Techniques in Materials Characterization

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Module No # 14
Lecture No # 59

X-ray Diffraction Profile and Analysis (Continued)

Welcome everyone to this NPTEL online certification course on techniques of material characterization. So we are in module 12 that is last week of this course and this is lecture 4 that is penultimate lecture. And we are discussing about extra diffraction profile and it is analysis and basically what we were discussing is a extra diffraction profile of real specimen. And how to analyze that how to understand various causes this kind of a diffraction profile from a real specimen.

So what we understood by now is that we can construct extra diffraction profile for any specimen if you know the crystal structure if you know the symmetry information and all those things. And if we from using that we can calculate the structure factor we can calculate the multiplicity factor etc., And we have the branch law which will tell us that exactly where we will be getting for particular lambda value where we are going to get the extra diffraction.

So we can virtually we can or we can construct the extra diffraction profile for any material if we know the cryptographic information. But then we have seen that real specimen the X-X-ray diffraction profile of a real specimen is quite different from the one that is generated theoretically by this method structure factor. And then using structure factor and using X-X-ray diffraction.

The most important difference is that whereas if you construct it theoretically you will be getting a line function. Whereas in a real specimen you have a finite width for a extra diffraction peak and the there are other differences like the diffraction intensity will not follow the trend and so on. But this broadening of the peak or a finite width of the peak expressed in terms of FWH and that is what is basically a representation of various effects that is causing that.

And if we understand what are these effects that is causing this widening of increasing in the width of the peaks then we will able to understand many more things other than crystal structure many more things will be able to understand for from that extra diffraction profile. So that is what we started and first thing we did is to understand the effect of the line instrumentation broadening the width broadening of the extra diffraction peak caused by the instrument itself because of this non-monochromatic beam non-parallel beam and so on.

And then we started understanding slowly the effect of the size of the specimen the size of the crystallites which is basically coherently scattering domains which are responsible for the extra diffraction for causing the extra diffraction. And the smaller this domains becomes or this crystallite becomes the peaks gets widened we understand that. And then we started discussing just started discussing about another effect that is the effect of strain in the material.

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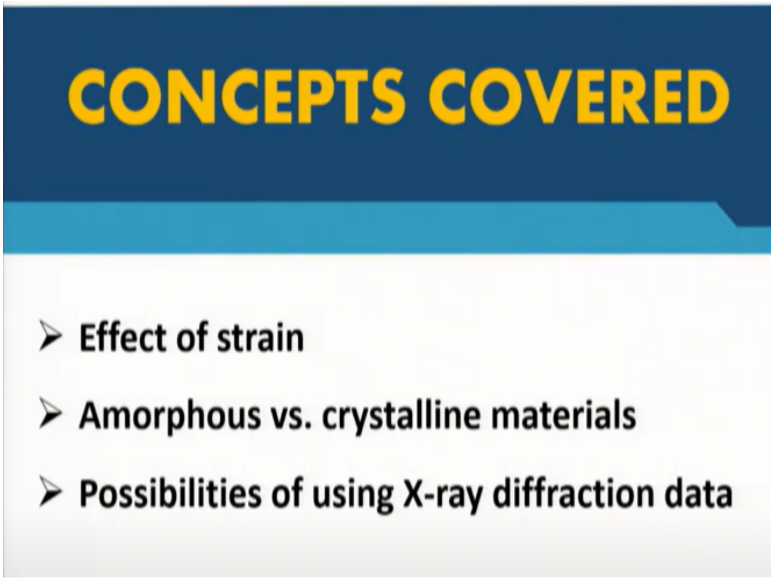

CONCEPTS COVERED

- Effect of strain
- Amorphous vs. crystalline materials
- Possibilities of using X-ray diffraction data

And we will continue that in this lecture as well the effect of strain and then we will see another important factor that is amorphous and crystalline different between amorphous and crystalline materials. And finally we will discuss about various possibilities of using this X-X-ray diffraction that are very briefly not going in any details about that.

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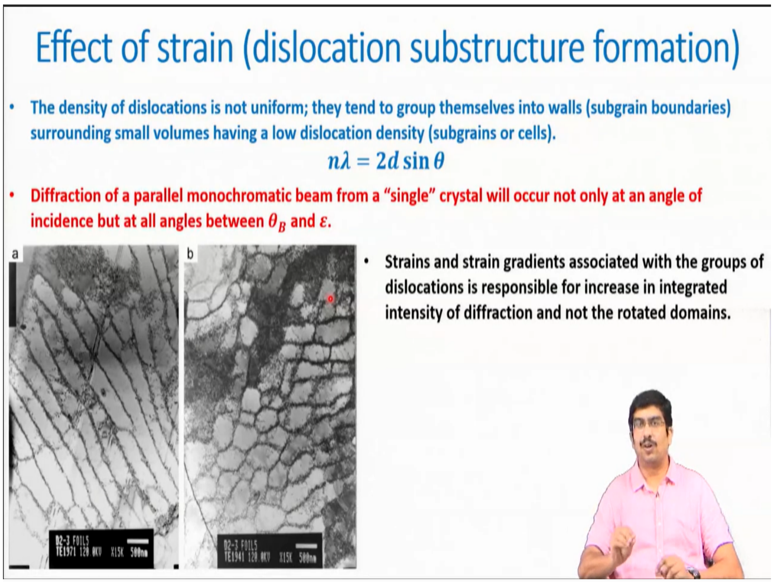

Effect of strain (dislocation substructure formation)

- The density of dislocations is not uniform; they tend to group themselves into walls (subgrain boundaries) surrounding small volumes having a low dislocation density (subgrains or cells).

$$n\lambda = 2d\sin\theta$$

- Diffraction of a parallel monochromatic beam from a "single" crystal will occur not only at an angle of incidence but at all angles between θ_B and ε.

- Strains and strain gradients associated with the groups of dislocations is responsible for increase in integrated intensity of diffraction and not the rotated domains.

So the first thing is effect of strain and in the last class we started that how people thought initially people thought that even the crystallites are divided into further smaller structures. And these structures they called it mosaic structure where mosaic structures are around 100 nano meter of size and misoriented by at the max 1 degree angle. So this small domains of small sub crystallite domains they thought that it is responsible for the beginning or for increasing the width of this X-X-ray diffraction profile.

And after the discovery of TEM so the discovery of transmission electron microscopy when people starting seeing the materials in great details their internal structure people are trying to say or people who are able to see. Then they understand that this mosaic structures are basically the structures or they resemble very well with the dislocations structure the dislocation if a material is heavily deformed then and containing huge quantity of dislocation huge dislocation density.

Then those dislocation goes and form their own structure within the material and then those structure size wise and misorientation wise those structures where very much resembling to this mosaic structure. For example if you see this TEM images which is showing the dislocations which are basically this black lines you can remember our discussion about dislocation contrast.

So these are taken at this dislocation contrast and what you can see is that dislocations are forming very nice boundaries here which are known as the sub grain boundary. So basically when the dislocation density becomes very high those dislocations forms this kind of boundaries within the materials and further divide any grains original grains. They further divide it into smaller sub grains and within the sub grains these areas are very much dislocation free.

So all the dislocations are accumulated at this boundaries that means the dislocation density or dislocation distribution becomes very non-uniform in this kind of materials and size of this as I said size of this dislocation cell this is called cell structure. Dislocation cell structure and this also evolves basically as the function of applied strains the dislocation structure also evolved.

Initially you have this band like structure and then you have the cell like structure dislocation cells. So this is different stages of evolution of dislocation structure but whatever it is what we understand is that? This kind of a structure is basically similar to mosaic structure and now onwards we will not be using the term mosaic structure will be using the dislocation substructure.

So what does this dislocation substructure does and remember the misorientation between these structures are very less that is expressed by a term eta. So that is the amount of disorientation between individual dislocation sub grains or cells and that is that eta is within 1 degree. Now if we put that in this n lambda = 2d sin theta and we imagine that we are working with a perfectly monochromatic beam perfectly parallel perfectly monochromatic. Then just because we have this dislocation cells which are disoriented within themselves by a very small amount what we will be getting is that?

We will get considerable intensity not only at the Bragg condition or the Bragg's angle theta b we will get it for an angle theta B + eta. So for theta B + eta being very small we will be getting considerable intensity from this because and this non-monochromatic beam and little bit non-parallel beam adds to this. So if we have a non-chromatic beam anyway it will be allowing little more Bragg condition to be satisfied for a much relax condition and that relaxation increases even with eta as all.

So ultimately what it will does is that it will cause this line functions it will cause them or to be a finite width of finite weight just because of this dislocation cells being there. So as a whole the strain so dislocation structure means strain. Basically the strain in the material that we are imparting in the material is causing the dislocations to evolve or dislocations to generate to generate in the first place.

And then the dislocation structures to evolve so the dislocations sub structure is a manifestation of the applied strain. So we can say that because of the strain in the material or strain or other words in other word we can imagine that the strain is of the material contains that applied strain in the form of dislocation substructure. So the effect of strain is basically going into broadening this X-X-ray diffraction peak.

The more amount of strain or deformation report in a material the more rapidly this dislocation structure will evolve this size of the dislocation structure will become smaller and so on and so forth. And the more broadening will be caused here so this is what the effect of strain largely we can think of is the effect of strain in the material in and it is causing this dislocation substructure.

And then the dislocation structure because of their small size and very small amount of mis orientation causing the extractive extra peaks to be broadened by sudden amount.

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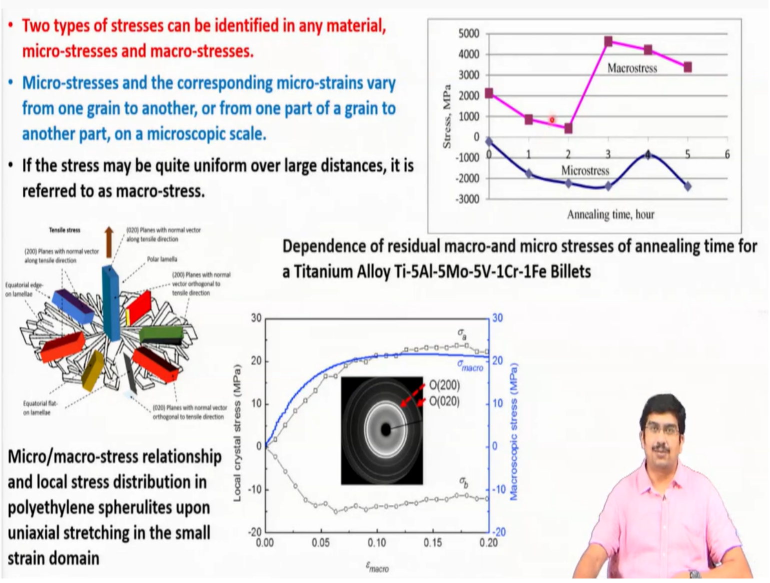

- Two types of stresses can be identified in any material, micro-stresses and macro-stresses.
- Micro-stresses and the corresponding micro-strains vary from one grain to another, or from one part of a grain to another part, on a microscopic scale.
- If the stress may be quite uniform over large distances, it is referred to as macro-stress.

Dependence of residual macro-and micro stresses of annealing time for a Titanium Alloy Ti-5Al-5Mo-5V-1Cr-1Fe Billets

Micro/macro-stress relationship and local stress distribution in polyethylene spherulites upon uniaxial stretching in the small strain domain

Now we have to understand how the stresses or strain is evolving or appearing in the material. Now this is what the route cause the dislocation substructure but we have to see that how this stresses are reflected finally in the extra diffraction profile. So we can basically divide this stresses in any material when we are putting strain and we are getting some stresses some dislocation structure we can imagine that there are 2 types of stresses which can be there in the material one is the micro stresses and the macro stresses.

So micro stresses are correspondingly the micro strain whatever you can call so micro stresses or micro strain they basically varies from 1 grain to another or even within one part of the grain to another part on a microscopic scale. That means on a sum microns scale possibly and if you think it in that way if you have a sum micron sized grain. Even within the grain you have this dislocation substructure formation.

And that dislocation of structure even varies with grain to grain because many grains different grains may have different orientation and dislocations of course will be completed different type of dislocations will evolve dislocation density will be different so on and so forth. Whatever it is so basically, we can imagine that this is happening the strain accumulation is happening in the material at microscale.

Compare to that is if the macroscopic stress is basically the stress you are applying on the overall materials. So overall the grains collectively together if you they have a uniform stress over a larger distance we can call that as a macro stress. Basically, it is the stress you are applying to the material and the material is showing the effect of the stress over the larger scale.

So if you think of this to be a grain to complete grain and this grain is having now different regions in different orientation dislocations sub stress you can imagine and the macroscopic stress is possibly applied on the all the grains or all of these grains smaller grains the macroscopic stress is applied and microscopically this individual grains different amount of microscope.

So ultimately what you can imagine the macro stress and micro stress basically does not correspond one is to one. It is not like if you increase the micro stress macro stress the micro stress will increase. Because that is these 2 are governed by completely 2 different links scale sorted together both in the micro structurally as well as in the mechanical respect. So completely different length scales are involved in these 2 types of stresses micro stresses and macro stresses and that is what it is shown here.

That if you look at a annealing with a titanium alloy relates the way macro and micro stresses varies with annealing this is completely different. So when the micro stresses are high macro stresses are very high micro stresses still very low. And when the macro stresses are something like started dipping up the micro stress is becoming increasing, or it is becoming higher.

So, this kind of relationship we can get between the macro stress and micro stress but ultimately, we can imagine that any material which posses 2 types of stresses. One extending to a larger distance several grain on the bulk scale another one is possibly within the grain itself or that kind of a length scale. So these are the 2 kinds of stresses at least from at an x-X-ray diffraction the way they are influencing the x-X-ray diffraction profile from that prospective we can think of these 2 type of stresses.

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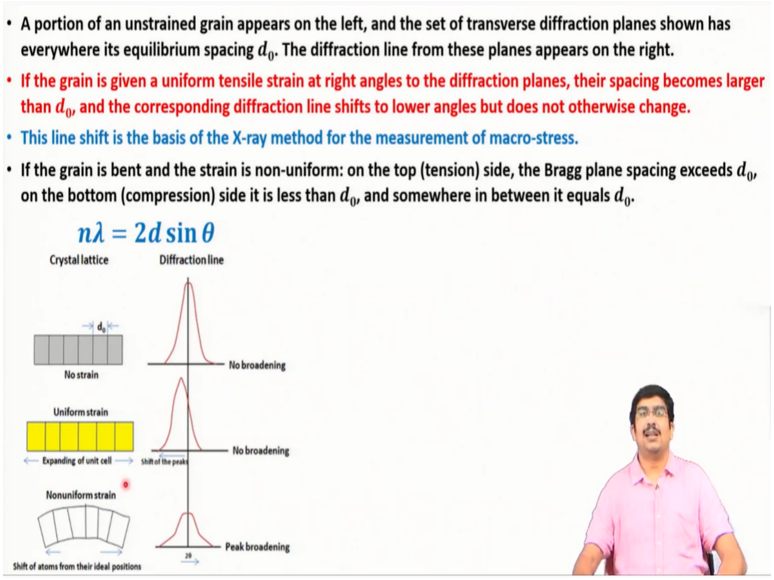

- A portion of an unstrained grain appears on the left, and the set of transverse diffraction planes shown has everywhere its equilibrium spacing d_0. The diffraction line from these planes appears on the right.
- If the grain is given a uniform tensile strain at right angles to the diffraction planes, their spacing becomes larger than d_0, and the corresponding diffraction line shifts to lower angles but does not otherwise change.
- This line shift is the basis of the X-ray method for the measurement of macro-stress.
- If the grain is bent and the strain is non-uniform: on the top (tension) side, the Bragg plane spacing exceeds d_0, on the bottom (compression) side it is less than d_0, and somewhere in between it equals d_0.

$$n\lambda = 2d\sin\theta$$

Now let us see that how these 2 stresses are acting on the x-X-ray diffraction profile what is their effect? What does they do and how we can make out the extreme or this entire thing is by the way is basically determined from the extra diffraction profile both the macro stresses and the micro stresses. And we can think of or we can discuss about how these things are determined.

So let us imagine this is the normal regular crystal or normal regular grain one single grain at equilibrium condition there is no stresses applied on this material. And this is having something like an inter atomic spacing which is d naught. So because of that we are getting now this x-X-ray diffraction profile without any broadening in the sense without any broadening due to strain.

Whatever the little broadening we are having it over so this is the 2 theta which is from the Bragg's law the ideal condition what we are getting exact Bragg's angle where the diffraction condition is satisfied and we should get highest intensity. So this is that line so if you do not have any stress on this material this will show exactly a ext3ra diffraction peak with a maximum intensity corresponding to the exact Bragg's angle.

And this whatever broadening we are seeing here that is possibly because of the instruments or because of the size we are getting a finite broadening here. Now let us imagine we are applying and uniform tensile strength on this material. Tensile strain mean we are basically elongating this material so now what is happening this d naught is increasing. The atomic plane are going further apart from each other.

So d naught is basically increasing if we put that and keeping all other conditions constant that means lambda becomes constant now we will be getting a sin theta which is less than the theta b the earlier exact Bragg's condition. The sin theta will be smaller because d is increasing so what will happen is the entire peak will be shifting towards the left. So that is the effect of a macroscopic strain or macroscopic stress.

If you are applying the stress on all of the grains or all of the atomic planes then the entire peak is shifting towards left if you are applying tensile strength if you are applying a compressive strain then the d naught will decrease that means all the atomic p into atomic planes all the planes will come closer together inter atomic distance will decrease sin theta will increase.

The entire peak will be shifted in the right hand side from the theta b earlier for a condition where there is no strain. So that is an effect of macro stresses that you can imagine what the macro stress will do to you extra diffraction peak without effecting the intensity it will just shift the peak either to a lower value or a higher value depending on whether you are applying extension or a compression.

Now let us imagine another situation where we are applying a bending now instead of a tension or compression we are applying a bending we are bending this entire crystal. What will happen we will get a tension on the top side and the compression on the bottom side. So this is like a 3 point bending you can imagine 3 point or 4 point bending. We are getting here tension on the top side and the compression on the bottom side.

So within the same material within the same crystal if we imagine is to be one single crystal or a grain whatever. If we imagine that then within the same grain or same crystal we are getting now 2 different regions where one is a tension one is the compression and the tension in compression is also constantly varying with a distance. So, what will happen is at certain regions the materials will have inter atomic spacing higher than d naught where the tension is prevalent.

And where the compression is prevalent the material will have it inter atomic spacing which is lower than d naught. And at equilibrium at some intermediate condition where there is an equilibrium stress no stress it will have something like d naught the inter atomic spacing will d naught. So now this entire material is divided into different stress state that means we are now generating a micro stress in the material not the macroscopic stress.

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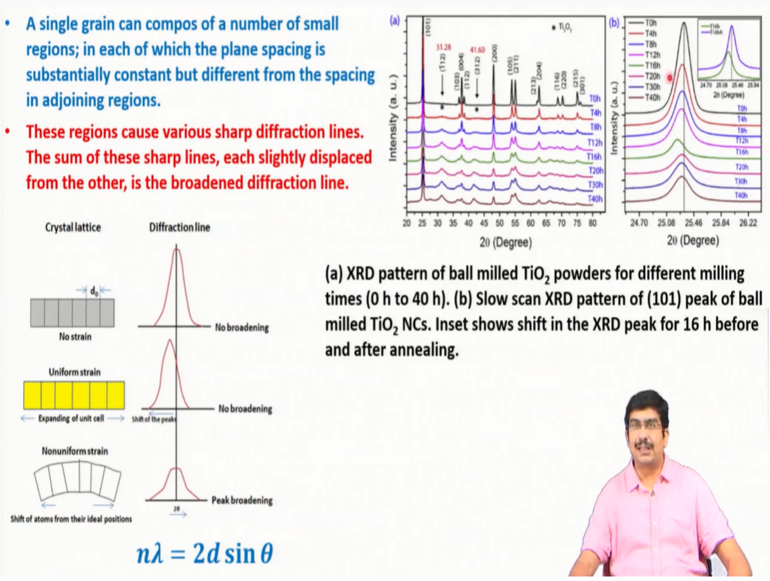

- A single grain can compos of a number of small regions; in each of which the plane spacing is substantially constant but different from the spacing in adjoining regions.
- These regions cause various sharp diffraction lines. The sum of these sharp lines, each slightly displaced from the other, is the broadened diffraction line.

(a) XRD pattern of ball milled TiO_2 powders for different milling times (0 h to 40 h). (b) Slow scan XRD pattern of (101) peak of ball milled TiO_2 NCs. Inset shows shift in the XRD peak for 16 h before and after annealing.

$$n\lambda = 2d\sin\theta$$

We are generating a micro stress in the material so how those effects micro stress we immediately understand d naught s, now different some places d naught the inter atomic spacing d is greater than d naught some places d naught or inter atomic spacing is lower than d naught. So, what will happen is that some regions because of that d naught being smaller than d beam smaller than d naught we are getting peaks will be forming higher than theta b or some regions.

Tension regions where d naught or d is greater than d naught the peak will try to form at a lower sin theta value than theta v. Ultimately this will effect in a larger broadening of the peak and intensity will also correspondingly decrease so that is the effect of micro stresses. Micro stresses will broaden the peak as well as it will decrease the intensity of the peak macro stresses will just shit that peak position it will not cause a broadening neither it will cross a diffraction neither it will cause a decrease in the intensity.

Now these are the 2 extreme cases and this is not what we expect in a real sense that there will not be any macro stress any micro stresses or there will be any micro stress only micro stress. These are the 2 extreme conditions that we are dealing with so in real conditions if we look at this kind of a situation where this is the XLD pattern of a ball made into powder for different milling times and this is the corresponding.

This is such peak 101 peak and what we can see is that? As we are increasing the milling time so more on milling time increasing milling time is more and more strain is important on the material. So what we are able to see is that without the milling is the peak position so exactly at the branch condition. The moment we started the milling now the peaks are getting shifted the intensity slightly decreases but more prominent effect is peak shifting towards the left.

So there is considerable amount of macro stresses generated in the material at the starting when we are continuing this milling operation for more and more time then we are generating much more amount of micro stresses as well because of that the peal intensity is decreased and as well as the peak is now getting broadened. So more than shifting of the peak this is now showing more amount of broadening so that is why we can call that now micro stresses are more prevalent at when we come or when we go for a longer handling time.

So basically this is what again showing the effect of initially it is basically micro stresses and towards higher annealing time it is milling time it is basically the micro stresses which are more prevalent. But all the times both the stresses are there and together they are playing but they are not going hand in hand which we have already saw here the micro stresses and micro stresses are not going hand in hand because of this kind of effect.

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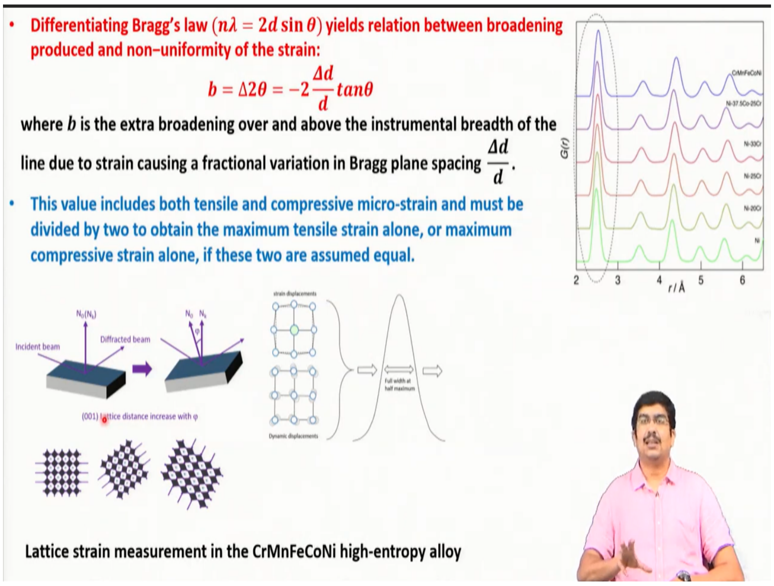

- Differentiating Bragg's law ($n\lambda = 2d\sin\theta$) yields relation between broadening produced and non-uniformity of the strain:

$$b = \Delta 2\theta = -2\frac{\Delta d}{d}\tan\theta$$

where b is the extra broadening over and above the instrumental breadth of the line due to strain causing a fractional variation in Bragg plane spacing $\frac{\Delta d}{d}$.

- This value includes both tensile and compressive micro-strain and must be divided by two to obtain the maximum tensile strain alone, or maximum compressive strain alone, if these two are assumed equal.

Lattice strain measurement in the CrMnFeCoNi high-entropy alloy

Anyway so how to get the quantitatively how to get this kind this amount of stresses this material there are many other ways but we are discussing about the most simplest of all how we can determine the amount of stress in the material. So what we can do is that we can take the Bragg's law and just we can differentiate. So we can take this in lambda equals 2 d sin theta well lambda we can consider lambda being constant and n being just a first order diffraction.

So n is 1 so if we differentiate that what we are getting is the width of the peak which is basically delta 2 theta means. If you remember our discussion in the last class, the theta 2 theta 1 – 2 theta 2 that is the broadening and ultimately we were getting b equals theta 1 – theta 2. So same thing we are now getting here that we are expressing delta 2 theta and we are differentiating this entire Bragg's law what we will able to write here is basically -2 delta d by d into tan theta.

So this b the broadening extra broadening due to the string over and above the instrumental broadening or size broadening the broadening cost by the strain is equal to minus 2 delta d by d into tan theta and delta d by d is basically the amount of strain the definition of strain delta d by d delta d. So this is if you know strain is basically the change in the dimension in any of the dimension the change divided by the original string.

So that is the original length that s what we can express that to be straight, so this is the strain. So we can write eta if you if we or some other value so we are writing delta d by d here this is the strain into tan theta. So from this we can determine the amount of strain in terms of the weight so tan theta of course theta is the theta b. We know that from the diffraction this curves we know that theta b and from by measuring the width of this or the broadening of this peaks.

We can determine the amount of strain present in the material so this is how we can get basically the micro strain in the material for measuring the one more important thing is that this strain basically. This strain includes both tensile and compressive so you can imagine that micro stresses as I just gave an extreme example the micro stresses contains both tensile and compressive.

And if we imagine that both of them are the same the amount of tension is exactly equal to the amount of compressive that is why we do not get any macro stresses tension tensile stresses in the material is exactly balance by the compression stresses. And we do not get any amount of macro stress if that is true that is an extreme of course which is not a really but that is in that case.

What we can imagine that this micro strain is basically composed of equal amount of tension and compression, and we can get either tension or compression by dividing this by 2. So that is how we are getting micro strength either compressive micro strain or tension tensile micro strength which is also done here. If you look at here this is the tensile and compressive part of the micro strength so one part is tension one particular compression and the of course the here we are the assumption is that both of them are exactly in tension and compression.

Other wise but that is not something what we see in reality that is why we are finally getting some macro stresses in material. For macro stresses determination of macro stress that is the comparatively difficult one to do basically you have to rotate this material that is something related to the residual stress determination and so on which is related to the rotation of this specimen along some specific axis phi axis psi axis.

And that is how you can generate something called rocking curves and those rocking curves will give you the amount of macro stresses we are not going exactly how this is done the residual stress management and so on. If you are interested you can always go through the reference books.

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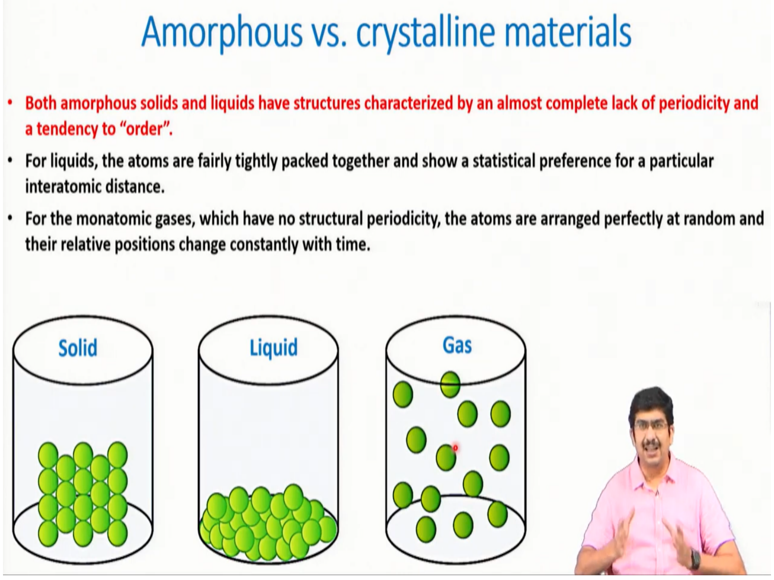

Amorphous vs. crystalline materials

- Both amorphous solids and liquids have structures characterized by an almost complete lack of periodicity and a tendency to "order".
- For liquids, the atoms are fairly tightly packed together and show a statistical preference for a particular interatomic distance.
- For the monatomic gases, which have no structural periodicity, the atoms are arranged perfectly at random and their relative positions change constantly with time.

So now that is what is strain is doing we will be discussing one last effect which again will change the extra diffraction peak. So this is basically amorphous versus crystalline material so about the structure or about the atomic arrangement within material. So this we have discussed about the little bit of that when we were discussing about if you remember we were discussing about the Bragg’s law.

We discussed how crystalline periodic arrangement how that is finally responsible for getting the constructive different so on and so forth. So for a solid materials we can imagine solid crystalline material we can imagine and completely periodicity in the atomic arrangement all attempts are fixed around their mean position and they are we have complete periodicity in the material.

For liquids of course the atoms are not having the periodicity liquid or amorphous structures we can think of that they are not having this periodicity. But they are still tightly packed together and this shows a statistical preference for a particular inter atomic distance which we can identify from the something called radial distribution function basically we are not going into that.

But got amorphous region we can find out we can express the same thing using radial distribution function. So their radial distribution function basically what it tells is that this atomic distances even in a liquid material or an amorphous material super cool liquid this inter atomic distances are not any random value. There is a preference for certain inter atomic distance values so that means this has certain level of order at certain level of order at certain length scales of course.

Mono atomic gases we can imagine that the length scale is really large that means the material the atoms are completely randomly oriented there is no periodicity and as such there is not any preference for inter atomic distance to be assuming some particular value.

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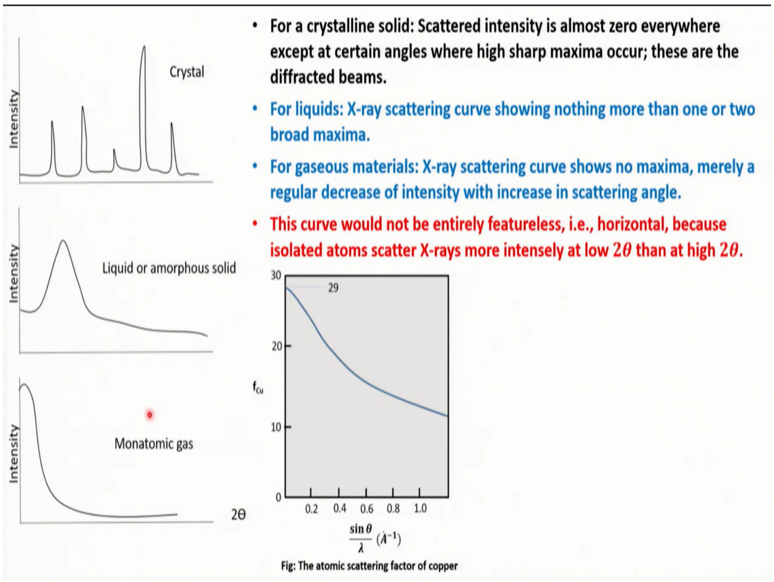

- For a crystalline solid: Scattered intensity is almost zero everywhere except at certain angles where high sharp maxima occur; these are the diffracted beams.
- For liquids: X-ray scattering curve showing nothing more than one or two broad maxima.
- For gaseous materials: X-ray scattering curve shows no maxima, merely a regular decrease of intensity with increase in scattering angle.
- This curve would not be entirely featureless, i.e., horizontal, because isolated atoms scatter X-rays more intensely at low 2θ than at high 2θ.

Fig: The atomic scattering factor of copper

So the way this is effecting of course because of this atomic arrangement we have already discussed how this atomic arrangement s responsible for producing this kind of a crystalline peak. This kind of a peaks at well defined angle for a crystalline material constructive interference will happen only along certain particular angle rest of the angles it is supposed to be destructive interference.

But of course there will be measurable intensity because of other factor we have discussed thermal scattering how it is attributes to the finally to the background materials. So basically the crystalline material you will be expecting this kind of sharp peaks in the middle. For liquid if you take an x-X-ray diffraction peak now what will happen is that? The inter atomic spacing is continuously changing so between various type various atom you are having a completely different inter atomic spacing.

There will be statistically they will be having a preference towards one single value but that will also be a large ring. So correspondingly what we will be having is this kind of extra diffraction peak where you will have a very wide and broad peak in the material. So this is you can think of as a one extreme of this size effect. So here the size is so small and size is varying in such a large way that you are getting a huge kind of broadening for individual peaks.

And then finally what you will be getting is one single peak possibly which is very wide and the extreme case is of course the gaseous material where the extra diffraction peak is possibly will vary like this. It will start with a higher intensity and it will continuously keep on decreasing now the point one point you should understand for a mono atomic gas even a mono atomic gas what you are not getting a completely horizontally you are not getting any extra diffraction at all.

What you can imagine for liquid or mono atomic gases you can imagine this is more like a extra scattering not any diffraction. We discussed it is a particular case of the scattering where we have this constructive interference Phenomena happening for a certain particular direction for this extra scattered extreme. That is not happening in case of a liquid or mono atomic gases in this case the extra intensity the intensity of the x-X-ray is basically varying from high value to low value because of the atomic scattering factor.

So if you remember the atomic scattering factor varies in this way with respect to the sin theta and Lamba. And for mono atomic gas basically whatever variation you will see with 2 theta the intensity of the extra beam is exactly because of this variation in atomic scattering factor with sin theta by Lambda. So that is how we are getting a difference between crystal and an amorphous material and the extreme is a mono atomic gas.

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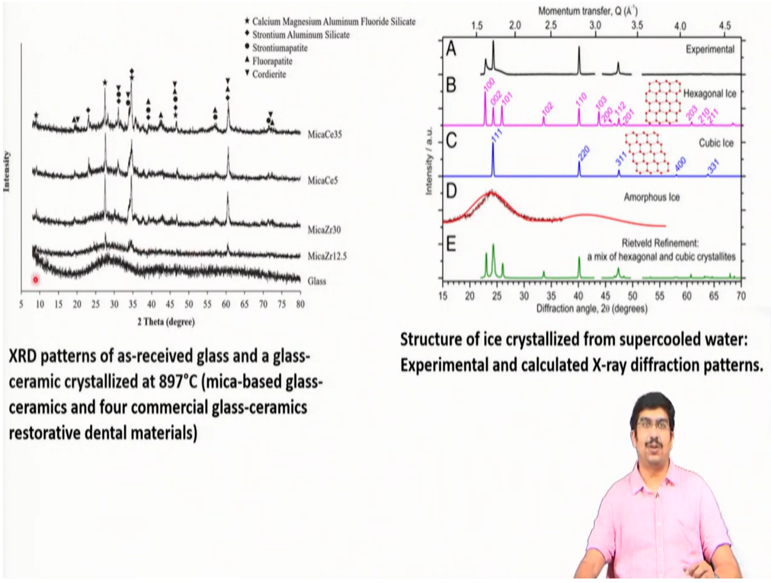

XRD patterns of as-received glass and a glass-ceramic crystallized at 897°C (mica-based glass-ceramics and four commercial glass-ceramics restorative dental materials)

Structure of ice crystallized from supercooled water: Experimental and calculated X-ray diffraction patterns.

So with this we are getting over so we will be checking some if you can use this information that how the x-X-ray diffraction profile will change from a crystalline material to an amorphous material you can use that for various studies. One such we are showing here so you have the glass that we do in our research group. So this is the x-X-ray diffraction profile for a base glass and you can see it is just similar to this liquid where you are getting one single very broad peak and mostly you get the background.

You do not get any sharp peak now if you know the glass is a metastable state it is in super cool liquid and for some glass systems you can basically promote crystalline into this. If you do a secondary heat treatment on the glass you can develop crystals within the glass itself. So if you do that then slowly you are doing a heat treatment and slowly you are increasing the crystal volume fraction you are generating crystal within that glass and that will result in this sharp peak.

So if you just take or if you monitor this process you can be able to see this change in their corresponding x-X-ray diffraction profile.

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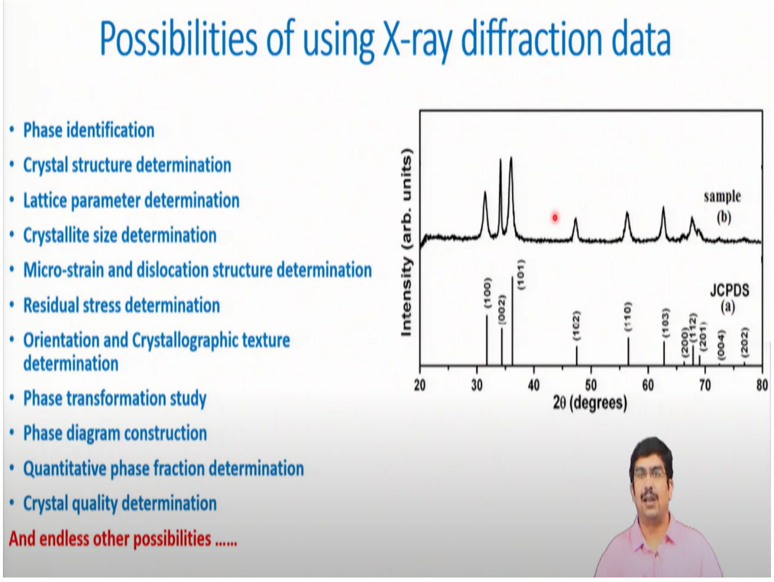

Possibilities of using X-ray diffraction data

- Phase identification
- Crystal structure determination
- Lattice parameter determination
- Crystallite size determination
- Micro-strain and dislocation structure determination
- Residual stress determination
- Orientation and Crystallographic texture determination
- Phase transformation study
- Phase diagram construction
- Quantitative phase fraction determination
- Crystal quality determination

And endless other possibilities ......

So this kind of studies you can do it and this is the last thing that we can possibly discuss about this x-X-ray diffraction profile x- X-ray diffraction course part of this course various possibilities od using the x-X-ray diffraction data. So now you can see that this is the kind of the specimen or this is the kind of x-X-ray diffraction profile that you can get from a real material. From this what you can do is the phase identification if you do not know what phase it is?

Then you can try to find or if you have a mixture of various phases multiphase material mixture of various phases then you can find out exact phase which phase it is from your extra diffraction profile. You can do crystal structure determination of course but normal crystal structure determination is done with single crystals and by some other method. But from an x-X-ray diffraction but the main underline phenomena is the extra diffraction profile.

So crystal structure determination also you can do if you do not know the crystal structure of any unknown material you can do an diffraction and since diffraction is related to atomic arrangement which you by now you must have understood. You can determine the crystal structure. And then similarly for the phase identification or for the crystal structure determination the next step is to determine the lattice parameter for this material accurate lattice parameter determination you can do.

For example if you are working with semi conducting materials with the thin film deposition and so on, Then you can think of or you can find out that how the lattice parameter change with change in composition change in your parameter of deposition and so on and so forth. So all of these things you can do with x-X-ray diffraction data. Basically the Bragg's law where you determine the d value.

You can of course do the crystallite size determination if you have a nano materials or if you have an ultra fine grain material you can determine the crystalline size using the (()) (31:28) formula or using much more advanced techniques are there well definement. Or you can do MWP multiple whole profile fitting all of these methods you can use find out the crystallite size.

You can determine the micro strain you can go a head another stage and you can determine the dislocation structure on the material again from this high end methods you can use some very simple methods known as Williamson hall method or you can go for very high end methods like this MWP CMWP all of these methods. You can go for residual stress measurement which is like the macro stress measurement which I discussed you can do this specific rotations.

You can use something called Euclidean cradle you can give some specific rotation to a specimen and from the peaks how the peaks are varying x-X-ray diffraction peaks are varying. You can determine the residual stresses in material you can of course determine the orientation and crystallographic texture. Again by giving some particular rotation which we also do which we very regularly use in our research use in our research group crystallographic texture determination.

But those are like a little advanced the lying phenomena is of course determined the x-X-ray diffraction. But there you have to go for events a little higher in term of instrumentation you have to give specific rotation in the specimen. And then you can determine some other things which like you can determine something called pole figures you can determine orientation distribution function and so on.

So we are not going there you can use extra diffraction in terms of phase transformation study we have already shown you one couple of example like you can check out this gamma to alpha. Or as a function how your different peaks are coming up and from there you can identify this phase transformation which phase is transforming to what? What is their orientation relationship and so on and so forth.

You can determine by institute study or by sudo method you can determine a phase diagram the change in the crystal structure as a function of temperature or pressure. You can find out the quantitative phase fraction determination which is very useful for people working in steel industry they often ask us to determine the detailed austenite volume fraction that is what they call it that how much austenite is retained in the material after at room temperature.

And from x-X-ray diffraction you can find out this is something like to do with the intensity of the x-X-ray diffraction peaks and then do a quantitative phase fraction determination. You can also use it for determining your crystal quality determination if you are developing a single crystal you can take x-X-ray diffraction. And find out that how much order is there or what is the imperfections are there in your crystal and so on.

And there are endless other possibilities exist where you can use this x-X-ray diffraction data so x-X-ray diffraction is possibly one method which is very useful method and powerful method developed possibly a long back almost 120 year or more than that time x-X-ray diffraction. But still people are using it and there are many other techniques many other applications possibly you can think of where you can use this x-X-ray diffraction data.

I request all of you to go through the reference books to know more about the possibilities or more about what you can do with this extra diffraction data and of course we will be happy to help you to if you have specific queries to know what where you can use this x-X-ray diffraction. So with this we are ending this x-X-ray diffraction part we have one more lecture left and there we will be discussing some special topics in the next class thank you.