Defects in Crystalline Solids (Part-II) Prof. Shashank Shekar Department of Materials Science and Engineering Indian Institute of Technology, Kanpur

Lecture - 14 Origin and Nucleation of Dislocations

So, today we will discuss about dislocation interaction, which leads to some mechanical behavior. So far we have looked at dislocation in a particular systems, we looked at FCC systems, then FCC, HCP, then the ionic system. And then the last one that we looked in the last module previous module was about the dislocations in super lattices. And over there also we will already started this associating, how this dislocations can lead to mechanical properties, and particularly the higher strength at higher temperature, so that is what is the unique property of super alloys.

$$\vec{F} = (\bar{\sigma}, \vec{b}) * \vec{\xi}$$

Now, here we will talk about one of the very basic phenomena that is attributed to dislocations, and that is work hardening. Now, this work hardening, when we discussed dislocation interaction, we said that this dislocation interaction is what leads to work hardening. So, the basic mechanism is dislocation interaction.

And the equation which describes this is Peach-Koehler equation Peach-Koehler relation, this we had discussed in part-1. And we will start from where we left that is we discussed how Peach-Koehler relation can be used for one to one dislocation interaction. And here we will start with one to one interaction to show, how it can be extended to the interaction of dislocation in a atmosphere or in our environment, where there are lot more other dislocations.

So, this one was given by sigma is a tensor, when we wrote this equation, the meaning of these various terms are like this. So, there is a dislocation on which we are talking about the force. So, the force on this dislocation which is F. b is this burger vector of this dislocation, and E is the line vector of this dislocation line.

What is sigma, sigma is the stress the net stress that is acting on to this particular dislocation. So, you can say that so I am drawing it like this, so this is for various reason; this could include internal plus external reasons. So, based on this sigma is the net stress experienced by dislocation line. Now, this stress can also be due to another dislocation, so that is where we are able to get the relation between one to one dislocation interaction, can also be due to.

So, here the now the picture will change if we say that, so you can now have something like this, and somewhere very far there is a dislocation. So, this has a stress field, so this will have with respect to this stress this will be at x, y, z. So, the sigma at this point will be sigma x, y, z. And then in this case, the stress will be because of another dislocation, it could have been a screw dislocation as well. So, it could be this or screw dislocation either of these are applying a stress, and with respect to that the location is x, y, z. So, sigma x, y, z along this point, and you will have to calculate it at per unit point of this dislocation. And but the burger vector and line vector would still remain the same ok. So, now that we remember this equation.

$$F_x = \frac{G b_1 b_2 y (x^2 - y^2)}{2\pi (1 - v)(x^2 + y^2)^2}$$

$$F_y = \frac{-Gb_1b_2y(3x^2 + y^2)}{2\pi(1 - v)(x^2 + y^2)^2}$$

So, let us go ahead, and use this equation to apply for a release for a pair of dislocation. So, there is a dislocation, which will call as 1, and there is another dislocation which will call as 2. So, here for the sake of geometry and make the making the geometry simple, we will take the line direction for both of them along the same direction. And assuming that the line direction this is z, it is 0 0 1.

Burger vector, so will assume that the burger vector is along x-axis. So, this will be along positive x-axis, this will be along negative x-axis, but we will not assign a sign as of now. It can be a positive dislocation can be a negative dislocation. We just want to know or this two dislocations interact. So, we will call this b 1, so this is along x axis. Similarly, b 2 which is along still along x-axis. b 2 could be a negative number, if it is a negative dislocation. And it will be a positive number, when it is a positive dislocation.

So, now what we need to find is force on 2 due to dislocation line 1. So, we will go back to our equation, which we know is sigma dot b cross E. And here since, we are trying to find a force and dislocation 2, so this will be b 2, this will be E 2. And this sigma 1 is because of dislocation 1, so whatever is the field being generated. And now without going into the details, which we explained in part-1, you can go back to the lecture to understand the full form of sigma how you can expand sigma dot b cross E. Here I will just write what is sigma dot b, and it will be so this is sigma dot b, and epsilon will be and remember these are for dislocation the line vector, and the burger vector are for 2.

And we know that here b 2 in the b 2 only x b x exists, and E 2 only the z exists. So, these turn out to be 0. And over here this term also turn out to be 0. So, you have these three elements over here, and these the only one element over here. Now, if you multiply it what you would find, so in the end we will be left with only two numbers and no z. And this we explained that there this two are parallel, so there will be no x no force along the z-direction.

And here we as I said this is for dislocation 2, and this is equal to b 2. And what is sigma y x equal to sigma x y, so it is with respect to one there is some x, and y for this point. So, this is what x and y are. And sigma x x is again equal to G b 1 y 3 x square plus y square.

Now, if you look at this is this has three terms, and which correspond to F x, F y, and F z. And now so we have written a sigma x sigma x y, and sigma x x, and we also know that b x is equal to the burger vector of the second dislocation, so that will become b x is equal to b 2. And therefore, from this we can say that F x is equal to and F y is equal to so I have missed a sign here. So, this should be minus over here, so this is G. So, these are the two forces F x and F y that are acting on the second dislocation. So, F x, this is F y. And clearly this is the glide force that is accessing acting and this is the climb force.

$$F_{x(int)} + f_x^{app} = 0$$

$$\frac{Gb_1b_2y(x^2-y^2)}{2\pi(1-v)(x^2+y^2)^2}+\tau b_2=0$$

Now, when we are talking about room temperature work hardening, then of course there is no climb, we are only interested in glide. So, what we want to know is how the glide interaction forces change, when the distance x and y are change. So, now what we are interested right now is only this term the F x part. So, we are only interested in F x, and this is due to interaction, because this is the glide force ok. So, this is our glide force.

Now, let us say that some external stress is being applied because of which the dislocations are moving ok. So, now here we are applying some external stress. So, let us say that this external stress, and since the dislocation that we are trying to move is the dislocation two. So, and it further according to the geometry, the only stress that can actually make a difference is sigma x y. So, you remember this is the sigma x y, this is the one that is actually making it in move which is glide in the plane, so that has to be sigma x y.

So, thus external stress which is applied to make dislocation line-2 move must be sigma x y. And let me put some super script a p p to show that this is applied stress. Now, this is at shear stress, so I can also represent it as tau. And if it is tau, then we know that the force which is or we can convert the since this is a stress the shear stress, we can convert it to the applied force on the dislocation. So, effect of the applied stress.

So, the effect of applied stress can be given as tau b. And what will be the burger vector again; this is the dislocation-2 that we are trying to move, so it will be tau b 2. So, this is because of external stress, remember this is because of the internal stress or the internal interaction, and this is because of external stress being applied.

Now, if this is the external stress being applied, and this is the force that is being generated on its own on to dislocation-2 to keep make it moving. So, now if I say that what is the stress or what is the applied stress required to keep dislocation line-2 a stationary meaning, the net force on the dislocation line-2 must be equal to 0. So, I can write it like this F x, which is internal plus F x, which is applied this must be equal to 0. So, this is a condition that from where we can derive other things.

So, this is telling us how much stress is required to balance the internal force acting on the dislocation. And therefore, it means that the net force are acting on the stress on the dislocation is 0, so F x internal plus F x applied is equal to 0. And now I can expand this relation to write it like this. So, we have already seen this is G b 1 b 2 ok so something I

missed here ok. Now, this should not be y ok. So, my bad as you can see their taking x sigma x y, so it is x. And similarly, now just now I noted this, so this should be x. So, G b 1 b 2 x x square minus y square by 2 pi 1 minus nu, this is the F x applied, so this is times tau b 2, and this should be equal to 0.

$$F_{x(int)} + f_x^{app} = 0$$

$$\frac{Gb_1b_2y(x^2-y^2)}{2\pi(1-v)(x^2+y^2)^2}+\tau b_2=0$$

$$\tau = \frac{-Gb_1x(x^2 - y^2)}{2\pi(1 - v)(x^2 + y^2)^2}$$

And from here you can see that what should be the shear stress acting on that plane. So, remember tau is the on dislocation line-2. So, how much should be that shear stress acting on dislocation-2, so I will take it take the whole thing to the other side. So, it will become negative. And then b 2 can be canceled as it is non-zero, so it becomes minus G b 1 x x square minus y square by 2 pi 1 minus nu x square plus y square whole square.

$$\tau = \frac{-Gb_1x(x^2 - y^2)}{2\pi(1 - v)(x^2 + y^2)^2}$$

Now, this is of the same form that we earlier drew for force versus the x distance x in terms of y we had earlier drawn it, and the form of the equation is same. So, overall this will we will get a similar relation over here or the similar variation, and how is that variation. What is y-axis, you can keep it as tau b or force. And what is x-axis, x-axis is actually x meaning how many axis, and it is in terms of y. So, this is at point x equal to 1 y, this is equal to minus 1 y, and so on.

And if you do the calculation, you would find that this minima occurs at 2.414 y. And this minima occurs at minus 0.41. So, accordingly this will be plus 0.414 y. Now, this is again to make things put things in perspective, this is when you have dislocation this is dislocation-1, and this is dislocation-2. So, this is how the forces are varying, when you keep changing the distance.

So, we are let us say you are trying, so what we are trying here is goal move dislocation 2 to on its glide pin itself, we are not trying to move it any along or we are not trying to move it out of the plane. So, move dislocation to on its own glide plane past dislocation-1. So, this one this one is coming from somewhere over here, it is you want or basically you want to apply stress, so that it can keep make it keep moving in this direction.

So, how much stress is required that is the question. We so now the there this is interact internal interaction, this plot is arising because of internal interaction. And the question I am asking is that how much stress would I need to apply to keep the dislocation moving along, so keeping dislocation to moving along this direction.

So, first let us understand what these different situations are. Now, when you are somewhere very far the forces are negative, so it means that if you had the dislocations like this. So, the forces are acting in such a way that, it wants to keep moving it for it the negative forces in this direction. So, it wants to keep for in dislocation moving in this direction. And what I am drawing here is 45 degree line, because it is special with respect to this dislocation configuration.

Now, when you what this plot is saying is that when the dislocation is far away, it wants to keep moving in this direction. And it when it comes over here, it reaches a 0 value meaning it is at a configuration, where no more forces are acting on this. Now, if it moves in this a little bit to the right, a positive force acts on to it which means that it mounts to make it back move it back to the other direction. When it moves to the negative direction or any a force in the opposite direction acts on to it, which means that it is trying to equally bring it to this particular position. So, this is a stable equilibrium, and where do we achieve this is achieved at point A.

Now, from here if the dislocations were moved somehow up to this point, then you can see our much larger negative stress is acting, which means it wants to keep it moving back. But, our goal is to keep it moving to the right, but the stresses are acting such that it wants to keep it moving to the left. So, there is a force or a stress acting against what you want to do. So, we must overcome, we need to overcome maximum internal resistance or a stress. And where is this maximum internal stress or resistance, it is at this point b which happens to be I am not showing the geometry now or not trying to calculate from the geometry here, but you would be able to show that it is at 0.414 y.

So, at this particular point, it will have the maximum amount of repulsive force. And if you can overcome that, then it means that you can keep moving the dislocation in the positive direction. Now, at position c what happens the dislocations are like this, and forces are 0. So, the forces are trying to if you if it moves just a little bit to the right, the forces are such that it will just move it all the more to the right. If it if the dislocation is a little bit to the left, forces are such that it will try to make it move more to the left. So, you can call it unstable equilibrium.

Now, let us come to the point C, if it comes somewhere around 0.414 y, then it experiences a maximum amount of force or a stress acting to the right. So, it is moving automatically on its right, you do not need to do anything. And that is a good situation just that it is not under your control, it just automatically the forces interactive forces are such that it will make dislocation to move to the right, but fortunately for you do not need to do anything over here.

Now, let us look at position D. So, position D is like this, this is again 45 degrees. So, as you can see the forces are again 0. If you try to move it to the right, it wants to come back to left. If you try to move it to the left, forces are such that it will try to bring it back. So, the configuration is such that it wants to retain this 45 degree angle between each other. And therefore, again we have a similar situation like a point A, and you can term it as stable equilibrium.

Now, from here if you keep trying to keep moving it to the right, you will get to a maximum shear stress which is acting in the negative direction, which is in this direction. So, what you what do you want to do is or what it wants to do is that it wants to pull it to the left, but I like I said you want to move it to the right. So, you will have to overcome this stress at this point. A fortunately this and this stresses are same.

And again we are not going through the calculations, but it is not very difficult to show that both these points are the minima. So, you will have to the easy way to do, it is take x and y in a non-dimensional parameter something like x by y. And then differentiate tau with respect to that parameter, so delta tau by del beta. Wherever you have the 0 you will get the minima and the maxima and you can show that at that position, the stresses are maximum. So, I have told you how to do it, I am just not doing it over here.

So, these two stresses happen to be the lowest. And therefore, if you, if your stress was high enough to overcome this, it will also overcome this stress. So, this is the amount of stress that you need to apply now what is that amount of stress. Now, let us look at it how do we find it, it is simple. We have here said that x should be equal to 0.414 y that is all you need to do. Once you put x equal to 0.414 y that will give you the maximum stress. And that will give you the magnitude directions or the sign can be obtained depending on whether you are selecting the two positive edge dislocation or two opposite signed edge dislocation. So, right now I will just calculate the magnitude of this of this shear stress.

$$\tau_c = \frac{Gb}{8\pi(1-v)h}$$

So, this tau critical and I am saying magnitude is nothing but tau at x equal to 0.414 y. So, whatever equation I have written over here, which is this I will put x equal to 0.414 y, and then I will get what I just explained to you. So, I can take out the y square common, and the whole square of this. So, there is a square inside, and also a square of the whole thing there is x square plus y square whole square, and therefore, y to the power 4 over here. So, now this y cancels y square, and this y, and you are left with one y in the denominator. And therefore, this can be written as so this minus sign goes off, anyways we are not concerned about minus sign like I said 2 pi 1 minus mu y.

So, this is 0.414 this comes out to 0.28286, and the denominator will come out to 1.372. And this whole thing is equal to 0.25 or basically equal to 1 by 4. So, I can write it as tau critical is equal to G b. And so we have a configuration like this. And if we assume the y will be, y is constant, because it we are talking about glide plane. So, instead of y, what we can do is we can say that this is some distance h ok. So, y can be replaced by this term h. And therefore, this becomes, and I am now dropping the subscript because we are assuming that it is the same burger vector all across 8 pi 1 minus nu h.

So, the tau critical what does this value imply, this implies the amount of shear stress that must be applied because of external loading onto that dislocation to keep it moving past dislocation one. So, let me write it, this is ok. So, this is a very good starting relation after describing how much stress is required for dislocation to move past one dislocation,

but rarely we will have only two dislocations in a material, we will always have a lot of dislocation.

$$\tau_0 = \alpha G b \sqrt{\rho}$$

So, there is what is called as the Taylor hardening formula. So, in this what we will assume is that there are lots of dislocations. And for the sake of simplicity, we will assume that the dislocations are arranged like this. This is called Taylor lattice. And what I am trying to show is that there are opposite dislocations arranged at periodic arrangement, a periodic spacing interlaced with dislocations of opposite sign.

So, the distance from here to here is h, and the distance from here to here is h. So, if you take a square like this, you should be able to get the dislocation density. Now, the area of this size is h square, and the number of dislocation in this cell is 1 plus one-fourth of all these four, so 1 plus 1, 2. Therefore, the density of density of dislocation when you have a Taylor lattice distribution is given by 2 by 2 h square. So, the area, this is h, this is h, 2 h, 2 h, 2 h square and number of dislocation here is 2 by 2 h square. And therefore, this comes out to 1 over 2 h square. Now, if that is the relation between this density and h, so we can say that h is equal to 1 by 2 under root rho, where rho defines density of dislocations.

Now, you would say that this will be only applicable should be applicable only for a particular case where the arrangement is like this. But what you have to realize is that when there is a large density of dislocation because of their repulsion between them. And if there is no there is no other forces acting on it, they will like to keep the minimum energy configuration. And when is the minimum energy configuration, when the interaction or the stresses acting on to each other is at the lowest. And this is the configuration where they will have the lowest stress. So, this describes on an average what will be the distance between different dislocations. And therefore, this need not be exactly like this, but on an average this is how any dislocation distribution can be described as.

Now, next thing that we will do is will assume that, and this is not without any basis, it is you can realize that the amount the stress equation that we derived in the previous part

where we said this is the amount of stress required to make a dislocation move through against or past a dislocation was of that form. We are what we will say is that there was only one dislocation against which it was working, now it has to work against a set of dislocation. So, the overall form of the equation will remain same only that the multiplication factor would change. And we will get that multiplication factor from this relation, because we know that on a on a local basis, it each dislocation has to pass through another dislocation. So, on the local basis, it is still the same.

What is different is that the h value is now being determined how the dislocation is distributed. So, we will assume that stress required for moving dislocation against several dislocation has same form as earlier. What will be different is the multiplication factor, only multiplicative constant changes. So, earlier what was our equation, so it was of this form tau equal to g b by 8 pi 1 minus nu h. So, let me write it down again here.. So, overall the constants here are g and b and nu. So, those things will remain same. What we are saying is that these constants 1 by 8 pi h is what is changing and that is again like I described h is now being adjusted depending on how many dislocations are there or what is the dislocation density.

So, I will say that now implies this implies that tau naught which is the stress for moving through the set of dislocations is equal to G b by 8 pi 1 minus nu and instead of h I will write 2 rho ok. So, here again I have missed a sign not a sign, but there is a square root over here. So, this can be further simplified as alpha G b root rho. And this is called as Taylor hardening equation or Taylor hardening relation.

$$\tau_0 = \alpha G b \sqrt{\rho}$$

Now, here when we have derive this alpha is of the is equal to root 2 by 8 pi 1 minus nu. So, it approximately is equal to 0.1.

$$\tau_0 = \alpha G b \sqrt{\rho}$$

And what people have found for example, if you take a copper as a function of different dislocation densities. So, let us say on the y-axis, you have b square root rho; and on the

x-axis you have tau over G. So, we go back to this relation. This is b root rho on the on this side and tau naught by G on this side. So, what you have is a relation like this tau naught by G equal to alpha times b root rho. So, alpha is a constant, therefore, if I draw a line like this, what I should get is a straight line and this is what has been observed people have observed straight line.

So, what are the implication that this relation Taylor hardening relation is valid. What is more the alpha value that we obtained as 0.1 is not really 0.1, but it ranges between 0.5 to 1.0. And how can we get like I said the slope is equal to alpha. So, this is y equal to m x or if this is actually x. So, this is the x. So, this is x equal to 1 over m y. So, this is our y; this is our x; and this becomes 1 over m. What is the other thing that we conclude stress filled of dislocation array meaning sigma i j is proportional to 1 over r. So, individual dislocations were proportional to 1 over r square, but sigma i j when it is a stress field of dislocation array is proportional to 1 over r.

So, we see that we have obtained a relation which describes and so the most important relation that we described in this module is this one, which describes how the shear stress required in keeps increasing with increase in the dislocation density. And this is clearly implying that you will have to apply more and more stress as dislocation density increases, and therefore, this is work hardening. In work hardening your dislocations are increasing dislocation density is increasing. So, the amount of stress you will have to keep increasing.

And if we what we so just to refresh or jog your memory, so if this is a simple stress-strain curve, and this is the yield point, if you keep moving beyond this you are applying some plastic strain on to the material. And as you keep improving in increasing the plastic strain and if you allow the material to come back, and then do redo the stress-strain test, what you will see is that this becomes the new yield point. So, the yield point has increased from here to here. And what has happened from here to here dislocation density has increased because of straining.

So, dislocation density increased which led to increase in the yield strength and now this can be directly correlated with this relation. And this relation is I can accurately predict how much you will get for at least the pure materials you it can very accurately predict how much will be the increase in the shear strength. And then you will have to correlate

it to the stress the tensile and compressive stress of a single phase or a single crystal, and then we will have to have models to extend it to polycrystalline material, so well and this module over here. Next time what we will discuss is that how is the dislocation density increasing. We said here that strain leads to dislocation density increase and it makes sense, but what is the phenomena that leads to increment in the dislocation density. So, we will look into that in the next module.