Defects in Crystalline Solids (Part-II)
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Lecture - 16
Interaction of Point Defects and Dislocation – Solid Solution

So, we will be discussing another mechanism of strengthening which is Solid Solution strengthening.

This particular mechanism arises because of interaction between point defects and line defects. So, it is in effect it is Interaction of Point Defects and Dislocations. So, we are talking about solid solutions. So, the first thing that we should understand is that there are two types of solid solution and we have already covered the types of solid solution in part one, we will just look at it to understand with how they will affect the point the interaction. So, the solid solution can be interstitial for example, in when we have carbon or nitrogen in iron or it can be substitutional, when it replaces one of the lattice atoms for example, copper in nickel.

So, now these are point defects why do this point defects interact with dislocation. So, the idea here is that whenever you have a point defect, whether you have talking about interstitial or substitutional point defect, they create a distortion around them so, around that point defect there is a distortion created. Now, this distortion interacts with the stress field of the dislocation and therefore, you have something called as interaction energy.

So, and this may and you would see why I have written may because there are conditions, where this may not actually interact may interact with and this interaction may raise or lower the overall elastic strain energy of the crystal. So, first thing is that this change can be termed interaction energy. So, I am sorry the change in the elastic the overall strain energy that is called a interaction energy.

So, this change in energy is termed as so, we have two types of solid solution interstitial and substitutional. Interstitial for example, in the steel carbon and nitrogen going to the interstitial sites, they do not replace iron from its position substitutional for example, copper in nickel, where copper replaces nickel atom and even otherwise we get even nickel in copper so, nickel replaces copper.

So, these are the two types of point defects now why do point defects cause strengthey the first thing is that, whenever there is a point defect there is a distortion field created around it. Now, this distortion field will interact with the stress field of the dislocation and this causes a overall change in the strain energy of the lattice. So, when the change in the strain energy is negative it implies that they are two the two are bonding, when the strain energy increases it means it is a repulsive or the overall energy of the system has increased and this change in energy is called the interaction energy.

So, this is what I have written here distortion is created by point defect and this may interact with the stress field of dislocation and may rise raise, or lower the overall elastic strain energy of the crystal. Now, this change in energy is termed interaction energy. Now, if E I is large and negative now what is what will that mean in terms of energy if it is something is large as well as negative.

If E I is it means that the two defects the point defect and the dislocations have bonded very well and therefore, you would need some additional energy to break the bond, what will be the amount of work required it will be equal to E I. So, E I is the interaction energy which is the amount the, which it changes and the same amount you must apply by additional work to separate the 2. And how would you apply that is additional amount? You will have to apply through most like E I stress. So, it means that increased stress will be required for the dislocation to move.

Now, we can explain this we can understand this interaction energy with the help of a simple model, in this particular simple model what do, we do we assume that the overall crystal is a continuum elastic follows a continuum elastic model meaning we are not assuming a discrete atom like structure, but that there is whatever property we define for the bulk is there uniformly across the bulk whether you go at the Nanometer level or Armstrong level Armstrong level or Pico metre level. So, at each and every level you have a continuum of material and each of them display the same property.

Now, with that model we will assume that there is a hole in the model and what is the size of the hole, here we will assume that there is a hole and a sphere of another radius is being inserted. So, the hole has radius r a and volume V h this is in the matrix and if you are talking about interstitial or a substitutional either way, another atom is being inserted over here and what is the distortion created it, we will assume only because of the change in the size not because of the modulus we will say that it is the distortion because of the size.

And therefore, the size of the sphere that is being inserted will be assume to be a little different, how can we say that or how would we take that mathematically will say that the size of the sphere that is being inserted has a radius r a 1 plus delta. So, a sphere of radius r a 1 plus delta and volume V s is to be inserted in the sphere in the matrix, clearly the sphere has a different radius and the hole is of a different radius therefore, a distortion will be created.

Now, delta can be positive or negative positive meaning you are putting or substituting, or whether or maybe interstitial atom are larger than the location over there when delta is smaller in size, then it would mean that you are substituting atoms smaller than the matrix atom. So, that way we will be able to accommodate into this equation, whether we are putting larger atom or a smaller atom.

Now, based on this we can say the misfit volume, meaning how much is the overall change in the value volume, when the two are separate right, now we are not assuming any elastic defamation for either the ball or the hole. Just as it is what is the misfit volume. So, will give misfit volume which is as V misfit which is nothing, but V s minus V h is approximately equal to 4 pi r a cube delta this will be when delta is much smaller.

So, what we are doing is basically 4 by 3 pi r cube here r will be r a 1 plus delta cube here 4 by 3 r a cube where r a is r a. So, this will be in effect 4 by 3 pi common and r a 1 plus delta cube minus r a cube, now here if delta is very small then 1 plus delta cube becomes 1 plus 3 delta and therefore, 3 by 3 and 3 in the denominator cancel out and what you are left with is only 4 pi r a cube delta. So, this is the misfit volume assuming that there is no elastic strain right now or there is no elastic deformation for the hole or for the sphere.

Now, because we are defining this we can now say that delta is equal to 0 greater than 0 it implies larger solute atom just like I said few minutes back and, when delta is less than 0 it means that the smaller solute atom is being added, one is inserting sphere in the hole V h changes by delta V h ok. So, now, we will assume that the size of the hole is being changed, because now we have this extra biosphere over here and there is a hole in the matrix.

So, you put the sphere of a different size into the matrix. And the change in that matrix would not be exactly or the new volume of the hole would not be exactly equal to the volume of the sphere, that you have put in there because there will be elastic deformation.

$$\varepsilon = \frac{1+\nu}{3(1-\upsilon)}\delta$$

So, the new volume we would say is equal to V h. So, the change is actually delta V h V h was the original 1 so, changes by delta V h to leave a final radius r a 1 plus epsilon.

You see that the new radius that is being defined for this hole is not 1 plus delta, but 1 plus another quantity epsilon and there will be some relation between epsilon and delta, because it will depend on their compliance how much is the elastic modulus of the material and what is the new and so on. So, this is the new radius of the hole r a 1 plus epsilon.

And therefore, if we define delta V h which is how much the volume of the hole changes then it can again be written like 4 by 3 pi r a cube just like I said for earlier it will be 1 plus epsilon cube, minus 4 by 3 pi r a cube and again this is epsilon is very small 1 plus epsilon cube becomes 1 plus 3 epsilon. So, all the quantities get cancelled and this only 3 epsilon gets multiplied by this. And therefore, what you are left with is 4 pi r a cube epsilon when epsilon is very small. So, we are assuming that whenever we are inserting a substitutional or interstitial atom, they are not very very different from the available space size.

Now, we need to find a relation between delta and epsilon and what we have assumed just keep in mind that G the modulus for the sphere and the hole are same. So, G which is the modulus of sphere and matrix are same. Therefore, we will not in our equation will not get the G term they will get cancelled what we will be left with is only nu which is the Poisson ratio. Now, this can be shown we are not going into the detail, but at equilibrium how would you obtain this basically there should be a equilibrium what could be that equilibrium, at equilibrium inward and outward pressure on sphere and hole surface must be equal.

So, let us say that the sphere is larger in size and the hole is smaller in size. So, when you insert there is a press pressure inward on to the sphere and there is a pressure on the surface of the hole on outside. Now, if you want to equate this which will be equated by calculating the strains and the stresses acting on to it.

So, the pressure term on both the things will have to come out same and from there, it can be very easily shown that delta V h will be equal to 1 plus nu by 3 1 minus nu this is basically coming from the pressure term into V misfit. Now, V misfit and V h we know are in terms of delta and epsilon so, we have a relation between epsilon and delta.

So, delta is the actual difference in the size and epsilon is after it has been fitted, now let us look at a few more things, if we were talking about infinite matrix then the total volume change, because of this one insertion would be equal to delta V h ok, but we are talking about small region plus the constraint at the outer surface there will be some bulk there. So, the outer surface the stresses must equilibrate and when you use this constraint what we get now this part is beyond the scope of this work will not be proving it here, we in this particular course will just.

$$p = \frac{-1}{3}(\sigma_{xx} + \sigma_{yy} + \sigma_{zz})$$

So, we will just write that actually the total volume assuming the these constraints would equal to delta V h 3 1 minus nu, while if we were considering if we considered infinite matrix, change in volume would be equal to because of this sphere being inserted in the hole will be equal to delta V h this is what we calculated delta V h earlier which is equal to 4 pi r a cube 4 pi r a into 1 plus 4 pi r a cube times epsilon.

So, this is what we obtained or this is what we know earlier, but we are saying that in under the constraints actual volume change is equal to delta V total and this delta V total can be written in terms of delta V h 3 1 minus nu by 1 plus nu again it is the pressure term which is coming, because there has to be stress relaxation. So, this term that you see over here is because of pressure.

So, delta V total the actual change that will come under these constraints is equal to delta V h times these, but what is this term we know from earlier this is equal to V misfit. So, this is equal to V misfit. So, you see that we started with V misfit which is when the two things are separate and in the end we see that the actual volume change is also equal to V misfit.

So, if you one had made a erroneous declaration at the beginning that is since the volume change between the sphere and the hole is V misfit so, all our calculation should have a total volume change of V misfit that would end up being the same being the correct, because we are at two places we are cancelling out the pressure effect. And therefore, and therefore, the total change in the volume comes out to be V misfit.

Now, if we want to calculate the interaction energy then it can be given as p into delta V total, pressure into volume that is whatever pressure additional pressure is acting on that small amount of volume that is the interaction energy that is the change in the overall strain energy, but what will be the pressure term equal to the pressure term will be equal to minus 1 by 3 sigma x x so, let us say this is a matrix. So, therefore, there will be this will be a tensor quantity so this will be the 3 terms sigma x x plus sigma y y plus sigma z z.

So, this is a interaction energy between defect and any other defect. Now, if it happens to be a dislocation then this will come from a dislocation. So, what will be that sigma x x sigma y y signal z z of a dislocation you will have to calculate the misfit now where do we calculate this pressure. So, where so now let me first so at the up to this point what we have talked about is interaction of a defect with anything it could be any other defect. Now, we will go into interaction of defect with dislocation we will invoke the properties of dislocation and put in over here.

So, what do we need over here? So, first thing we want is where do we calculate the sigma x x sigma y y sigma z z, where do we calculate pressure, because you have a dislocation at different points you have different sigma x x sigma y y sigma z z. So, when we talking of interaction of dislocation and point defect we want to know how do we calculate or where exactly we do we calculate these values of sigma x x y y and z z the answer is at the location of point defect.

So, let us say this is a dislocation line over here and there is a point defect over here. So, you have to calculate the sigma x x sigma y y sigma z z, because of this dislocation at this particular point. So, sigma all the x x y y z z x y z so, whatever is the x y z with respect to this dislocation at this point is what you have to calculate to be able to find the pressure acting on to this point defect and then you would be in a position to say what will be the E I at this particular point. So, now, what we need is so this is from dislocation. So, now, what we need is the stresses from dislocation?

Now, if we are talking about the stresses from dislocation, we know that there will be two types of dislocations one will be the edge and other will be screw dislocation, what is the stress matrix for edge dislocation, it has while on the screw dislocation we have something like this.

Therefore, we will have pressure which is equal to will have some finite quantity over here in fact, you can easily show that this will for a stress for a edge dislocation this will come out to and like I said these terms that you see 1 plus nu 1 minus nu these come when we are talking about pressure. So, this is the pressure term that we have when we are talking about the edge dislocation, where you can put x and y for a particular point defect which may be x and y distance away.

For a screw dislocation what will be pressure all these terms are 0 these are the terms that we said that that we used to calculate pressure. So, the pressure is equal to 0, which would mean that E I would be equal to 0. So, the substitutional defect that we are talking about here that one we will create a pressure equal to 0. And hence the interaction energy for a substitutional defect does not interact with screw dislocation.

So, that is the fact that will learn and see in mathematical terms. So, this substitutional defect gives a pressure 0 and therefore, E I is equal to 0. On the other hand substitutional defect can interact with edge dislocation, because edge dislocation has a pressure term and therefore, this will be a finite quantity and which we can further calculate like this.

$$E_I = \frac{4Gbr_a^3 \epsilon \sin\theta}{r}$$

So, you can say that E I is equal to p delta V which is equal to p V misfit. So, will have p misfit equal to 4 pi r a cube delta and the p term would be 2 by 3 1 plus nu by 1 minus nu G b by pi sin theta by r so, sin theta is with respect to the dislocation. So, let us say this is the particular point defect we are talking about and this will be the x and y with respect to this. So, this completely explains the terms in the equation this particular plot and we will have equation like this which can be further simplified to something like this.

So, here we earlier we wrote in terms of x pi x square plus y square. So, which can now also we written as sin theta by r. So, this is the equation of interaction energy of sin, interaction energy of substitutional defect with edge dislocation. Now, we can further see some important results with respect to this edge dislocation.

Now, let us say this epsilon is greater than 0 then what do we see that E I so, if epsilon is greater than 0 all the quantity is here are positive as long as theta is on the top half of the plane. So, if theta is between 0 to 180 this term remains positive and everything remains positive. So, E I is positive for sites above slip plane, on the other hand E I is negative for sites below slip plane.

Let us see what is the meaning of this so, when is epsilon greater than 0 it means you have a larger substitutional atom and when that is the case E I is positive for sights above the slip plane meaning there is no bonding, when E I is negative it means there is bonding. So, the larger atoms like to bond on the lower side of the slip plane so, they will like to go somewhere below the slip plane. Now, let us look at the other scenario when the substitutional atom is smaller in size so, here bigger in size and their so when epsilon is less than 0 E I is negative above slip plane and E I is positive below slip plane.

So, now what do we see here if you have a defect which is smaller in size than the substitutional atom than the matrix atom, then energy is negative for above the slip plane, meaning those smaller atoms would like to segregate on the top side of the or above the slip plane. And on the bottom side it is positive so, there is no bonding and it will like to move away from over there. If I could simply draw a simple structure, let us say this is a edge dislocation and let us say we draw certain.

Now, let us say I put a small atom then where does the small atom want to go the small atom wants to go somewhere over here. So, it would like to go over here this is smaller atom. Now, if it were a bigger atom then that bigger atom would like to go over here so, this is also very obvious as you can see that larger atom will like to go in region, where it has where there is tensile stresses because it itself will be creating compressive stresses so, that will cancel out. On the other hand smaller atoms will go in a compressive region, because it will create a tensile stress so they will cancel out so, that make sense.

Now, that is for the substitutional atom how would it be different when we are talking about interstitial defects.

So, will the overall equation or the form of the equation for the interstitial equation interstitial defects would be a little complicated. So, will not be able to derive all of it will just understand what is physically happening. So, let us say we have octahedron in a BCC so, this is BCC. So, there is one atom of here one atom is over here and now let us connect these so, that you can see that approximately an octahedron is created now you can have a atom over here. Now what are its nearest neighbour? So, this is our which is octahedral site what else do we know about this, that this will create asymmetric now let us see will really if it is asymmetric distortion.

Let us look at the nearest neighbour for these this particular atom. So, let us mark A B C D let us mark these as E and F. So, which are the nearest neighbours for this particular defect it is A or E and F A B C D or E and F. So, as you will see that the distance between these two is actually root 2 A while the distance between this is A by 2 so, A by 2 is smaller. So, the nearest neighbour is actually E and F which is at A distance A by 2 and A B C D are actually a little bit farther away which is A by root 2. And therefore, this you can as clearly see that this is asymmetric.

Now, if this is asymmetric now if the that would imply that it has more space, over here in the region from over here while it has lesser space in this particular region. And therefore, it would mean that even it tries to push, a large let us say this interstitial atoms was a little bit larger in size, more than the space available. So, large interstitial which will be more than a minus 2 r produces distortion.

Now, it will first displays the nearest atoms which are E and F by displacing E and F more strongly than A B C D which are the next nearest neighbour. In fact, you can calculate what would be delta x x delta y y delta z z, but what is more important is that because of this asymmetry it creates a shear strain.

And now if it is a shear strain, then it means it can interact with edge dislocation it can also interact with screw dislocation, because screw dislocations earlier we saw they do not have pressure term or the hydrostatic terms therefore, they were not able to interact with the substitution, but interstitial defects because of their asymmetric distortion, they create shear strain.

And this shear strain is able to now interact with the screw dislocations, while edge dislocation interaction is still there because the pressure term is still there. And therefore, and here what you would get in effect is you will still get a relation which is of the form.

E interaction which is equal to 1 by r f theta just that this theta f, theta term would be very complex. So, as a summary we can write. So, let us say when we are talking about interstitial defects, then this is interacting with both edge and screw, what about the substitutional defects, it interacts only with the edge dislocation and not with the screw dislocation.

So, which one would you expect to be stronger. So, this will be stronger strengthening effect, relatively weaker effect is what you will observe over here. And in fact, this is how it has been observed people have seen or calculated for the delta sigma which is the approximate change in the strength with change in percentage concentration. So, people have seen that something like carbon which is interstitial or nitrogen which is also interstitial the effect is much more pronounced.

On the other hand so, this is carbon is nitrogen. On the other hand if you look at the substitutional atoms like vanadium, niobium silicon, so they have these are the substitutional atoms they have a much much smaller strengthening effect. So, here you have to changing the concentration and the amount of change in stress or the yield stress that you observe.

So, here clearly atoms like carbon and nitrogen which go in the interstitial site, because they are interacting with both the edge and screw dislocation are giving more strengthening effect while atoms like vanadium silicon niobium which go in the substitutional sites substituting the iron atom over there, they do not give as much strengthening effect.

So, we have looked that the strengthening effect, because of the interaction of the point defects and edge dislocation. So, will close this chapter here next time will come and look at another affect which is created, because of the presence of point defects and again it is will start actually somewhere where we left which is that the E I is equal to F theta by r. So, we start from there because of that will see some more interesting phenomena taking place particularly the yield point phenomenon. So, thank you will see you in the next module.