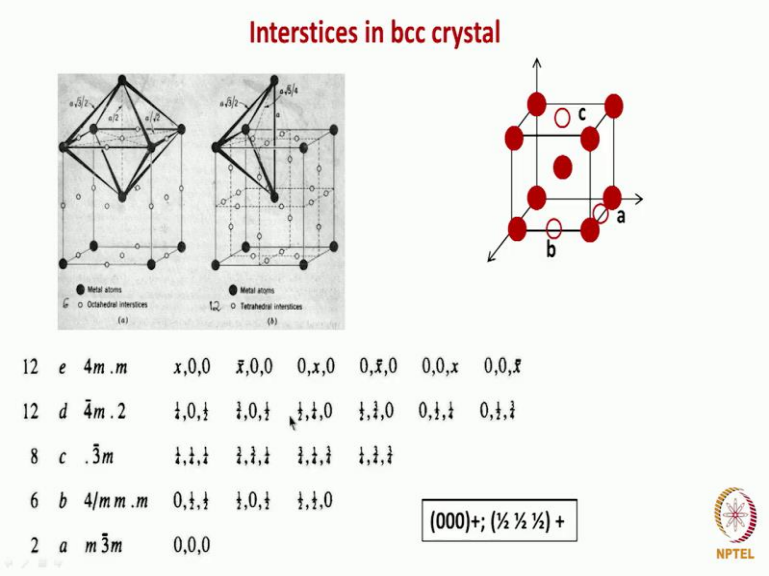

But let us look at the case in b c c material; the b c c material what happens here the 6 octahedral sites are there, in this particular case if an interstitial atom is put here to this interstitial site, the distances if we consider it the atoms on this phase are at a distance a by root 2, and atoms at the top and the bottom are at a by 2. There is an asymmetry which is associated with it and you look at the site symmetry corresponding to this this is essentially 4 by m m m. So, it is like a tetragonal symmetry; and what are the other equivalent sites which are there these sites are one here and another one here. So, if an interstitial atom occupy this position then this is the tetragonal distortion which is going to be there, that is because with which the distance is a by 2, the direction which is perpendicular to it the adjacent atoms are going to be at a by 4 correct.

So, the direction of here the distortion is along the c axis direction more, in this the distortion is along the b axis direction in these the destruction is along the c axis direction correct. So, that is what essentially I had shown marked it as a b and c, the interstitial positions three positions which I have shown with respect to b c c unit cell. And similarly if you look at the tetrahedral sites also; with respect to interstices position which interstitial occupies all atoms are not at the same position, and we look at this site symmetry corresponding to it, it is also shows that the tetragonal symmetry.

Now, let us take the case of octahedral one, as b c c material we are adding some impurities; this could be carbon, nitrogen or oxygen, atoms which I have got very small

size they go to interstitial positions then we can make out that three distinct positions are there depending upon the distraction which it will introduce correct; there is one a position, b position and c position because the strain which is if an interstitial comes here is going to be more in this direction compared to the directions which are perpendicular to this.

In this particular case what will happen; by probability if we look at it, any impurity which is added it has a possibility of occupying either a b or c position, if we add n impurities interstitials are added n by 3 will occupy a type position, n by 3 will occupy b type and n by 3 will occupy c type position. So, now, they are randomly distributed correct and each site will give rise to some extension in the sample, some tetragonal strain which will introduce. So, overall the tetragonal strain which is introducing introduces each one of them is going to be the same in all the three directions. So, overall there is an expansion which we see that sample correct there is no other change.

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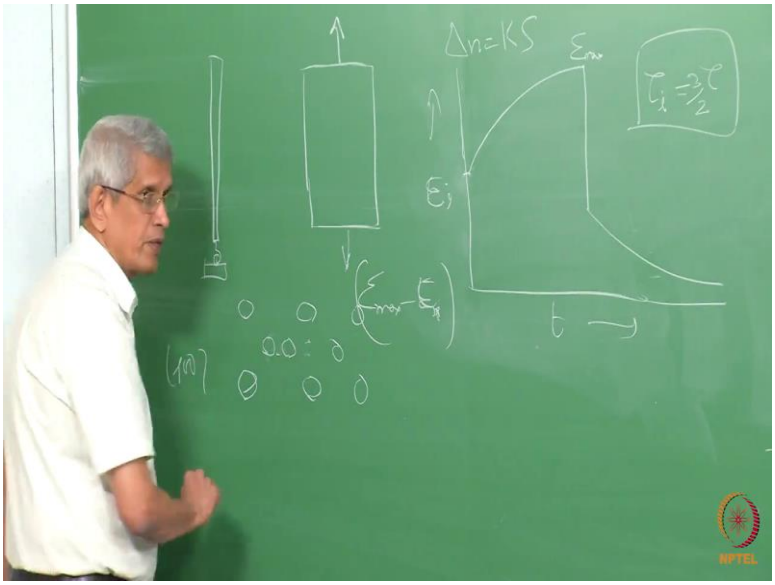

Now, the scenario will change suppose we add we apply a load like in this case if we apply a load then what is going to happen is that, and this load which is applied is very small. So, it is an elastic distortion, so the whole crystal is getting elongated in this direction the cubic one becomes slightly a tetragonal one right. So, when there is an increase in lattice parameter along this direction, now an interstitial occupying which

occupies this position the c position it finds that the energy which is required the strain is getting reduced.

So, there is a gain in energy it is easy for that to occupy that position correct whereas, in these 2 positions which is a and b type of a position, in this since elongation is going to be there and in this direction there is a slight compression is going to be there, if an atom tries to occupy that position the more energy is required to be there because a lot of compression is coming. What it will try to do naturally it will try to jump out from that position and try to go into an another position, but we know that the number of sites which are there are quite large all the three sites, and the concentration of that defect is much small compared to that, and we assume that there is not much of interaction between the defects that is the basis on which we are talking about this experiment.

Now, an attempt will try to jump from here to the both from a site as well as b site will try to jump into the c site; because only a few c sites are being occupied by interstitials correct. So, that depends upon what is rate, how many c sites are now still available for a interstitial atoms to jump from a and the b site correct and as they jump and try to occupy that site the number of sites available gets reduced, so an expression which we will get it is the rate at which it is going to reach that site that number is going to be an exponential form of an relationship it will come.

So, each site an interstitial atom is occupying, that is going to generate delta m equals some constant into some stress it will locally introduce correct. Or if an atom jumps from a this site to this site if it jumps, the strain is going to increase in that direction when interstitial atom jumps; that means, that there is going to be an elongation which is going to occur, and this process takes place as a function of time right. So, what we have done it is we have applied a load; when we apply a load what it will happen, that is an elongation that is we take a sample the hook which is there, I just put a load here very small load so that had very small increment in strain which is there introduce elastic strain. One should understand that one should distinguish it between the 2 types of experiments which we perform in a conventional machine tensile stress when we do, how you how do you do the stress.

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It is you control the strain the rate at which you are pulling the sample; here in this experiment what we are doing it is we are just applying the load, so the strain is instantaneous. So, if you try to plot time versus the strain, what is going to happen is that immediately corresponding to a load dictated by Hooke's law it will achieve that much of a strain.

Once that has been reached all the in that direction the lattice has been elongated, now the interstitials which are occupying a and the b positions will gradually try to jump into the c site position. Every time one of them jumps it will add to some increment in strain. That means that at that constant load as a function of time, the strain is going on increasing. So, what will happen we will be seeing that the strain gradually it is an exponential one it will and finally, be reach when all the atoms have jumped then it reaches a maximum value this is epsilon maximum we can tell.

So, the epsilon maximum the difference between this is an instantaneous load, instantaneous strain this difference is proportional to the concentration of the defects is it not. So, what is essentially happening is that, after the load has been applied and the material has deformed to that extent the elongation has taken place, now as a function of time there is an expansion of the sample which is going on this is called as the anelastic deformation.

Now, suppose we remove the load then immediately it will reach some value corresponding to this value what is it going to happen? That corresponds to that is to get dictated by this Hooke's law, how much corresponding to the load when we remove it will try to come back now, the lattice is being coming back to the original cubic symmetry. Now all sites are probable, so atom preferentially occupying one site is does not because it is going to be a strain which is going to be more, now it will try to jump to a as well as b sites, this will give rise to again an anelastic deformation, and it will be trying to come like this right this is the way the strain will look like central portion means.

Student: Determine the (Refer Time: 19:08) position does not have any symmetry (Refer Time: 19:09).

But if any interstitial has to occupy a particular position it will require a very high energy, if I any position which is available the symmetry and the energy is related what

is the energy which is required for that position to be occupied, only if all other positions are occupied then you can prefer to go to that position.

So, the delta n the number of defects which are jumping when the load is being applied that is proportional to n 0 into exponential minus t by 2, this sort of an expression which we can write we can write it.

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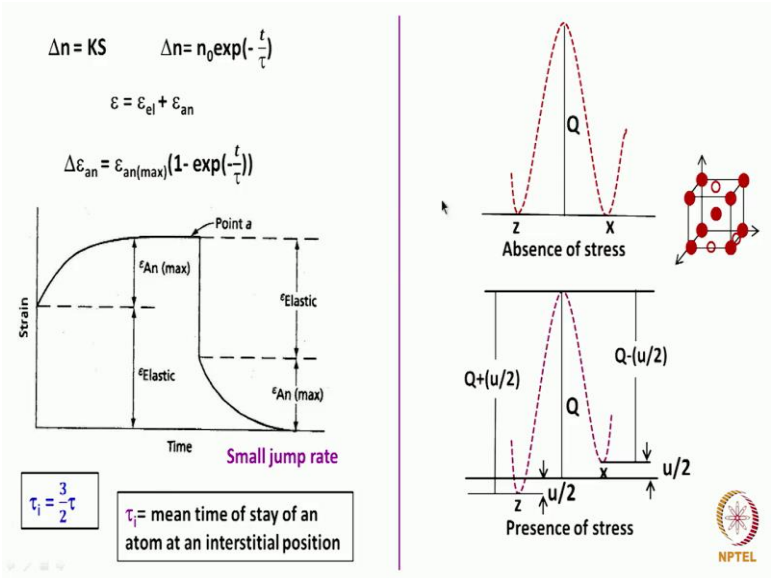

So, the total strain now equals for the same load in normal tensile stress it is essentially stress is proportional to strain, here not only that after the stress has been applied the strain takes some time for it to reach the maximum strain value; that means, there is a lag which is taking place between the stress and the strain. Some time difference which is happening and the total strain equals the elastic part plus the anelastic part. If you look at how the anelastic part will come because this delta in max depends upon delta n. So, similar to this we can write on another one expression correct for the strain itself; in any experiment which we perform tensile stress experiment we can immediately find out from the nature of this plot the tau can be determined.

And generally this tau is related to the rate at which the atoms jump by this formula, this tau this is the sort of relationship this part of the derivation I am not going into how these are related. This is related to atom jumping from one site to another what is the value which is required is tau I jumped it that is determined upon what the tau which will determine from this plot these are this is valid for all these experiments. The same thing

we can consider it from an energetic point of view also, here if we look at it when in the absence of a stress if an atom jumps from an a site to a b site, it is going to reach a position which will have the same energy right only thing is that it has to overcome an energy barrier.

Suppose the load is being applied now how it modifies the energy barrier? Already the atom in the a site the strain is more. So, it requires less energy to jump from that site to a c site, and if you look with respect to a potential which is from the c site under the application of the tensile load if an interstitial atom has to jump to the a site, the potential barrier which it has to overcome is actually q plus u by 2; where u is essentially is the energy corresponding to applied strain.

So, from this we can make out that probability wise even under the application of the load that is a probability that atom can jump from c site to a site or b site, but from a site and b site also it can jump to this one, but that is a bias towards jumping from a and b towards c site is more compared to that of the one from c site to the other site. Using this information only this derivation has to be made, but that part of it I am just leaving it, but let us get along with this experiment.

In this experiment if you have to measure this anelastic deformation, suppose it moves very fast, the jumping of the atom from a site and b site to a c site is occurring from this site to this site occur so fast takes a fraction of a millisecond, but what happens by the time we have applied the load you find that that is also occurred. So, the total strain as a function of time we are not able to see it, if the jump rate is rather slow takes minutes or hours then we can see that gradually the sort of the change could be measured.

Suppose m rates are really fast, this experiment this sort of experiment will not give accurate information about the rate at which atoms are jumping, for which the cyclic deformation test is used which is essentially nothing, but a torsion pendulum. In a torsion pendulum what is being done, the wire is taken of the sample it is held rigidly at the top or some specific length, then at the bottom we have an inertia bar to which we can apply some load also.

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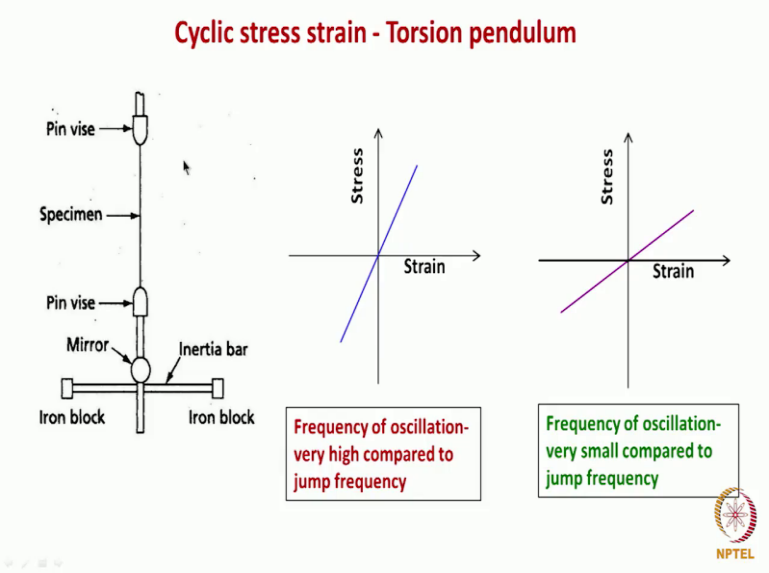

Then what you do it is we just twist the bar a little bit, depending upon where we keep that load and twist it we can change the frequency with which we are trying the, but this is like a pendulum this pendulum will go on oscillating correct. What will happen if you do this experiment in this room then since the air is going to be there everything this pendulum moves like this, that air gives a damping resistance; because of which after some time it will come to 0 amplitude will get reduced to 0, but at the same time when that amplitude is extremely small damping amplitude, the frequency is not getting affected.

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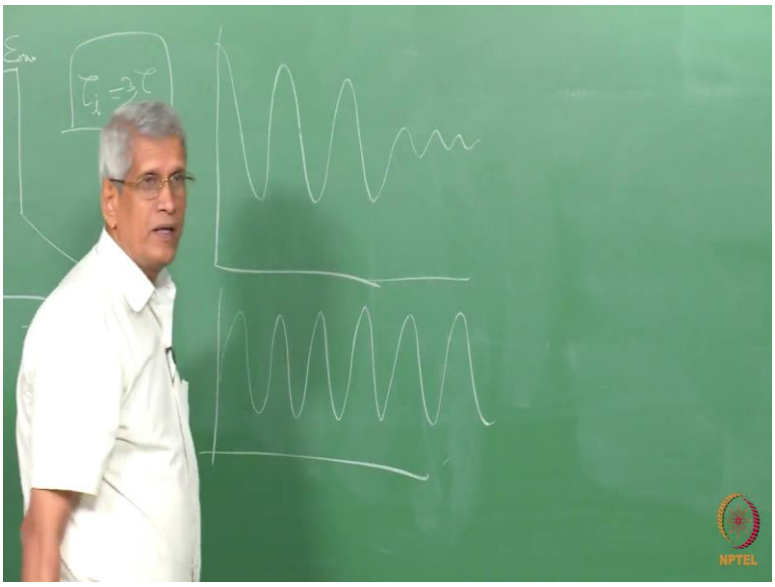

But the amplitude of this pendulum if you look at it, it will start from here, but with the same frequency it will just like this reaches 0 value correct.

This we have to talking with respect to a damping externally; suppose in the material itself there are some defects which are jumping from one to the other which is taking place, this jump itself is if it is random that can generate a preferential jump which it takes place it can also produce a damping in the material, this damping also will try to bring down the amplitude. So, if you can measure how this damping is taking place, look at this plot we can get some information about the migration energy, this is what is done in this experiment.

Now, we will talk about the details about this experiment; let us consider a few cases one case is that I am doing this experiment, the oscillation is being done with a frequency which is very fast. If I do this experiment at a very fast frequency what happens is that, the rate at which atoms are jumping is rather slow then it will not be able to follow this moment. So, it will behave like an ideal pendulum then how will the stress strain plot look like it look like, because it is going from one to other compression to tensile it will be essentially nothing, but a straight line correct this is how the plot will look like.

Now, we do an experiment in another way where the frequency of the pendulum at the period with which we are doing it so large, that the pendulum is able to accommodate or the frequency in which the jump take place is such a much faster rate compared to the oscillation frequency of the pendulum. And in such a case at every instant of time when we do this for applied stress, the full anelastic deformation is also able to take care of it. In such a case how will this stress strain plot look like corresponding to this one you have any idea?

Student: (Refer Time: 28:38).

No the stress is applied stress that remain. So, the strain increases. So, the plot will look like this right the slope of the plot will come down this is the way it will behave correct.

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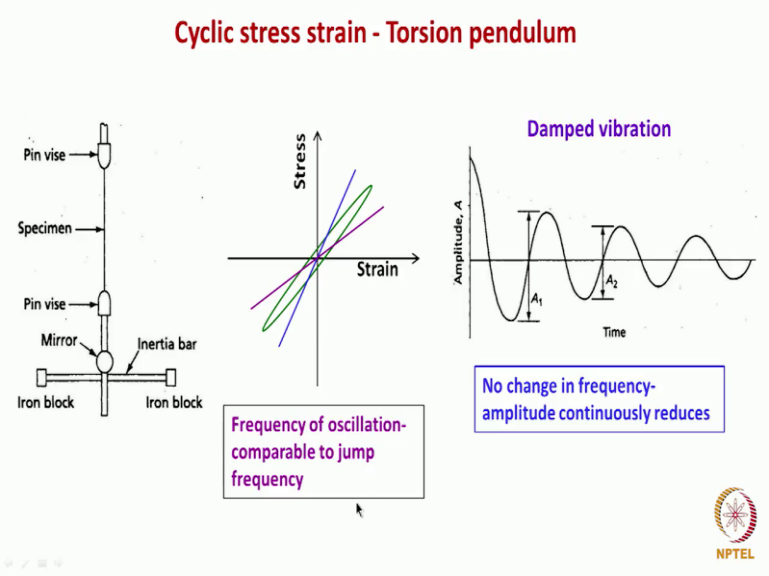

Now, let us see the case where the oscillation frequency and the jump frequency are close to each other. In such a situation what we are going to face is essentially that the hysteresis loop will come, it is not completely able to move its trying to move in the direction. So, now, it will look like a like fatigue test when we do, we get a or get a hysteresis loop this a type of a loop will take.

That is during each part of the cycle there is a loss in energy; in a pendulum in a normal hysteresis cycle especially in a fatigue test how do we find out that half amplitude of the stress into strain we can find out the energy, here what it will happen what is the manifestation of the hysteresis loss.

Student: (Refer Time: 30:02).

Area under the curve, but in the experiment amplitude is getting reduced. Where the amplitude is coming down if there is no resistance damping is there it should move with the same amplitude right in a case where that there is no damping, it should have been for an infinite time it should move like this. Now what is happening is that when since it is going to be there this gradually gets reduced; for any cyclic test how do you find out the intensity? Intensity is proportional to the area which you can take strain a squared correct.

Student: (Refer Time: 30:50).

Yes.

Student: (Refer Time: 30:51) group also circle (Refer Time: 30:54).

It will happen gradually it will happen. So, essentially what I just wanted to show you that it is an energy loss which is going to be there. So, this if we try to look at it this is the way, so the energy loss per cycle.

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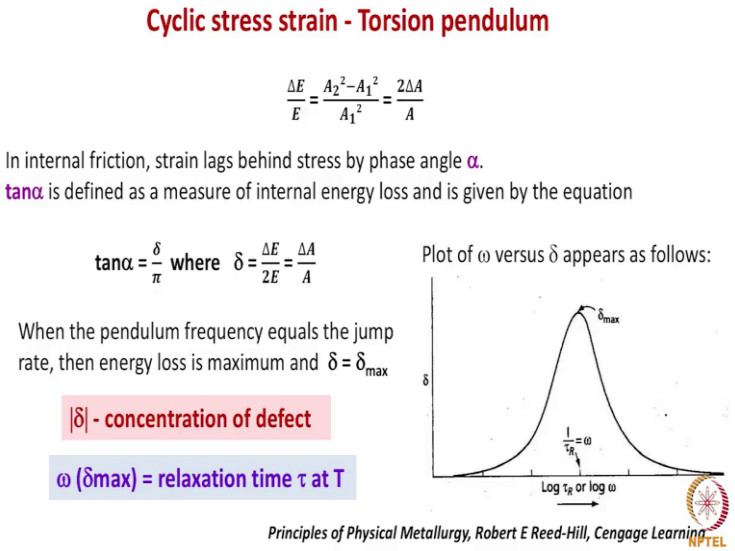

How we can generate it is that, what is going to be the amplitude on each of this location. If it this is the amplitude here is e a one and here is the amplitude e a 2, amplitude square is a relation to the energy then a 2 squared minus a 1 squared by a 1 squared this formula, then if we do some simple algebra we can find that this is twice delta a by a. What is delta a is the difference between the amplitude of successive cycle divided by the average amplitude, this is nothing, but equal to the energy loss per cycle this is how we can relate it.

And this is same thing if you look with respect to time what happens? When the stress has reached a maximum, the strain has not reached a maximum strain reaches a maximum after some time correct. So, in any electrical circuit we say that when the voltage and the current when they are not in the same phase, we it that is a lag which is there. Similar to that here also we can denote it by a lag, how much is the lag which is going to take place.

Student: (Refer Time: 32:42).

Anelastic two part of the deformation.

Student: (Refer Time: 32:46).

Anelastic part of it; so the same thing which we are calling is the tan alpha, we can define exactly in the same ways using the electrical circuit we can this how it is being defined.

This I had just written the essential value and generally in electrical circuits what we say that this is by a function delta we denote it, that is nothing, but equal to tan alpha pi into tan alpha.

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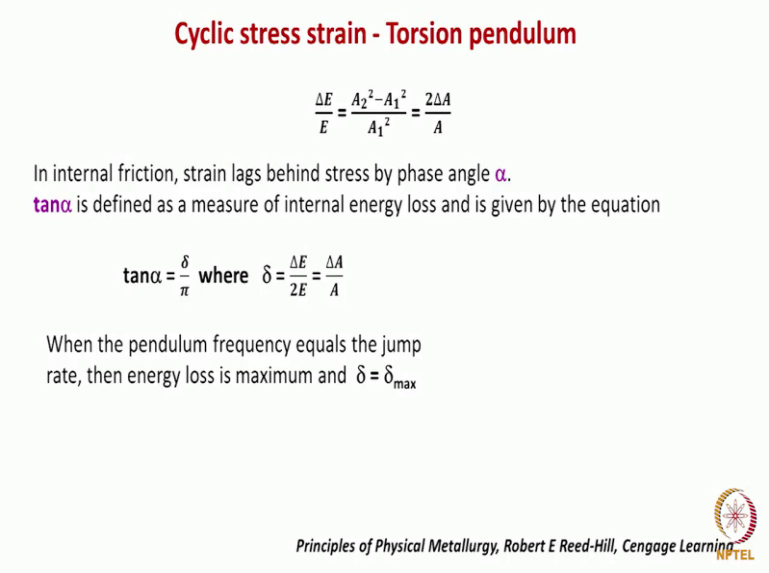

So, what we are able to when the rate at which the pendulum is moving. If the frequency of amplitude of the pendulum what we are giving it turns out to be the same as the rate at which it is jumping from one site to the other site, if the jump frequency they match perfectly, then the delta will have the maximum value will come delta max that is the lag will be maximum.

So, this lag itself is a measure and that depends upon how many of the defect concentration or the interstitial concentration is present. The experiment what is it being done we do not know what is the concentration of the defect, so what we do is that, you

ki at a particular temperature do this experiment at one frequency; you find some delta value will come lag then you do it at another frequency. That means, that the amplitude at which these are going to change the ratio of the amplitudes is continuously going to change depending upon the frequency at a particular temperature correct, and that is a measure of the delta also. Then if we just go on doing it for some time, it will reach a maximum value lag and again it will decrease. So, if you plot this delta versus the applied frequency, these are all the terms which are used do not bother about that we will be getting a plot like this right.

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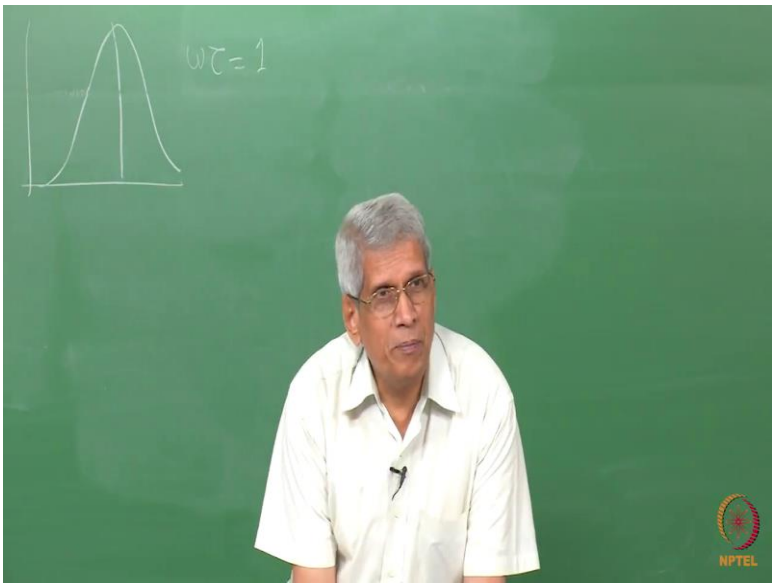

This plot is essentially. So, what we can find out is at a particular temperature to reach the maximum delta value, what is the frequency the oscillation frequency of the pendulum.

Now, and this frequency can be related to directly to the jump rate also. So, essentially what it will be that this omega into this one, equals delta equals one this is how the expression will be. I do it this experiment at another temperature just varying this frequency, then what will happen the frequency at which the maximum of delta occurs, oscillation frequency external oscillation frequency which you are imposing on the crystals that will be different under sample. So, not only this so delta is a concentration delta and omega at maximum delta max depends upon the relaxation time tau, these are all the 2 factors which we get it.

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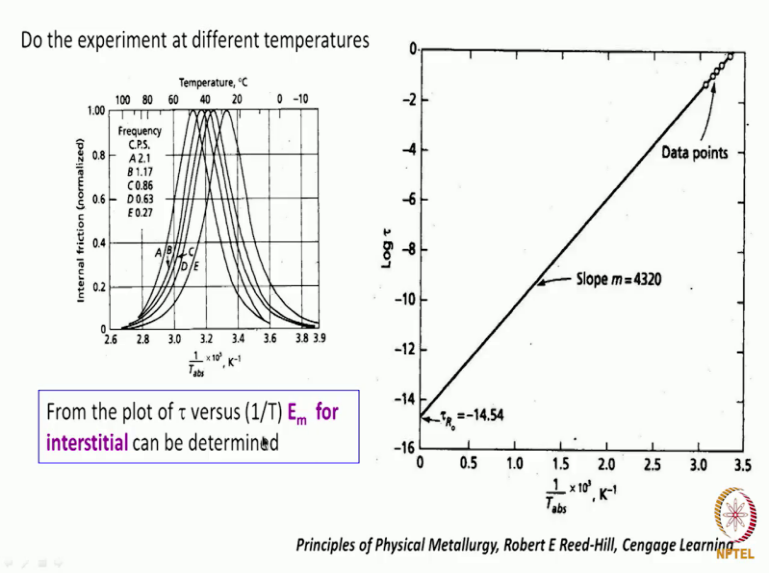

Now, if you do this experiment at different temperatures, this is a sort of a plot which we will be getting it and this delta is called as the internal friction coefficient that represents the internal friction. So, the maximum value at each temperature for different that is frequencies are going to change. In this particular type of experiment what they have done if they have done it in a different way because it is a data can be collected by doing experiment in a different choosing a different matrix format, what they have done?

They have kept the frequency constant and then just change the temperature; at each temperature you find out how the amplitude is varying, then do with another frequency just vary the temperature whichever way we do it, it is a matrix which we are generating with respect to frequency and temperature and trying to have this plot. From this plot what we can get it is the frequency which we are corresponds to a frequency of oscillation, with which you are able to find out when the delta max bit that is the internal friction coefficient become a maximum that corresponds to the jump rate.

We know that the jump rate is corresponding to inverse of temperature. So, if you try to plot the log of tau versus one by t, the slope of this line will get information about the migration energy correct. In these the defect concentration is already decided it is already has been added to the sample correct. So, essentially what this relationship depends upon is only on the migration correct, but in this experiment what is it which is very important about this experiment is that how exactly this experiment is done.

In the pendulum which is there at the end of it we attach a mirror, this is the mirror which is attached. When the pendulum moves this mirror also moves, the same oscillation it, moves what is being done is that you have a torch light a not torch light a laser beam which is falling onto the pendulum and that is most it will be deflected you have you can have position sensitive detector and collect this oscillation, and since it is kept at a distance it is magnified information which we get it. So, that this amplitude variation could be measured very sensitively, that is what is very important to get accurate information correct that is what essentially is being done.

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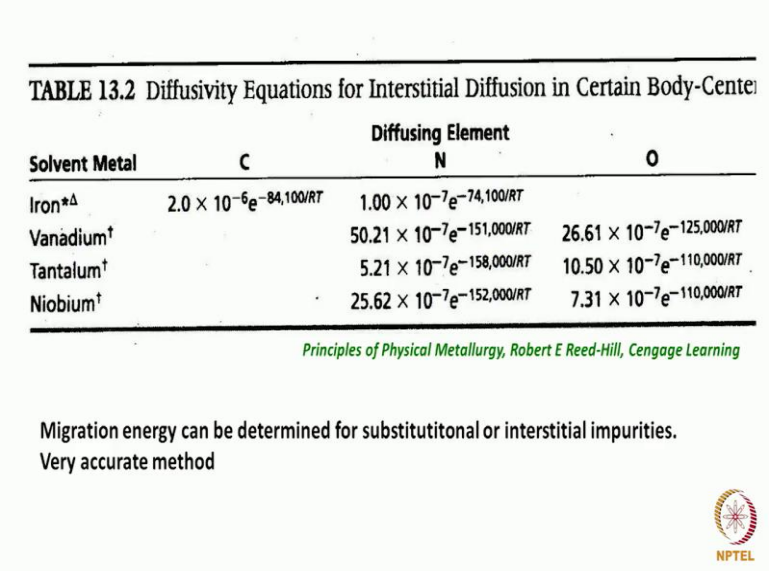

So, with this experiment what we are able to do is that we can measure the migration energy for different types of interstitials which we can get it. This is what the value which is being given for one more here, these around the 74.1 kilocalorie, another is for vanadium in which carbon nitrogen oxygen different elements it has been determined. Not only that since we are talking about defects moment, even in substitutional impurities the same thing could be done, only thing is that that jump rates will be at the higher temperatures correct.

So, this experiment could be performed for the interstitial or substitutional impurities we can find out, and another is says suppose a self interstitial is there the self interstitial when it occupies a position it is not occupying the position which is dictated by the crystallographic or the geometrical crystallography. It occupies a position like for

example, in a simple cubic 1 1 0 0 says if you look at it, or the inner c c if it is going to be here, this is how the 1 0 0 phase the atoms are looking like if you add an interstitial it will be coming to this position. So, essentially what it does it is that since the position of atoms are quite closed by; now it takes a position where right when this sort of a position which occupies if you look at the adjacent atoms they are not all at the same distance correct.

So, it has changed a distortion which it has introduced. Now this itself we are looking at one what are the possibilities with respect to other phase it could be, it could take place with respect to this direction there are many three possibilities which exist correct. So, essentially when these defect have to move, it can something like this can move like this, like this like this like this it can move, if you have a different way in which it will be moving correct.

Student: (Refer Time: 42:35) coupled moment.

Coupled moment then similarly if you have a not only single interstitial, suppose it is a complex which is moving then it will have a different jump rates. So, by doing this experiment we can identify now if you know that if not only the way the defect is somewhere looking at the migration energy, we can get some information about indirect information the structure of the defect configuration itself.

What is the basic problem essentially which is being seen is a very nice simple experiment, but you find that this experiment is hardly only very few places this sort of setup and the setup is very simple to do correct. It does not take much of a time or a energy to setup, what is important is that the room when we do the experiment it will not be there even a small vibration then you will not be able to get the measurements. That is a precaution which has to be taken to doing this experiment; otherwise it is a very neat very accurate method with which we can find out both the concentration as well as the migration energy.

So, now if you look that what we have done, we have these are all the things if you summarize the last 4 lectures we have looked at the point defects starting from the different type of defects which can be present, the defects in metallic, ordered alloys as well as in ionic materials, then what is the type of a theoretical calculation or equation which is available for finding out the equilibrium concentration of vacancies, then what

are the experimental techniques which are available and their relative merits and demerits also, with which we can get information about the concentration of the defects their formation energy as well as this migration energy.

So, basic information which is the both experimental as well as theoretical information, which is necessary to characterize point defects we have covered in this last 4 lectures. Now we will go from here to talk about that other type of defects like dislocations we will start, before that some basic information which is necessary regarding stress and strain and the nature of stress and strain these aspects we will start discussing in the next few classes.

We will stop here now anyway I will give some assignments also by working out that assignments one will get much better idea about this topic.