Defects in Materials
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Lecture - 23
Chemical Force on Dislocation

Welcome you to the course on defects in materials. In the last class, we have discussed about the forces, which are acting between dislocations; and also in the presence of an external field or external stress what is the direction in which the force will be acting on the dislocation, this we have looked at for a pure screw and a pure edge dislocation.

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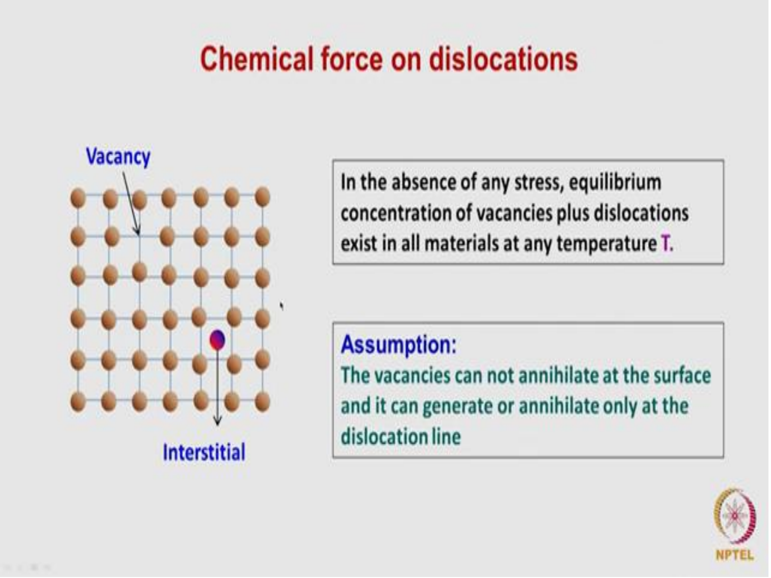

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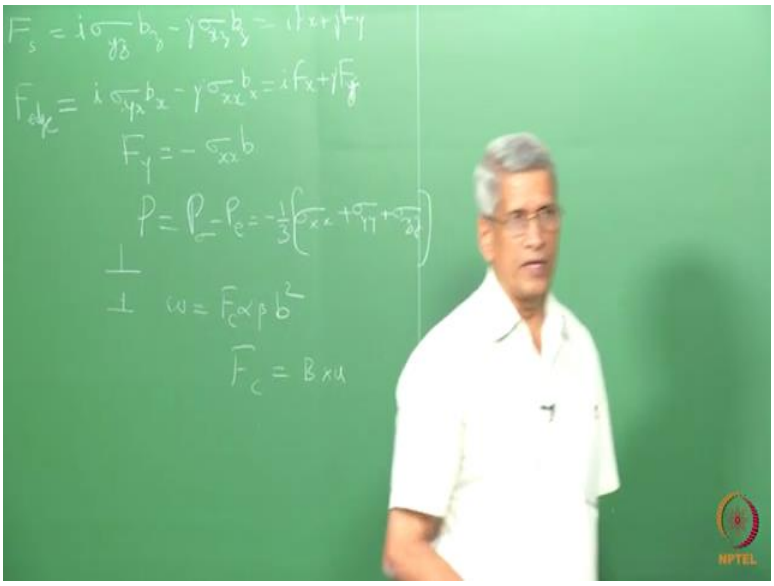

And what we will do today is that at that time when we looked at these defects in material, one important thing which was there was there when we looked at the force on a screw dislocation, we had one component i sigma y z into b z j, these are all both are shear stresses. So, this force and can be written as nothing but i into F x plus j into F y correct these are all the components in the x and y-direction. But if you look at the components in the x and y-direction, it is essentially a shear stress which is acting on the dislocation. Whereas, when we derived an expression for the force acting on a edge dislocation in this case it is, in this one if you look here this is a shear stress the application of the shear stress that develops a component of a force is i into F x that is force in the x-direction. Whereas, the tensile stress which is being applied to the material that generates a force essentially in the y-direction correct, y-direction means that x-direction is where that slip plane slip direction is there this is perpendicular to the slip plane your force is generated.

This does not happen in the case of a screw dislocation it is only a shear force, which is coming. Whereas, here we have a force which is perpendicular to the slip plane is coming that is if a edge dislocation has to move in that direction, the first thing which has to happen is that some vacancies have to be generated. What will be the consequence of this vacancies and this itself generates a force, which is called as a chemical force this is what we will discuss in today's lecture.

So, here what I have done is I had just shown the two-dimensional lattice with a vacancy as well as an interstitial, this is what we call it as a generally as a Schottky defect. We can find out the concentration of the vacancies, which are going to be there, because earlier when we derived the equilibrium concentration of vacancies. We assume that the material contains only point defect correct that is the way we did it. But normally the material always contains dislocations, and dislocations and vacancies both are present and they are in equilibrium.

If we apply a stress like any tensile stress if we apply to the material, then vacancies can be generated correct. The derivation which we are going to follow, we make an assumption that the vacancies which are generated by the moment of the dislocation, they can annihilate only at the dislocation that is the vacancies cannot escape out of the sample surface. This case can happen in real materials, when we consider temperatures below 0.5 t m vacancies may be mobile, but the excess vacancies which are being produced. The mobility is not sufficient for them to come out of the sample surface. We can consider that as one particular case where this sort of a situation can happen. Here we make an assumption that whatever the vacancies which are produced by dislocation moving up or down vacancies which are produced or annihilated, these vacancies the sink also is only the dislocation that is the assumption under which all these derivations are being done.

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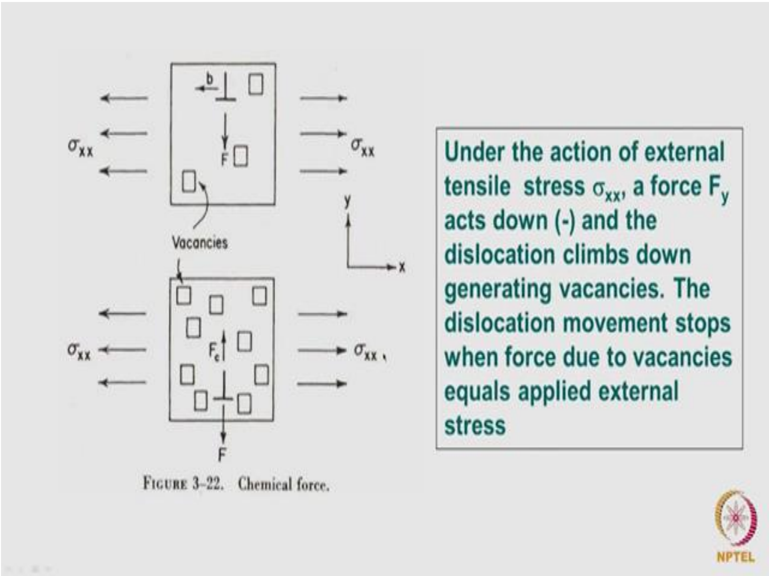

This picture essentially shows that in the absence of a stress, which is being applied the vacancies and dislocations are in equilibrium. Let us physical picture, we will try to have then we go into the mathematics of it. And if we apply a tensile stress sigma x x, as we mentioned in the last class, when a tensile stress is being applied, in the case the extra plane will try to come down. If the extra plane has to come down means essentially it is equivalent to some atoms from the bulk of the material come to the end of this dislocation and join together here a row that is way the dislocation, this will be equivalent to the dislocation a line going down correct, this is exactly what will happen. So, if that happens, when an atom has been removed from the lattice, vacancies are created. Now, the dislocation is under the action of this force this force the expression is already given by this equation that this force F y is equal to minus sigma x x into b that information is already available.

So, as the dislocation comes down, when the vacancies are created, these vacancies will try to generate, because if they are not going out of the sample surface. This is going to generate a pressure inside the material or some sort of a force that force will try to act in a direction, which is opposite to the direction in which the external force is acting on the dislocation. With these two forces become equal then the dislocation will no longer move. So, essentially what happens is that lots of dislocations will be generated in the material by non-conservative motion of dislocations; this is essentially what is being written here.

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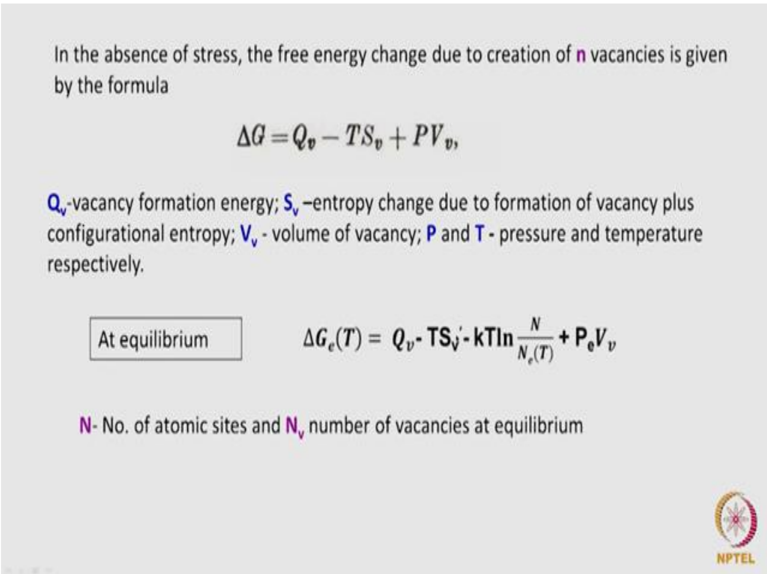

Now, what is the methodology which we follow to find out the stress which is going to be generated by the action of an external stress, what is the concentration of the vacancies which will be generated? These are all the information which is required the concentration of vacancies which are generated on applying load that is what we are trying to look at it. We know that under thermal equilibrium condition, when no external stress is being applied, the free energy change which is going to take place depends upon the energy which is required for formation of a vacancy for a single vacancy. Then S v is essentially the T into S v is the entropy term look at the contribution due to a entropy energy, where S v is both corresponding to the change in the vibrational energy plus the configurational energy.

Since, lot of vacancies are there creation of each vacancy some volume is being added to it that is what we have added as the V v is essentially nothing, but the volume of the vacancy. One should understand this volume of this vacancy is different from the size which an atom is going to occupy in a lattice side, because there is some.

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Relaxation is going to be there, so it is not that same.

So, at equilibrium this is how the value will turn out to be correct. This expression we have derived in the case of a point defect earlier. When we derived for the point defect at that time we did not consider this part is P into V is essentially nothing but a mechanical energy. This is internal energy change, this is the entropy change, this is the mechanical energy change, these together decide the free energy change. So, here if we now try to look at in this N is the number of atomic sites N e into T is the number of equilibrium vacancies which are generated. The P is the equilibrium pressure which is there the normal pressure; all the terms have been explained earlier.

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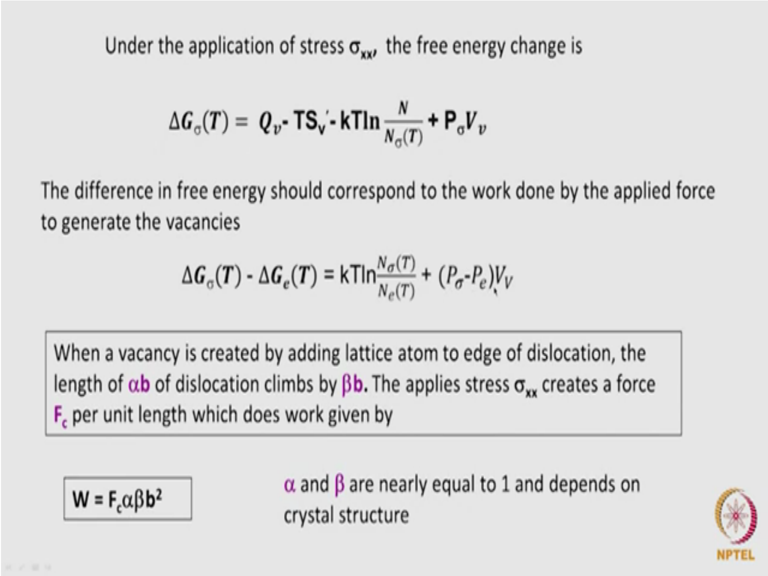

Now, what will happen under the application of a stress? When we apply a stress by a mechanism which we talked about earlier, lot of vacancies are going to be generated in the sample. When vacancies are generated in that sample, now the concentration of vacancies is more than what it should be, when the stress is not applied under thermal conditions. And this excess vacancies, they are going to the volume per vacancy we know, so because excess vacancies are created, there is going to be a hydrostatic pressure which is going to come in the material. These are all the terms essentially which is coming into the picture. This is with respect to when a stress is being applied.

If we take the difference between these two free energy change, this will give the change in free energy which is occurring as a result of application of mechanical stress. That free energy change if you take the difference between the one corresponding to under the action of the stress and one in the absence of stress, this difference will turn out to be k T into log N sigma T is the vacancy concentration on application of load. This is the equilibrium vacancy concentration at the same temperature. And P sigma minus P is the one which is under thermal equilibrium condition. This is corresponding to the stress which is going to be, this is the hydrostatic pressure when the load is being applied.

The stress which is being applied is this hydrostatic pressure, this we can write it as P equals P sigma this will be, we know this expression the hydrostatic stress. So, P sigma minus P can be replaced by P, and we can write it. So, this tells us what is going to be the free energy change, which is occurring because of the generation of excess vacancies due to moment of dislocations as far as what we consider. So, this should be equivalent to if you have when we know the external stress that has been this is F y, this is essentially nothing but the force per unit length of the dislocation. This will be essentially equivalent to the work which is being done to move a unit length of dislocation; under the action of this that dislocation is moving in which direction the dislocation which is being present is moving from here to here.

So, let us consider one atomic displacement of the moment of the dislocation if it is taking place that means that one row of vacancies has to be added to it, or even if at one atomic site, if a dislocation has to climb row one atom has to be added to that site. Then only the dislocation will climb them or if a dislocation has to climb up, one atom has to be removed from that and we have to create a vacancy.

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One row has to be for a full row, otherwise at one particular point it will be creating a essentially. For this to happen a length alpha b of the dislocation we assumed that for one atom position its climbs, and what is going to be the burgers vector corresponding to that beta b we take it to be. So, essentially if this is equivalent to generating a force on the dislocation opposite to the force which is being applied for the dislocation to move that will be equal to that force we call it as F c. So, F c into this one will give the energy which is required, so that is what essentially we have written as W equals this alpha and beta are parameters which will be depending upon the crystal structure, their values can change. And they are mostly close to one in many calculations we take it to be 1, and take that is how it is being taken.

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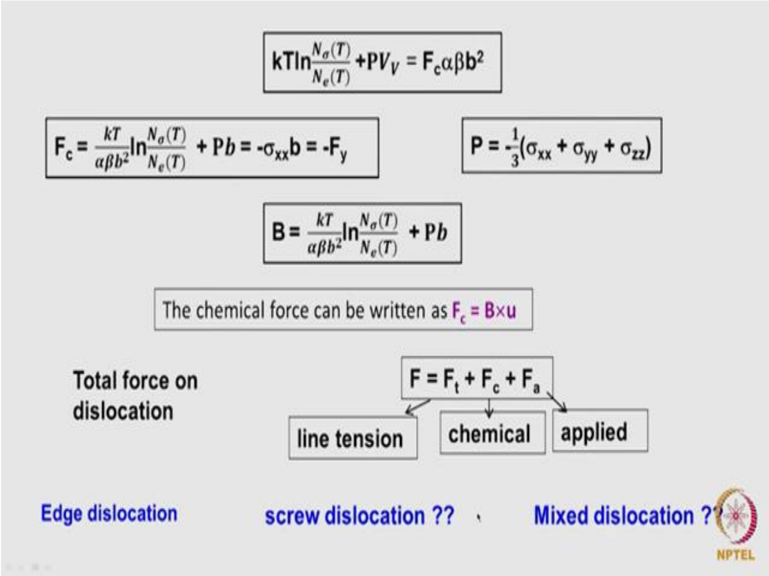

So, now what we should do is that we should equate these expressions that is this we calculated the free energy change, this is equal to the force which is being applied. So, this if we take wanted to find out F c we take it to be under this side. So, then we will be getting an expression like this. And this is equal to nothing but the applied force, this is how we can write it. And P as I mentioned equals minus 1 by 3 sigma x x. So, essentially in the present case the stress is sigma x x, the pressure P will be minus 1 by 3 sigma x x hydrostatic pressure. So, what I have written is that this force F c is written I just written as B, just denote it by B, it does not matter one can use F c also as the notation. This force is the chemical force what is the direction in which this force will be acting this F c equals this B cross u is the line direction of the dislocation perpendicular to it, it will be acting.

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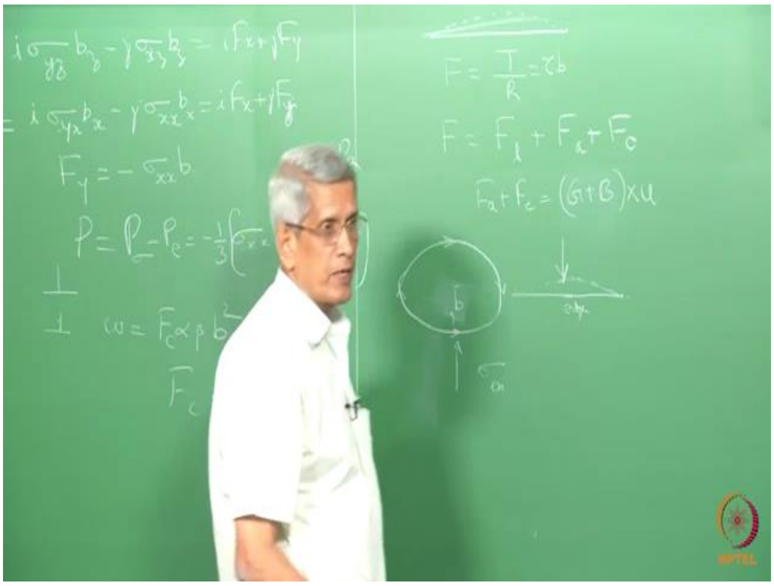

So, far what we have considered is three cases, one if we take a dislocation a straight dislocation line, and if the dislocations are being anchored at two points. If we apply a force, the dislocation will bend into this shape. Then the force which is going to act will be equal to T by R, which is equal to applied stress into burgers vector that is one force which is acting on the dislocation. Other force is that external stress as it is being applied on the dislocation that generates the force on the dislocation to make it move that is the applied stress that is what the essentially it is. In addition to it, when the applied stress turns out to be not shear, but it is tensile. For the edge dislocation, now we have a force which is chemical force which is also acting on this. So, these are all the three forces which are going to act on a dislocation.

These two forces that is F equals due to a line tension F l plus F applied plus F c. So, these two together applied plus F c, we can write it to be equal to B plus or I should write it the other way around G plus B cross u. But what we should remember is that the chemical force acts only on edge dislocation, because for the chemical force to be generated essentially a tensile stress which is acting and the tensile stress has an effect to make the dislocation only an edge dislocation to climb up or down, it has no effect on the screw dislocation. So, this one should always remember. So, on a screw dislocation, what is going to happen is that it will hardly have any effect. Screw dislocation only the line tension and the applied stress will be having that effect.

What happens in the case of a mixed dislocation, what do you think will happen to a mixed dislocation?

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Yeah, mixed dislocation what will happen is that suppose we have a dislocation which is I just on drawing a cross section of a dislocation. And its viewing direction is there is the plane of the dislocation is perpendicular to this direction. This is just a cross section. Suppose, we assume that this side this part of the dislocation, this is the projection of the dislocation is an h component and these two N's which we see the part of the, because this is essentially nothing but a dislocation circular dislocation. We are just looking at that dislocation from in this direction, then we will be looking at the dislocation in this way correct, this is how the line direction of the dislocation is. Then.

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The burgers vector will be in this direction or the dislocation. Then this is an edge part of it. This is going to be a screw component of it. If you apply a stress that stress could be a shear stress or it could be a stress which is a sigma tensile stress tensile or compressive stress. If you apply a tensile or a compressive stress then what is going to happen is the edge part of it depending upon, whether it is a tensile or a compressive what will happen is that the dislocation may climb up. This process will occur only at high temperatures, where the vacancies are mobile, because at room temperature though there may be forces which are acting on the dislocation in the y-direction because a tensile stress has been applied. It is a mobility of the vacancies is so small that nothing much happens, only at intermediate temperatures this sort of a process will occur.

So, essentially when we look at it which was only a like this. Now, we observe that this has bent like this, the edge part is still in the slip plane. Whereas, the screw part of the dislocation has just climbed up, this is what essentially will happen in the case of a mixed dislocation. So, in fact, these sort of micro structures which they come, one has to be very careful when one looks at electron microscope, then one has to identify which is the slip plane which is the burgers vector all the information one has to obtain to get correct information about which is the way this dislocation is moving.

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What are the consequences of this sort of a generation of vacancies in the material? We will take one what will be the effect of this chemical force that is we are comparing between a mechanical stress, which we are applying, and the chemical stress which is generated. These sort of a chemical stress can be generated in a material by radiation, when we radiate it, interstitials, and vacancies are produced. Interstitials can diffuse very quickly to the surface, but excess vacancies will be generated within the material. When if the two options are there for the vacancies, one - the vacancies can go to the surface and get eliminated to reach equilibrium concentration, or the vacancies can go to the sink which is present within the material which are dislocations and that dislocation can glow go climb up or down. That means, that these vacancies are trying to put a pressure on the dislocation that way we can consider it.

But essentially in this what one has to look at it is that, what will be the sort of a vacancy concentration which will be required to put stress on the dislocation, whether very high concentration, if you look at this expression, this B we know for a dislocation any typical material we can take it, k is the Boltzmann constant. T is the temperature correct and N sigma by N t is, if we calculate this value, this is an energy. So, this will be equivalent to a force which it will turn out to be. And that value turns out to be about 2200 with respect that is this value of the stress generally turns out to be in few GPa plus you have a log N sigma by N e is there.

This ratio if we take it most of the time even if you take this value to be about the something like close to one or two that is if the vacancy concentration is raised by just double.

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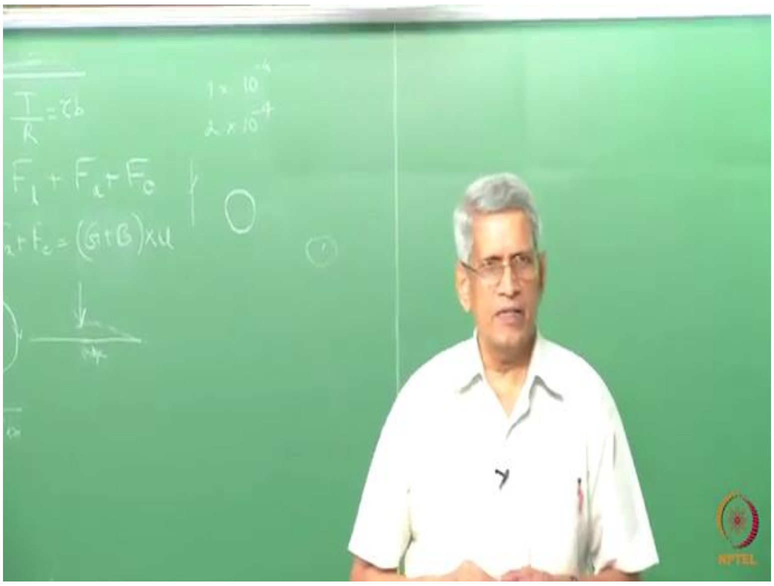

Double means that generally at melting point we consider vacancies to be typically around 1 into 10 to the power of minus 4, it is increased to 2 into 10 to the power of minus 4 the vacancy concentration. Just this increase in concentration will be putting a stress which will turn out to be much above the theoretical shear stress. This one can do this calculation and just work out. That means, that even a small increase in vacancy concentration can generate the type of stress even by mechanical force we will not be able to generate that sort of a stress we generates which is equivalent to theoretical shear stress of the material or much above the theoretical shear stress.

What is the situation in which we will be facing this sort of a stress condition in a material?

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One of the things, which one can think of immediately is yes high temperature allotment we take a sample keep it close to a melting point to solutionize the sample. Then we quench the material most of the time to generate to retain the high temperature microstructure that is what normally done by solutionizing treatment. When we do this quenching, what will be the sort of vacancies, which are generated close to melting point it is of this order? If we bring it to room temperature, what will happen, orders may be 10 to power of 6, 10 to power of 7 or 8 of that order vacancy concentration will be produced, no material will be able to accommodate this sort of a vacancy concentration.

In fact, what happens in most of the material is that the vacancy concentration is reduced considerably. How that happens is that as the sample is being quenched, many of these vacancies when they are mobile, they are try to come to the surface and equilibrate it. And beyond a particular point when this cannot happen these vacancies which are closed by a short distance movement they can agglomerate and form vacancy loops in the material. This is what I called as a quenching stresses.

So, in fact, in most of the material the best example is that if you take aluminum or copper it is a very well annealed structure. If we take it too close to a melting point and then quench it, then if we see, we will see a lot of dislocation loops will be there. These loops are essentially frank loops. In FCC on a close packed plane, if vacancies condense on a close packed planes that means, atoms are removed from that layer this will be equivalent to generating a frank dislocation. So, by in this process a lot of vacancies have been accommodated and dislocations have been generated in the material, this is what essentially happens. With this, what one will observe is that the concentration of vacancies is brought down considerable.

So, the consequence of it will be that if we take any material, we quench it from a very high temperature, when the vacancy concentration comes down that we assume that the vacancies are retained that does not happen, instead lot of a dislocation loops are generated within the material. This loops also will generate some stresses in the material, these stresses are what we call it as the quenching stresses. The effect of these sort of stresses where we can see where we do not allow material for expansion to take place or a contraction to take place, can you imagine, can you tell me a situation where this occurs? This is what we call as weld cracking.

What is a weld cracking are, you weld the material and just what happens is that after that when an expansion is going to happen that there are tensile and compressive stresses which are being generated. Quickly we quench it then what will happen is outward, you saying that the crack has developed. So, the stresses which can be generated are of this order very high stresses which could be generated. Similar phenomena, in fact, we can think especially ceramic material if you consider it, ceramic materials should never be quenched you know that. If you try to quench it what is going to happen is that the whole material will shatter into pieces.

In the case of metallic samples, where it cannot plastically deform and accommodate, there some dislocations will be generated, but there are cases under situations where we find that this is not able to happen in such cases the material cracks are observed. Otherwise, in most of the materials, the quenching itself produces sufficient dislocations and stresses are generated that is if I take a material the best experiment which we one can do to verify this. You take a sample which maybe is a deformed sample take, it to high temperature it is annealed slowly cool it, so that at every instant of time we are allowing the vacancy concentration to equilibrate, and then take some sample which is quenched very fast. If you observe these two samples, and try to find out the dislocation density which is going to be there in these two cases, the one which has been quenched the dislocation density will be very large.

These dislocations, this excess dislocation density because they are the vacancies are getting equilibrated at the confrontation. So, when it cannot happen these stresses only way they can relieve the high stresses which are generated due to excess vacancy concentration. These vacancies which are close by in some region, they all come together and condense and a small loop will be formed that is the way they can generate this they can relieve this stresses, this we will observe this material.

So, from this, what we have considered that is in all these the last few lectures 3 or 4 lectures, what you have looked at it is that what is the force which is acting on the dislocation. The various components which we have consider one due to a bending of the dislocation, and another due to the applied stress to find out the direction in which the stress the force is going to act on the dislocation, the Peach Koehler equation was derived that is an elegant method with which we can immediately using that equation. We can immediately find out what is the magnitude of the stress and in which direction the stress is going to act. Then when excess vacancies are generated in the material, what will be its effect on generating stresses. And as we discussed just now these stresses even in a small increase in vacancy concentration, it is going to generate very high stresses, and what all the implications of this stress this is what we have considered in this lecture.

In the next class, what we will do is that we will talk about some dislocations in some specific systems, which we will consider like, for example, in FCC where both perfect dislocations and partial dislocations are going to form. These aspects we will look at it in the next few classes. We will stop here now.