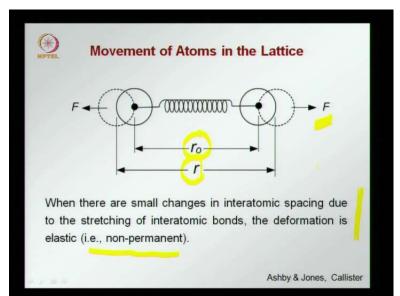
Modern Construction Material Prof. Ravindra Gettu Department of Civil Engineering Indian Institute of Technology, Madras

Module - 2 Lecture - 4 Movement of Atoms in Solids

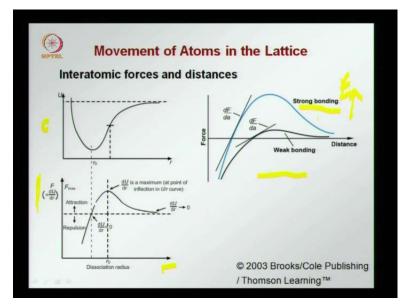
Welcome to the fourth lecture on modern construction materials, we are covered until now atomic bonding how material structures formed. And today will go on to see, how atoms moves within these structures and this is interesting, because it leads on to ah givers the understanding ah of diffusion. The movement of atoms and particles due to stresses; and then we go on to talk about mechanical behavior will understand better the mechanism, which cause that kind of a behavior.

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Now, when we have small movements within the lattice; we have the bonds being separated from the stable ah the minimum energy distance r 0. As you remember from the quantum most diagram, we said r0 is where you have the minimum lattice energy within the ah lattice. Structure and that also gives the highest binding energy of the attractive forces between the atoms. Now when there is a small change between the spacing going from this to the dashed positions. We have the distance now as r and if there is a small change just like you would have a elastic

spring. There is an elastic behavior and when this force is removed the atoms go back to the original position, so when there are small changes in the inter-atomic spacing. As the interatomic bonds are stretched the deformation is elastic; elastic means that the deformation is nonpermanent when you release the note the atoms go back to their original positions.



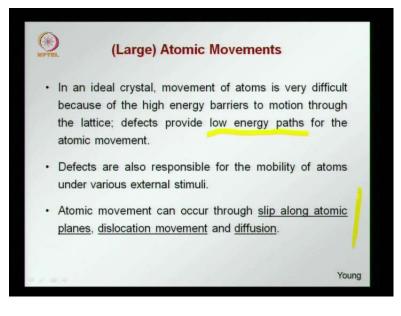
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But they could be movements or changes that are larger larger changes in inter-autonomic Spacing; and again using the quantum most diagram. We can explain what could occur, so here on the top we have quantum most diagram. And you have the energy versus the inter atomic spacing r. And you have indicated here r zero, which is the stable inter atomic spacing corresponding to the minimum energy. In this curve the minimum potential energy or the minimum lattice energy now from this we saw in the earlier electron. How we can derive stress spacing diagram by differentiating the energy curve. And here you have now this curve, which gives us the force f which is du derivative du ah derivative du by dr and this is the distance or the how much the atoms are disassociated?

Now this curves tell us the behavior between the spacing r and the force and we find here that over a certain range that corresponds to distance less than r zero. We have repulsion or compressive type behavior here; the atoms are closer to each other than this stable distance r0. And then as there is no tension or the separation of spacing with r being greater than r0; you have this is curve, which is on top of this dashed line. This point corresponds to the place, where you had the minimum energy and this corresponds to the zero force situation. Where the atoms are separated a at stable distance; now has you separate the atoms more you have a linear part. And then a non linear part and a maximum part; So this as we said earlier give us the tensile strength; further separation encounters less attraction until the atoms have no attraction anymore. And they can be fully the separate, this behavior is better seen here; where you have the this blue curve showing us the case of strong bonding the force versus.

The distance diagram and you see the here, that initially you have straight-line a behavior or a linear behavior both in compression and tension for-week bonding also. It is a similar case but the slope is less, so here you would have more resistance to separation initially. Here they would be less resistance to separation or in other words the model is of plasticity for the case of strong bonding will be higher. You have higher young modernist, and here for a week bonding you have a lower young's modernist. There is less resistance to movement and beyond a certain stage you have a non-linear behavior.

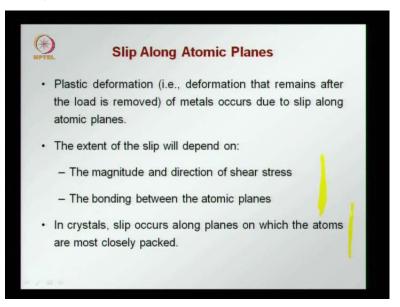
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And then finally failure or complete separation of the bonds will occur; now when we go to large atomic movements. There are some mechanisms, which controls such movement ideally in a crystal the movement of atoms will be very difficult. Because of the energy barriers the high energy barriers to motion through the lattice, that is the energy required to have movement of atoms through an ideal crystal is very high. However the effects provide low energy paths and we find that lot of times defects dominate the autonomic moment.

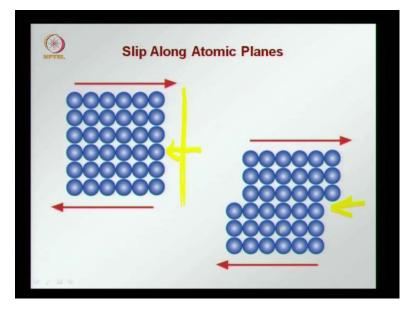
Because they provide this low energy paths the defects are also responsible for the mobility of atom sunder external stimulate. That is temperature stresses chemical action and so on so you find that the defects; that we saw in the previous lecture the point defects the line defects the surface defects and so on. Effects how the atoms can move within the crystal structure, the lattice structure. There are three basic mechanisms, which are important autonomic movement can occur through slip along autonomic planes dislocation movement we talked about dislocation already and diffusion.

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Now you look at these types of movements in further detail starting with the slip along autonomic planes. We have what is called plastic deformation that is permanent deformation or deformation that remains after the load is removed in metals due to this slip along the autonomic planes remember a couple of slides back. We have looked that elastic deformation, were when the remove the load the positions of the atoms returns to the original state. That is the atoms return to the original locations and there is no deformation that remains after the load is removed. Now in plastic deformation there is permanent deformation or deformation that remains, even after the load is removed. And this is the amount of the deformation the amount of slip that occurs between the autonomic planes.

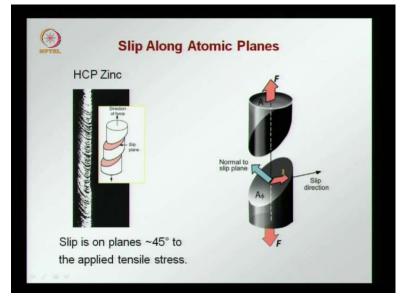
Repulsion on two things how much is the external stimuli in terms of stress or the magnitude and direction of the shear stress shear stress is what causes slip the magnitude. And the direction in which the shear stress acting, which is based on the external loads and stress causing phenomena. The second aspect is how very the autonomic planes are bonding better the bond stronger the bond less will be the extent of slip under the same stress. This is what we saw aha slide earlier and also, what is important is that? When we have a lattice structure in a crystal the slip occurs along planes in which the atoms are most closely packed.



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That is if you have close packed structure along planes slip will occur along those planes not across those planes, but along those plane this we see better in this ah diagram. So you have here structure with closely packed atoms so all these planes. Here are the packed planes and if, you

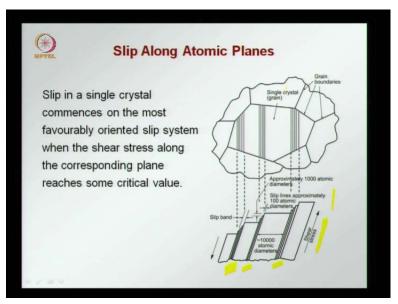
apply a shear force, then what we will see is that the slip doesn't cut across the closely packed planes but along those like what we see here.



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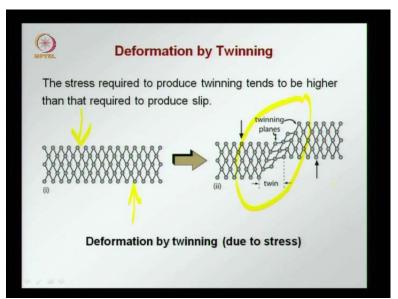
So here you see how slip occurs the slip is occurring along the closely packed structure; and not against it or across this is done. This happens because this requires the least energy or creating the slip in depended of how the load is applied slip may often occur in a certain direction for example here. We see a bar of zinc being pulled and we've seen that the slip across at forty five degrees to the apply tensile force. So even though the force is acting here; vertically we find that this slip is occurring forty five degrees. Because that is where you have the shear stress acting slip requires sheer stress and slip occurs in the direction of the shear stresses. So that is why in this case you have slip occurring along the plane at a forty five degrees to the direction of the applied tensile stress.

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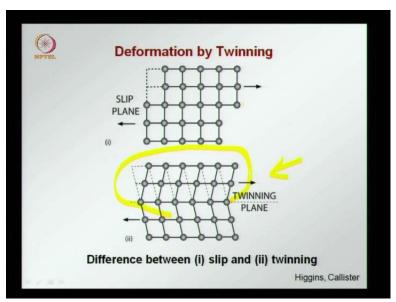
Now when you take a crystal they will be several atoms packed together in a crystal slip in a single crystal now commences starts. In the most favorably oriented slip system and we have already discussed the slip will occur along the plane were you have a close packing. So slip will occur along the most favorably oriented packed plane and this when the shear stress along that plane reaches the critical value. Where resistance of that is not enough to keep the atoms from sleeping; so, if you have if you look at this material and you look at just this crystal or grain they could be closely packed atoms along these planes, which start s sleeping so they form is slip band. So these are different slip bands, which occur due to the sheer stress. Which is given rise to by the applied stress; these slip planes are very small almost in the atomic scale and also separated by a certain distance. This is me in a certain distance now we should keep in mind that the crystal planes will not co inside from one crystal to the another. We already looked at this when we discussed poly crystal and material.

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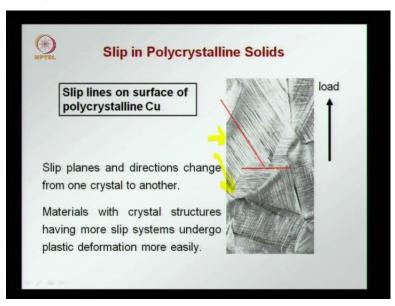
So the slip which occurs in one grain when it as to be continued in another grain might have to change direction to accommodate direction of the planes, in the adjacent in the crystals other than slip you can also have deformation within the lattice due to twinning and here. You see what happens when you have a structure here, which is subjected to shear. So you are trying to make the material shear then this give rise to a structure like. This where you have a twin form over a certain distance; and here you can see the symmetry about this line and that is why it is called a twin.

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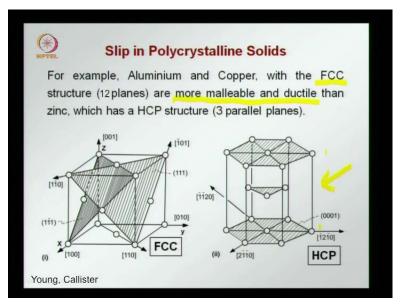


And this is called the twining plane, so this is also a sizeable deformation plastic deformation that can occur the material. And this mechanism does not requires slipping, because it occurs due to twining when we compared the two we can see the difference here slipping occurs. On the plane where the shear stress is applied with atoms; now shifting by one lattice spacing twining on the other hand requires a lot of deformation to occur. Like you see in the bottom diagonal, this is twining you find that a lot of this spacing as to change for twining to occur. Here you just have one atom shifting each time at each step to have the slip occur.

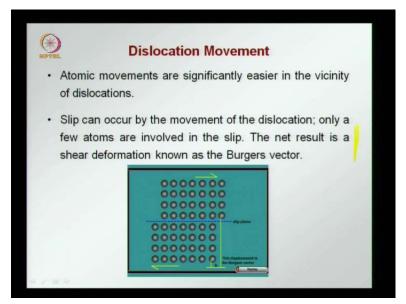
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Now when you see a poly crystalline materials such as a copper you have now different crystals and you can see the crystal planes along. Which slip will occur and if you loan you find that slip will occur along this red line. In this crystal but to continuity will have to change direction and slip to occur along another direction in the adjusting crystal. So slip panes and directions change from one crystal to another and materials therefore with more slip systems will undergo plastic deformation more easily. That is if this adjusting crystal as a slip plane along a similar direction is this and then the continuation of the slip will be easier. And there will be more plastic deformation or plastic deformation will occur more easily under a certain load. (Refer Slide Time: 16:12)

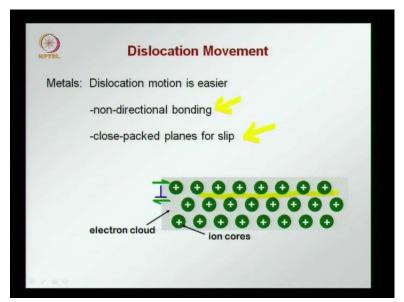


This can be explained more by looking at this diagram, where we are comparing two structures the FCC structures the phase centre cubic structure and the hexagon a closely packed structure on the right aluminum and copper have the FCC structures. And you see here is shaded different planes along which slip can occur and you see that these planes are having different orientations. The HCP structure has three parallel planes and all of them and since they are along the same direction will offer more resistance to an arbitrary slip system forming. So we find that materials with an FCC structure are more malleable and ductile, which requires a lot of slipping to occur. When sharing the occurs within the system, so HCP structure structure material for mental will be less malleable and ductile, because the formation of the slip plane is more difficult in a poly crystalline material which has the HCP structure. (Refer Slide Time: 16:12)



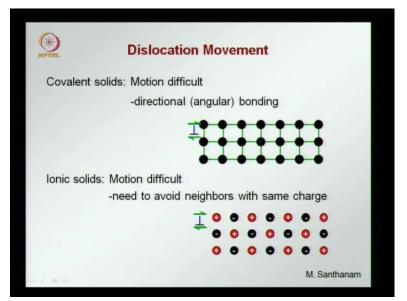
Now another type of movement is dislocation movement were they have the defects moving within the system. You see here in the bottom animation that there is a dislocation moment, which ends with slip occurring along this line. And ultimate displacement in the system, which is called burgers vector there was a dislocation here, which moved across and ended up with this sort of a permanent deformation equivalent to the burgers vector. So atomic movements are easier when dislocations are present atomic movements are significantly easier in the dislocations. This clip occurs by movement of the dislocation across we saw the dislocation moving across here with only a few atoms involved in the slip.

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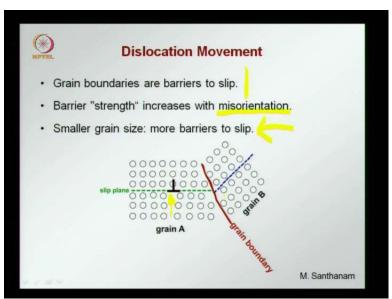
At each step there was only one bond be broken in form and finally the net result is a shear deformation permanent deformation called the burgers vector. We have discussed basically how dislocation move within metals how deformation occurs within metal. Because dislocation moment in easier in metal; because the bonding is non directioning. So dislocations can move without hindrance due to the directionality; there are closely packed planes which facilitate the slip so that is if i dislocation here.

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It can move across move across and slip can occurs along this plane easily. However when we look at covalent and ionic solids. It is obvious that it can become very difficult the motion due to the dislocations can become very difficult, because if you see here the covalent solids will have angular bonding directional bonding and when the dislocation. As to move then the directionality will have to change. And this the movement of the dislocation, because these angular bonds have two have certain direction. And these cannot be broken so easily in slip cannot occurs; in this plane very easily in ionic solids. If you remember we had both the cat ions and irons ions in certain array; and now when the dislocation. As to move across it will find that there will be neighbors with the same charge. So if this as to move you will find that the cat ion will have to come. Here at some stage and there will be a repulsion between the cations and this will again impede the dislocation within an ionic solid to move.

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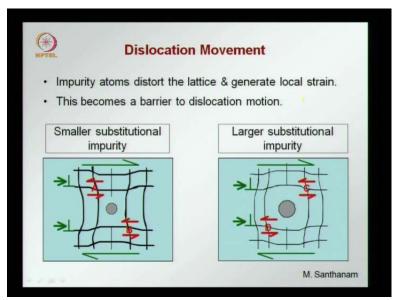


So we have basically moment of dislocations in metallic solid because of the type of bonds; and because of the type of structure that occurs in metals. We also saw earlier that in poly crystal line materials there are green boundaries and at the grain boundaries we had discontinuity of the crystal structure. That is what we callas surface effect where there is a gap between the edges and atoms adjutant at ions in a metals. And the slip plane does not continue across to the neighboring grain so in grain a if this was the lattice structure and here you have dislocation here. You have a

dislocation this crystal plane does not continue into grain b there is a green boundary here and if this dislocation.

Now as to move across slipped to the grain boundary and continue due to substantial you find that. Now it to change direction this offers more resistive so there is a greater force will have to be required to create shear that will continue onto drain p so this gives rise to a very important aspect, which is that grain boundaries are barriers to slip more grain. Boundaries means, there are more barriers and what happens is this barriers strength that is which requires a more ah higher force to move the dislocation from one grain to another increases within the miss orientation. That is the angle between the crystal planes across the grain boundary here you see between the green line and the blue line. There is an angle, which is not at one hundred eighty degree if it was one hundred eighty degree the dislocation would just move across.

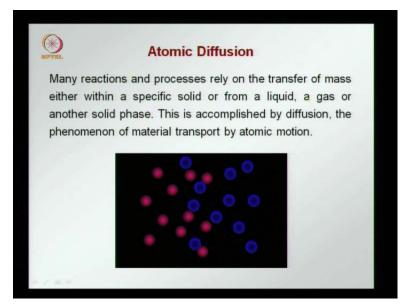
Now but now the dislocation as to change direction and move across the blue line for the split to continue to occur, so the one strength of the barrier increases with more miss orientation more different the angle is from one hundred eighty degree you have ah higher barriers strength and there is a very high probability. That this will occur in a poly crystalline metrical consequently what we find is smaller grain size within the structure more barriers to slip.



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And the strength of the materials or the resistance of the material to slip increases, we find that impurities or defects that distort lattice also offer barriers to dislocation movement. And this we can understand from the figures below you can have a substitutional impunity, where either impurity or the atoms is smaller than the other atoms of the in both the cases. You have a discussion of the crystal planes so when the dislocation. As to now to slip across it encounters ah surface. That is not plane that it distortion so the dislocation now as to surpass this distortion and move across.

And therefore the require ha higher share stress than when they would be no defect and the slip plane is straight; Here also you see that there is a bump, so the dislocation. Now as to surpass this bump and go across, which requires a higher share stress than, if this slip plane was plane. So impurity atoms atoms that are introduced into the lattice distort a lattice; and therefore generate a local strain. And this becomes a barrier to dislocation; so we saw this earlier in the example of copper with different atoms introduce that distorted. The lattice and therefore the strength the heel strength increased, because h e l depends on the slipping and the sharing along the crystal planes.

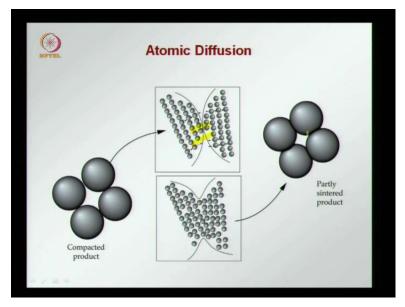


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Another type of movement with the materials is done by diffusion is due to diffusion lot of reactions lot of processors that we have in materials, which define how the material structure

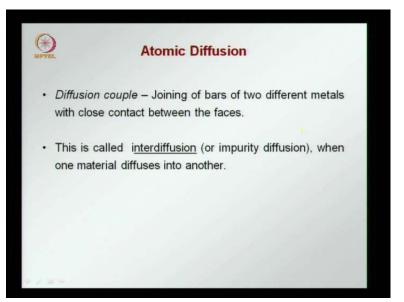
forms and also materials behave in time depends on atomic diffusion. So, many reactions and processes rely on the transfer of mass within a solid or a liquid or a gas another solid-phase and this transfer accomplished by diffusion, which you see in the animation below where you have the diffusion of the red and the blue atoms occurring in time so this phenomena of atomic motion is called diffusion.

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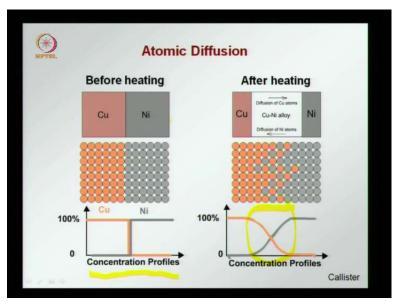


And this is important for several reasons, we can have diffusion joining particles through sintering. Where you have the upper diagram articles that are pushed together probably heating is applied and you find that the atoms. Now move across and you have a neck being formed in the sintered product the diffusion.

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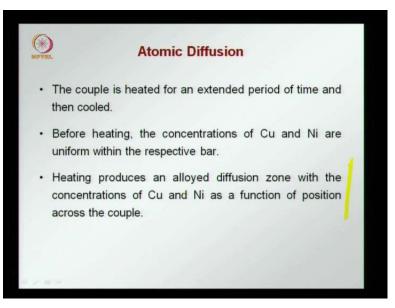
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Now has joined these particles together to form a more solid structure diffusion can also occur in metal. And an example is in diffusion couple where you have bars of different metals closely in touch with some heat applied and the diffusion now occurs between the two bars this is called inter diffusion or impurity diffusion and that you see. Here in these figures more clearly we have copper and nickel two bars of copper and nickel. Put next to each other they are pressed together and heat apply before diffusion occurs, we find that hundred percent of the left-hand side is copper on the right. You have hundred percent nickel, so the concentration profile looks like this you have hundred percent copper and hundred percent nickel on the right-hand side.

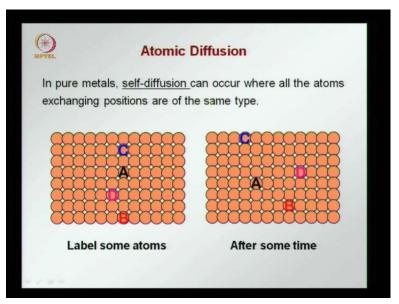
Now when diffusion starts because of the pressure applied and the heating copper atoms start moving from the left to the right equal nickel atoms start moving from the right to the left. So, the concentration profile; now changes there is no sharp difference between the copper part and the nickel part. But you have an area, which as both copper and nickel atoms or an alloy is formed or a solid solution is formed with both copper and nickel were the concentration is now like this.

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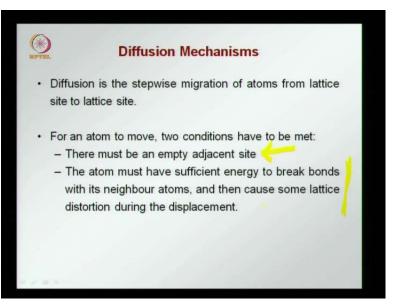
So, diffusion as created an alloy in the middle and also bonded that two bars together; so, to recap we have a couple two bars of different metals pres together heated for an extended period of time and cool. Now before heating the concentration of copper and nickel in the respective bar in the previous figure, we saw on the left it was copper, right it was nickel. And heated hundred percent copper concentration of copper on the left and hundred percent concentration on nickel on the right but due to diffusion.

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Which is occurring due to heating the and alloy is formed in the diffusion zone with a combination of copper and nickel to the concentration is higher as we move away from the diffusion zone of one material. And is a mix at the diffusion zone itself diffusion can also occur within the material in a pure material, also you can also have diffusion occurring where atoms move around responding to external stimulated. If, we have label some atoms A B C D like you see in the left hand side are diagram after some time due to the application of heat stress you can find. That they have changed locations and now they are in the new locations which are shown.

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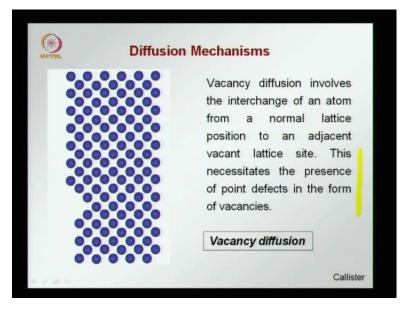
So this is called self diffusion, so diffusion can occur within a certain material or due to one material moving into another material diffusion. Therefore stepwise migration of atoms from lattice site to lattice site within the lattice structure step-by-step the atoms are migrating, this is called diffusion. Now for this diffusion to occur or the migration of atoms to occur between the lattice structure two conditions has to be satisfied, first they should be an empty adjacent in side; because the atoms has to shift their the atoms should also have sufficient energy. This can come stress being applied heat being applied the atom must have sufficient energy to break the bonds that is keeping it in his place it to break the bonds with this neighbor atoms cause some lattice distortion and moved to new site.

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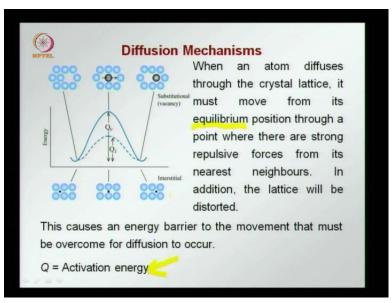
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So these are the two conditions, which have to be met we have two possible ways the diffusion can occur interstitial diffusion is where the atoms migrate. In the space between the parent structure, so interstitial diffusion involves atoms that migrate from one interstitial position to a neighboring. One that is m so you see that in the lattice form by the blue atoms you have these small red atoms moving in the interstitial. That is this space between the blue atoms and this occurs a lot in the case, where impurities defuses in material. (Refer Slide Time: 30:48)



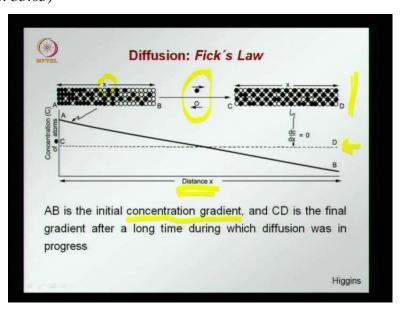
For example diffusion of impurities such as hydrogen carbon nitrogen oxygen, which have atoms that are small enough that they fit into the interstitial space. So this is interstitial diffusion vacancy diffusion is where you have an atom moving to a space which is un occupied by in any other hand. So, you have here see the blue atoms moving to a space, which is empty; this is called vacancy diffusion. And this involves the interchange of an atom from a normal lattice position to an adjacent vacant lattice site.

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And this obviously necessitate the presence of point different, if there were no vacancies then this type of diffusion cannot occur. When we compared with to the substitutional or the vacancy diffusion and the interstitialyou find that the interstitial will require less energy less activation energy Q here is activation energy. Qi is in the case of the interstitial diffusion you have a small atoms moving from one interstitial to the other and this requires now less energy than a substitutional or a vacancy diffusion were the born has to be broken. And they has to be significant energy for distortion to be overcome and a new position of this black atom as to take place.

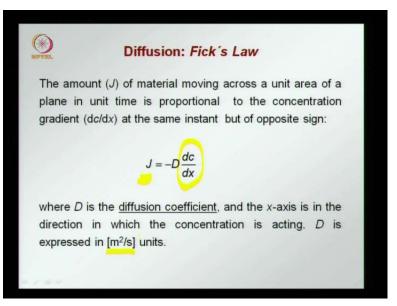
So when an atom diffuses through a crystal lattice it must move from its equilibrium positions, where it was before the diffusion occur through a point. Where there are strong repulsive forces from its neighbors and in addition the lattice as to be distorted this causes and energy barriers. This hump you see is the energy barrier the energy that is required to overcome this is called the activation energy then we find that the activation energy for a substitutional are vacancy diffusion is higher. As we see here, whereas interstitial case the activation energy is less. (Refer Slide Time: 33:05)



Because this ah time is small enough the distortion is less and the diffusion occurs more easy diffusion is governed by what is called the flicks law. And this dramatically is seen here, you can have a case where you have ah change in concentration of what I shown here is black-and-white atoms with more black atoms on the left-hand side. And less black atoms on the right-hand side or more white atoms, so there is ah difference in concentration of the black atoms through this distance x work diffusion will be is tried to make the concentration.

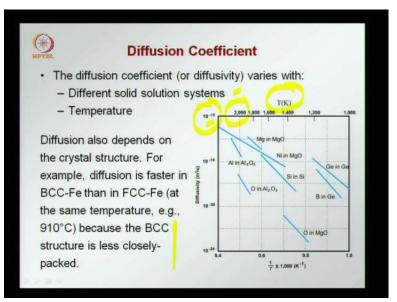
This same throughout the distance X by having the black atoms moved to the right and the white atoms moved to the left. So, eventually reach a system like this, where you have an equal distribution of black-and-white atoms throughout the distance X. So, the concentration changes from A B of the black atom to something like this C D the concentration is same everywhere over the distance X or the gradient now drives the diffusion until the gradient becomes zero. A D is the initial concentration gradient C D is the final gradient after a long time so you see the flat dash line.

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This is represented by ficks law were J is the amount of material moving across the unit area of the plane in unit time this is proportional to the concentration gradient given by dc by dx the proportionality constant is D and there is an negative sign, so J is equal to minus d dc over dx d is called the diffusion coefficient.

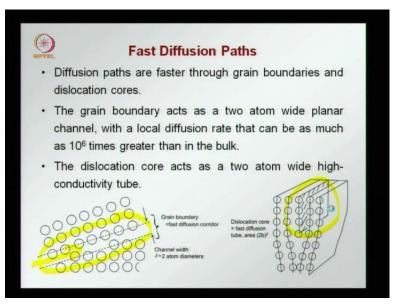
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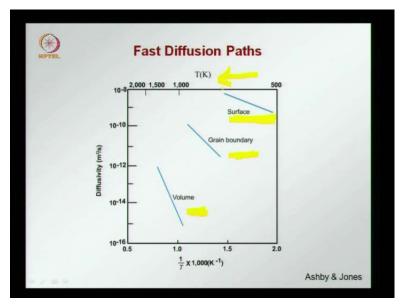
And here X is the direction along, which the concentration is acting or diffusion is occurring the diffusion coefficient is expressed in meter squire per second. These diffusion coefficient varies from one material to another, how the solutions are occurring. That is want the diffusing in what defines the diffusion coefficient; and also importantly we will be find that temperature also controls the diffusion; You see here on the right hand side diagram several of these blue lines showing different materials diffusing in other. For example this is magnesium diffusing in magnesium oxide nickel diffusing in magnesium oxide. And you find the values are very different and you find that all of them are sloping such that you find higher the temperature. Higher is the diffuse on the Y axis's here we have differential usability and you find than the values are higher. When the temperature is higher, so higher is the temperature diffusion occurs faster there more diffusion coming back to the first aspect.

We find that the diffusion depends on the crystal structure through which the diffusion is going to occur. For example, we find that in the BCC iron diffusion is faster than the FCC i at the same temperature, for example in 910 degree, there is a equal possibility that there is a BCC iron and FCC iron. And the reason is that the BCC structure is less closely backed. This we saw couple of lectures back that BCC structure was least of the closely packed structures. That we saw so when the structure is less closed packed diffusion can occur more easily.

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Because the other atom can move more freely in the lattice structure; there are also other cases where you can have fast diffusion paths. And this becomes very important when we look later at corrosion and so on. Because we find the diffusion occurs more rapidly diffusion path are faster along grain boundaries and dislocation course, and if you remember these are the defects that occur. In the lattice structure grain boundary being a surface defect and dislocation being line defect; the grain boundary acts as a two atom wide leaner channel, so you have the grain boundary here, which is now like a path a channel or diffusion occur. So diffusion occur very fast through that grain boundary also in a dislocation core here, you find that the diffusion will act fast dislocation core acts as a two atom wide high conductivity tube. (Refer Slide Time: 38:46)



So through this because of the higher energy the diffusion can occur fast and this is seen here in this diagram, where you see diffusivity on the Y-axis temperature. On the x-axis and hear you see how the behavior is diffusion is occur at the surface grain boundary and in the bulk value within the crystal. You find the diffusivity is very high on the surface, because you have discontinuity. There you have surface that is exposed next will come the diffusion along the grain boundary again, because with the surface defect will allow the atoms to defuse around the grain boundary. Whereas within the bulk of material diffusion will be slower diffusion less diffusion will occur in all the cases diffusion will be higher at higher temperature.

Here you see temperature increasing to the left in this diagram and you find that as the temperature increases we find that diffusivity. The speed at which diffusion is occurring will be more, so to conclude we have looked. At different ways that atoms can move within a lattice structure, we saw how small movements leads to elastic deformation, that is when the force is removed the atoms go back to their original structure. Then we have larger deformations occurring plastic deformation occurring due to large strains within the lattice structure dislocation movement.

We also looked at how diffusion occurs where atoms can move over large distances to the crystal structure and we look that different types of diffusion and so how diffusion is the effective by temperature. What we saw is that diffusion is faster through certain defects like dislocation course and grain boundaries. We also saw the diffusion was higher, when the temperature is

higher and one interesting aspect that came up was how grain boundaries are barriers to dislocation movements. So, we found that because of the miss orientation of crystal planes across the grain boundary the dislocation cannot move through one grain. And onto another and therefore we concluded that if we have lot of grain boundaries like any material, which as small grains they would be higher barriers or more energy needed for sharing of that material leading to higher heel strength.

We also look at how impurities seen alloy can increase the strength, because they cause the slip planes to be non planar. There is a distortion of the lattice and therefore we found that the dislocation movement is hindered and therefore you have higher strength in a alloys than in a pure material in the next lecture. We look at how ah the micro structure develops, we look at how phase changes occur in different material; and that will lead us on to understanding the behavior of the materials a surface properties. And the mechanical properties of different materials thank you. We will now look at few questions that could arrives regarding the lecture on the movement of atoms sir you have discussed. that A in closely packed planes why is it that it is easy in closely packed planes and want it is loosely.

Packed see what happens is it's not that the slip occurs in the plane, but along the place so when you have a very closely packed structure. Slip is very difficult to occur across these planes, so the plane planes, which are closely packed slip against each other. So the ah sleeping occurring along the planes, because it is very difficult for slip to occur across these planes, where more bones have to be broken, now if you have a closely packed plane. Then the slip will occur along those planes rather than any other plane, which is more loosely packed okay; can you explained what is the effect of grain size and grain boundaries on the ductility of material?

See when we look at ah the movement of dislocation, we said that the dislocations are hindered by the grain boundaries. So when you have a lot of grain boundaries, there is more hindrance; so there is a restriction of sleep or you need a very high shear force to cause slip to occur. And this is the reason, why we have strain hardening after a certain amount of slip or heeling the hindrance by the grain boundaries to the dislocation and this leads to strain hardening? Because more energy is required most shear forces are required to continue with the script, that as occurred due to your linear. So the ductility is affected by the amount of grain boundary, that you have more grain boundaries. You would expect the metal to be less ductile in the sense, that final allocation at failure will be less. But the strength will be higher, because you have more hindrance to the dislocations more barriers to the dislocation. So, the stress that is required for slip to occur that is high so the strength will go up but the allocation would normally decrease. If, you have small grains leading to many grain boundaries in the system.