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# Module - 2 Lecture - 3 Part 2 of 3 Structure of Solids – II

Will continue with the structure of solids and till now we have looked at different crystal structures forming due to ionic metallic and covalent bonds. Now well go on to see how defects occur in the crystalline structure; and we will also look at non-crystalline materials, which a call amorphous solids.

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Classification of Crystal Defects		
Туре	Specific Examples	Influence on Material Properties
Point	Interstitial Substitutional	Solid solution strengthening Swelling of clays
Line	Dislocations	Ductility in metals Work hardening
Surface	Grain boundaries	Grain size strengthening
Volume	Pores	Sites of stress concentrations and crack initiation
	Inclusions	Precipitation hardening

So, when we look at defects that occurred in crystal; there are different types of defects. And these are classified as point, line, surface and volume defects; point defects are where you have defects occurring in the particle level is could be interstitial that means that within the gaps in the crystal structure. You can have a defect meaning that there is either a vacancy or there is a foreign atom are a foreign particle in the structure.

Substitutional is where one atom of particle is replace by something else and this gives rise to a substitutional point defect. These have influences on material properties for example the point defects can affect solid solution strengthening, solid solutions or where you have alloys forming mixture of different materials. And this could lead to strengthening because of the defects, even though we call it a defect it could have some beneficial effects like strengthening. Then we have swelling of plays that can also be attributed to defects where you have some other ions being introduced into the clay this could lead to the absorption of water and therefore swelling. Line defects are basically dislocations, where you have a discontinuity in the crystal array and this has a lot of effect on ductility in metals and work hardening, because these are related to the movement of dislocations under stress.

Surface defects are grain boundaries where you have a discontinuity in the crystal lattice planes between one grain and the other and this we discussed it to some extent in the previous lecture. Where we saw how crystals nucleate and start growing and when their growth interferes with the crystal. That is growing next to it then you have a grain boundary form and this again as influences on the material properties. We will see later how dislocations are impeded or slow down by grain boundaries.

So, we find sometimes that when grain sizes are small there is a strengthening, because of the higher impedance to where this dislocation movement finally, we have volume defects in crystals volume defects could be the pores. Where there is an absence of material this could give rise to stress concentrations crack initiation at that point and these defects propagating as cracks. We could also have inclusions which can be considered as volume defects and this also could increase the hardening effect call precipitation hardening in a in some materials.

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So, as we said wind effects or certain points in the crystal lattice where an atom is missing are an extract atom is present or an atom of a different size replaces the expected atom that is the crystal structure is distorted at this point. By something that is missing an item that is missing a particle that is missing or an extra are and additional atom of particle being introduced or something of a different size that causes distortion of a crystal lattice. At that point line defects are imperfections in the crystal lattice where a line of atoms becomes mismatched or discontinuous.

So, there is a mismatch with the surroundings surface defects are grain boundaries; so, there is an area of defect concentration. We see the there is a large discontinuity in the crystal lattice at the grain boundary. So, there is an area of defect concentration in the interface between the crystals are the grains. Lastly we have volume defects which are three dimensional yeah either absence of material. That is a voids or a different a foreign material in extraneous material that is introduce in the material which is an inclusions.

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So, these are the different defects and we look at them in detail starting with the point defects in the crystals. We see solid solutions a mix of different metals there is a base metal; and then there is a different metal, which is introduced. And becomes a solid solution just like we have liquid solutions a solid solution is a homogeneous mix of two different materials. And we can have two types of point defects interstitial that is what we have in the animation at the top where we have this purple.

Atoms a particles being in the interstices that means, the voids between the blue particle. So, these are called interstitial defects in the solid solutions. Where you have small atoms are small particles fitting into the space between that larger particles or atoms. That is what we see here? Then we have the substitutional type of effect which is seen the bottom of the screen, where you have the blue-atoms substituting some of the purple atoms. So, here in the substitutional defects; we see that some atoms of the base material at the host material or replace by atoms of similar size in chemistry. Now it has to be of a similar size in chemistry other ways. They will not fit in very easily in the lattice sometimes you can have atoms of different size in chemistry.



And they have to be forced in the lattices distorted we look at that kind of effect in a minute the point defects distort. The lattice structure of the crystal and this leads to additional strain being introduced in the lattice. This increases the energy of the crystal and the lattice binding energy is decreased, if you remember from the previous lectures. We said that always a stable structure is that which as the lowest energy; because when the lattice energy is lowest other potential energy lowest you have the highest binding energy. But here what happens is when we introduce defect there is a stream created due to the distortion this train increases the energy.

That is you move away from the lowest point in the condones most diagram and this decreases the binding energy, which is holding the lattice together. Therefore, there is limit to which point effects can occur in the crystal beyond this beyond a certain states the crystal becomes unstable and cannot continue to exists. However as longest point defects can occur you can have some beneficial effect like in the case of alloys in alloys. What happens is we have a base material are a host metal in which different atoms of other materials other metals are introduced.

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And you have a solid solution, which eventually leads to strengthening are better properties of the alloys. This on this screen you see the example of copper being alloyed with beryllium in and zinc. On the right and side you see a graph showing the hill strength on the y-axis and the percentage of alloying element on the x-axis. And if you see this case at the bottom this is brass, where cooper is alloyed with zinc and in the crystal lattice this is represented as the hollow spheres being those of copper.

And then this solid sphere being that a zinc and you find that zinc atom is slightly bigger than the copper atom. So, there is some distortion after lattice not much distortion; and we fine that as be increase the percentage of zinc. In copper giving brass you have the yell strength increasing, now the question is why does it increase one way to visualizes is that when a material set has a metal yells. There is slip that is occurring in the crystal lattice that is one plane. In the crystal slides over the other plane leading to hearing on yielding now when you have local distortion like you have here.

So, you have a local distortion which is occurring here you find that there is a bump created here. So, as this plane and this plane slip over each other they will be bump. So, there is a little bit a more force needed to create this moment compared to when this was not there, if this was not there both the planes will be smooth. So, they will be easier to slip occurring between the two planes; now as this zinc atom is introduced you have a distortion in the plane. So, when slip as to occur we can imagine that this slip planes now i bumpier or rougher. So, more energies required for the slip to occur.

Now as the zinc atom is not very different in size in chemistry from the copper atom you find; that we can introduced up to about twenty percent of zinc in brass and till the material can become unstable. And up to that we fine that there is an increase in the yield strength from about seventy five mega pascal to say about hundred mega pascal with about twenty percent of now in the case a bronze. Then you have in being introduced the in atom is larger than the copper atom and also the zinc atom. So, what happens here when we substitute one of the copper atoms with the tin atom there is a higher distortion of the lattice around you can see that there is more distortion here. So, this means more strain is introduced and this has two consequences one is that this imposes a load limit.

And how much tin can be introduced in copper to give you a bronze beyond a certain limit be on a certain limit up say here it looks like about eight-percent the system; becomes unstable you cannot put in more tin atoms. Then about eight percent you other consequences now you see that the crystal plane is rougher. There is over these planes then you will need more energy took create a slip here. So, therefore, the yield strength goes up even high the yield strength is a consequence of the resistance to slip offered by the material planes or the slip plane.

And what we find here is now this surface is now bumpier and when this surface as to sleep on this surface you will need more energy to do. So, and this drives up the yield strength to say about hundred and sixty hundred and seventy mega pascal. We can also have the case of smaller atoms replacing the copper atom; in this case we have beryllium, which is a very small atom compared to the copper atom. So, when we remove one copper atom and we put in a beryllium atom you see that there is a very big distortion of the lattice. There is lot a stream created and they the limit to which you can introduce beryllium.

In copper is very small in the order of one or two percent beyond that this system becomes unstable because we have introduced a atom of a different size in chemist. So, this gives a graphical view of the limits of how much alloying we can do how much extraneous of foreign atoms can be introduced in the lattice structure and also the benefits of doing. So, why the yield strength material alloying increases when compare to the host metal; we find that when the introduce and atom, which is different from that of the host.

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Material we find that there is a distortion of the crystal lattice; and this creates the mismatch in the atom size. And the crystal planes by the slip planes become rougher and this leads to strengthening. Now points defects can occur in other materials like place here, you can have a point defect leading to a charge imbalance where and ion of one charge substitutes an ion with a different charge.

So, take the example of a smug tight here at the top; so, this is a spec night can made up of sheets of silica and aluminum hydroxide. This is the t o t e structure, that we have discussed earlier tetrahedral octahedral tetrahedral structure and these layers a bonded together by ionic bonds. And the clay is now made up of several sheets like this now suppose, we have aluminum substituting for silicon atom what happens is now there is a charge imbalance created. So, this meg tight could become probably muscovite or monbrnorillonite, because now we have other cations. Which are introduce to satisfy the charge imbalance these charge imbalance. That has been created you to the substitution of the silicon by aluminum has to be compensated by other cat ions, which get now introduced into the structure. There are cations, which get introduced; now in this structure and this can lead to changes the material behaves.

For example, when the silicon is substituted bellmen you can have potassium ion potassium cation being introduce between the clay sheets. This gives as mica muscovite or you can have calcium cations being introduced between the sheets. And the difference between these two is now with the introduction of the calcium cat ions this space between the sheets is no bigger you can see here. That is one point five nano meters, where as when potassium cat ions at there is there is only one nano meters. So, this pace here between the two sheets now is bigger this gives the possibility that water molecules can enter between the sheets. And when water molecules enter between the sheets the sheets lose some of their bonding and start separating and this gives rise to the expanding behavior of some place.

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So, as we said the partial substitution of aluminum in the silicate sheets of the plate leads the layered with a negative charge. Since the aluminum three plus replaces silicon four plus; therefore, external cations must now be located between the layers to balance the charges. So, there is the change in the charge because we have the aluminum cation replacing the silicon cation; and now you see that there is a loss of just. And so external cation have to know come in between the layers to balance the charge; and these cations are of different sizes and charges size and charger of the cations. Now determines the distance between the layers and this distance between the layers determines whether water can enter or not and this changes the behavior of place. And we saw earlier some clays absorb what are explained other not.

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So, the reason why this happens or these defects, which get introduced in the heat structure. And change the nature of death behavior it is also interesting to note that point defects occur in pairs to avoid charge imbalances. For example, here we have two cations together. That is one cations missing here and this is compensated by another cation here. You can have a case where there is a vacancy; there is one anion missing and to compensate that in terms of charge there is also a cation missing here. So, we find that lot of times the point defects occur in pairs. So, that there is less charge imbalance or this charge imbalance is compensated by another point defect also occur. And this also leads to minimum strain in the crystal lattice caused by the defect, that is the distortion created is reduced by the defects occurring in pairs.

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So, this is about the point defects, now we said that the next set of defects are line defects. Line defects are where you have a line of atoms instead of in the point defect we saw that only one point was changing here line of atoms becomes mismatched its either missing are introduced. So, these are called line defects line defects are known as dislocations we will see.

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How these occur and how these affect the behavior in a minute; now there are two types of dislocations first we will look at what is called edge dislocation and edge dislocation is and extra plane of atoms in the lattice. So we have a lattice here, which as a regular rate; but you will see that there is now these two atoms. Which have been introduced there is a discontinuous plane, where is a set up atoms. But it does not continue this is as if it has been wedged into the crystal lattice. So, if you can imagine how a wedge works, if you push this here then you will have pension developing here and compression developing and. So, that is what is shown here; so as this extra atom plain as formed you find that. There is compression here and pension; so, there is a distortion in the stress field whenever a dislocation occurs and this we can see on. So, in microgravity this is a crystallographic plane showing the dislocation aluminum.

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Here you have plain of aluminum atoms inserted in this otherwise crystal of aluminum this; obviously. Has been magnified millions of times and you can see; however, this very clearly this dislocation in aluminum these dislocations move under slip. So, when you have here see a crystal lattice with a dislocation here. And we are trying to shear or make this zone slipped this dislocation now moves towards and edge. So, you see here in these diagrams one by one they bond is broken and created.

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So, you need step we have one bond lost and one bond created this dislocations slips until it reaches and edge, this is called the slip plane. The dash line is called the slip plane this gives raise to yielding and sheering within a crystal. For example, in metal another type of dislocation is a screw dislocation, where you have region that is distorted instead of a line being introduced. You see here that at the plane has been shifted slightly that there is this line, which just moved up you have here. At line of atoms which has been moved up; so, this crew dislocation is a region of distortion in the crystal lattice in the form of a spiral ramp of atoms.

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So, you see here that it spiral right this plane i spiral it down here; it is higher here and here it this lower and this screw dislocation also moves under stress. That is what you see in the bottom diagrams you see here; a screw dislocation and when stresses applied again. If we are trying to shear this material to try to make it to yield you will see that the screw dislocation moves until it completely covers, and edge now we looked at how individual defects form and move, but in reality you will have lot of these dislocations accruing together and probably. In a mixed manner in this case you see here a screw dislocation at the edge and here in the middle you see and edge dislocation.

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So, now as the material is being sheered both the screw dislocation and the edge dislocation move. And till the reach the edge of the materials and till the structured inside his uniform, there is deformation. And this deformation becomes the slip that occurs in the material due to the stress. These are pictures again from the manchester materials science center site showing images from electron microscopic showing dislocations. In some materials on the left you have nickel and these lines that you see or the dislocations that occur and that you can see under magnification.

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Now this one on the right is aluminum there again you see the lines; and these spots or dislocations that are occurring in the surface. Which can be seen in the through the microscopy a third type of defect is a plain defects until now we looked at what happens in a point defect in a line defect. Know you have a surface, which is acting as a defect this occurs mainly in poly.

Crystalline solids where you have several grains are crystals forming this solid together; the interface between the grains are the interface between the deferent crystal, which is called the grain. Boundary represent area of defect concentration that there is lot of defects occurring in a grain boundary defect meaning that the crystal plain is becomes discontinuous and you see that. There is a gap between a edges in atoms in a grain boundary there is no continuity.

You can see in this diagram at the bottom that along the grain boundary between the white circle and the grain circle you see that. There is no continuity of the crystal plans there is a discounted, so this is called the grain boundary. And this is a defect a large concentration of the defects occurring in the grain boundary, when you see this diagram you can imagine how each of these crystals or grains as a different orientation of atoms then its neighbor. So, since each of these has crystal planes in different direction when these crystals meet when the grains meet. There is a mismatch and there is no continued. So, add those planes we find that the atomic spacing for the inter atomic spacing will be

larger than the than that corresponding to the minimum. So, you have actually higher energy at the grain.

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Fiane Den	ects. Grain Boundaries
Various degrees of cr adjacent grains are po	ystallographic misalignment between ossible.
Not all atoms at the grain boundary are bonded to other atoms.	Angle of misalignment

Boundaries and as you know higher-energy means that there is instability we see that explain further here. How what occurs at the grain boundaries so, here you have two grain boundaries. This is one and this is another where you have three the intersection between three different crystals. In this one you have the crystal planes running like this; in this one you have the crystal planes running like this. And hear that you have the crystal plain running like this and when they meet in this case there is some angle difference a small angle is what is there between the plains of these two crystals. So, you find that the distances between the atoms at this grain boundary or more then inside the lattice. But not too much, but if you see here at the top you see a bigger misalignment on mismatch this plane is going this way.

But now the adjusted plain as a bigger angle much more than one eighty degrees yeah you see that there is a big angle here. And therefore, you find that along this grain boundary there is more there are more gaps between the atoms. And there is lot of discontinuity; so, this increases the energy at the grain boundary instead of being at the minimum you are at higher level of and its and as we said always a material will look to minimize the energy decrease the energy and when the energies.

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Higher it is unstable and this is the reason why you have the fusion occurring along the grain boundaries. And you have chemical reactions occurring first along the grain boundary. So, as we said and grain boundary there is mismatch, which depends on the angles of the crystal planes of adjacent distance. There is therefore grain boundary energy or an interface energy which is now created and due to this interface energy. The atoms at the grain boundary are chemically more active, because they are not at the minimum potential energy or the minimum lattice energy. And to decrease the energy they react with atoms coming from outside the element; we also find that whenever they impurity atoms get into the material. They also concentrate on the interface, when you look at a metal which is corroding you generally will notice that corrosion starts at the grain boundaries. Because the grain boundaries add at a higher energy level the act more easily; so, corrosion starts a lot in the grain boundaries.

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Later on when we look at the stress corrosion you will see that stress corrosion cracking develops also along the grain boundaries. Another type of defect is a queen boundary where you have a distortion of their crystal plain again occurring, which is called a mirror lattice symmetry there is a symmetry here.

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But there is again an angle of more than hundred and eighty degrees between the adjacent crystal plains; this is called a twin. Now the twin can occur because of application of your forces on heat imagine, that you have a crystal structure like this.

Where you are shearing your plane shear force and you can possibly create a distortion here like the twin. So, you see the symmetry here, this is the plane around which you see the symmetry. This symmetric to this is a symmetric to this and so on.



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So, this is called twinning which can also be considered as a defect along this boundary between the two parts of the lattice. Now this type of movement requires more energy than just sleeping at the top here. Now you have a slip plane say you have a dislocation moving and slip occurring along displaying and you see here. When this slip is accruing at each step only one bond is broken an a new bound is crated. But when you have twinning you see that many bounds to changed.

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So, that the whole crystal lattice can get distorted like in the bottom diagonal, this is called a twinning plane. And this requires now highest stress to produced this than slipping, which you see the lost type of defects is three dimensional defects region of defects call volume defects. And they can be of two types, they can be voids which means that there is an absence of material or they could be an inclusion. Where there is another phase are another type of atom being introduced in a large volume. And these are usually be considered to be outside are external to the crystal structure you have a crystal structure. And there is a gap in the crystal structure that is outside the crystal structure or there is a volume that is introduced again outside the crystal structure. There is no continuity of the crystal structure through the volume defect due to voids and inclusion.

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So, as a said voids or pores or incomplete feeling of available space inclusions are region of a second phase. Some other material be introduced within the single grain here; you see a picture of grain cast. Iron cast iron is an alloy of ion with four percent carbon by weight. On the left you see an electron micrograph from the manchester material science center. Where you see that the microstructure has two constituents the background are the matrix is the alloy all pearlite. This pearlite is a mixture of ferrite, which is the phase of iron and iron carbide which givesp; that were me are the stripe structure.

Other than that you see these long plane flux, this is graphite which is precipitated due to an excess of carbon. In the alloy and this forms flaks inside the great custom; now this is an inclusion within the rest of the structure. The graphite is now an inclusion, so what happens when this material is subjected to stress. We find that the cracks develop along the graphite because the graphite this week we have seen how graphite behaves it cannot slip very easily does not offer a lot of resistance. So, cracks propagate very easily through the graphite. So, that is why cast iron it breaks very easily.

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Because cracks can propagate through it, even though the rest of the material is done here we see mild steel with another type of inclusions. The structure itself is made out of two major constituents ferrite; the alloy is made out of ferrite, which is the light color space the light color crystals of ferrite. And the striped regions up pearlite, this is pearlite this is pearlite and this is ferrite. So, this forms the bulk of the material; however, you have small inclusions here. The sports here this sports year are impurities, which are now included outside of the individual crystal lattices.

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Which could be oxides all sulphides, so, this is also another type of volume defect introduced in the material. So, we have seen now different types of crystal; crystalline structures and how defects occur in the crystalline structure. Now we move on to materials, which are not at all crystalline. They do not have any orderly structure, and they are called glasses are amorphous materials and to compare. You have two structures on the screen on the right is crystalline silicon you see an orderly structure. You have an ordered structured here and you can see better here. This same silica can occur as the glass very disorderly structure; you do not see any order at all no particular arrangement. And this is now a non-crystalline are amorphous structure; so, we call whatever has and orderly structure as a crystalline structure. As a crystalline structure and which has a completely deserted structure.

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As an amorphous or glassy material glosses are amorphous materials palm; for example, from mates when they rate of cooling is very we saw before when we talked about crystals. There are different stages of growth in the crystal from a melt first you have a nucleation and around this nuclei slowly. This crystal start forming than one crystal meets the other and a grain boundaries; now for these to occur a certain amount of time is required the rate of cooling has to be slow enough. So, the new nuclei conform and the nuclei can grow into orderly crystals suppose. We do not alloy the material to cool slowly we cool the material very fast. Then there is no time for this ordering of the structure to occur and you have a glass form.

So, that is what said here when the rate of cooling is too fast to allow nucleation. And the growth of ordered crystals a glass is formed an amorphous structure is full, because for crystal to grow. That is an orderly structure to farm enough atoms must come together. In the right packing to create the minimum energy only then a crystal its form in a stable view until now this happens, the energy will have to be used to overcome repulsion the atom slightly to separate and until now you have enough energy, they will not come together.

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So, this results in a nucleation barrier that has to be overcome; when crystal growth can occur thermal energy are heat can help atoms overcome the nuclear energy you need a certain amount of heat for the nucleation to occur. And that is shown schematically here, where we see the potential energy; how it is changing as the status changed. This is the potential energy and we go from a molten state to solid-state passing through a nucleation state.

So, for this you need some amount of energy to be sup past you have the nuclei forming and if the cooling is too fast you get a glassy is state. You do not go to a crystalline orderly state only, if that from the molten state to the cooling you allow for enough time. You can reach the crystalline state, this can be thought of in terms of thermal energy also thermal energy is of the only when it is large enough compared to the nucleation energy. Which has to be overcome you can have spontaneous nucleation occurring leading to crystal form if the thermal energy is in the same order as the nucleation energy. You can have the system go one way or the other nucleation occurs; when the cooling is slow no and glass formation are amorphous structure. Formation occurs, when the cooling is very fast if the thermal energies much less than the nucleation energy only a glass will form.

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So, basically what we have to remember is that there is necessity of thermal energy to a nucleation, which is required for crystal formation. And if the cooling is very fast there is a higher tendency for a glass to be formed and amorphous structure to be form now amorphous structures like glasses also. Even though then they have a random packing can be considered as ideal.

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Defect free structures like in the case of fused silica; there is a random arrangement of silica tetrahedral. But they did not necessarily be defects in the structure. On the other hand in soda glass, we have the sodium cations replacing some of the silicon atoms the arrangement is disrupted by the sodium ions. And instead of the silicon oxygen silicon born, we have a silicon oxygen sodium bond like you see here. There is a distortion here there is an distortion because of this defect caused by the sodium cation replacing this silicon. You do this distortion, what we find is soda glass? When compared to fused silica has a lower binding energy. And therefore, melts at a lower temperature remember when we talk about ironic material.

We said that higher the binding energy higher will be the melting point here, what we find this glass changes. When silicon is the replace by the sodium you have a distorted structure; you have a low binding energy. And therefore, you have a lower melting point now we've covered different types of defects; we've also looked at the amorphous structure of some material. And in the next lecture will continue to look at more of amorphous materials will talk also about polymers. Polymers can be partially crystalline a partially amorphous and we look at what are the specific characteristics of the polymer materials and polymer chains; and see how this gives rise to the elasticity the viscosity of parliament's.

Thank you.