**Texture in Materials**
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Module - 03
X-ray diffraction phenomena
Lecture - 08
Structure factor and diffraction extinction criteria (Contd.)

A very good day to everyone and this is lecture number 8 of Texture in Materials. So, this is lecture number 8 for module 3 X-ray diffraction phenomena. So, in this lecture, we will try to understand Structure factor and diffraction extension criteria we will continue that right.

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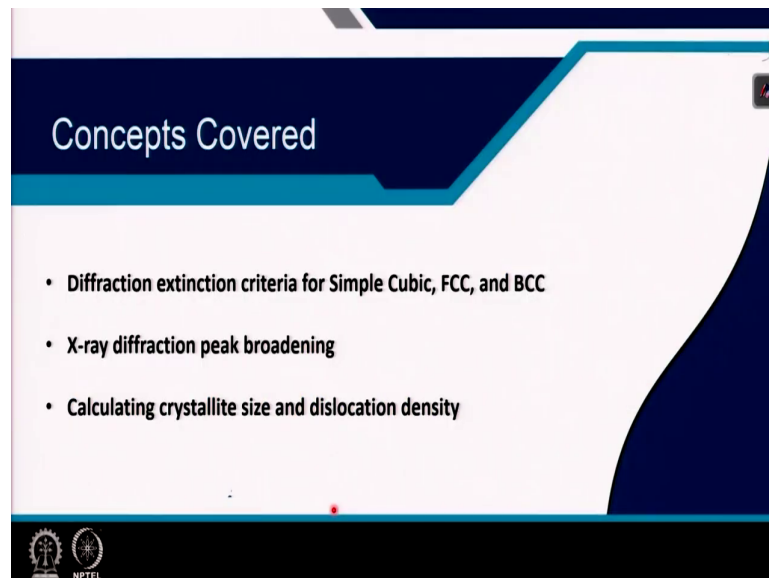
So, that the concepts that we covered in this course are in this lecture is diffraction extension criteria for simple cubic, face-centered cubic, and body-centered cubic. X-ray diffraction peak broadening and calculating crystallite size and dislocation density.

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So, that in the last lecture we found out how a structure factor for a crystal structure is being calculated.

we use the orthogonal crystal system, we did it for the two-dimensional system and then we took the analogy to three dimensions for a particular h k and l plane and we considered u v and w are the positions of the atom with respect to the unit cell.

So, that if we take a cubic unit cell we found that atoms positions are at the corners of the cubic unit cell right. And if we consider this what we found out that the origin of the cubic unit cell if it is here then this is at the position 0 0 0 right and the other atoms are also at the position 0 0 0 with respect to different unit cell right. And now because each of these atoms is being shared between 8 of the unit cell. So, it is said that the simple cubic has no missing reflection and let us see how ok. So, let me take the pen right and that the position of the atoms in the unit cell of a simple cubic is 0 0 0 right.

So, if we consider f for a particular hkl plane then this has to be equal to the atomic scattering factor which is n 1 n is equal to 1, because here there is only 1 atom present at 0 0 0 that is then it is 2 pi times i h times 0 plus k times 0 plus l times 0 right. So, so any hkl plane either it is 100, 110, 111, 200 each and every plane will diffract if it is for the simple cubic crystal structure right.

Now, let us take this for the BCC that is body-centered cubic crystal right. So, a body-centered cubic crystal has present at their corner and present at the center of the body-centered cubic. So, it is said that in body-centered cubic the 100, 111 are the missing diffractions and because F is equal to 0 that is a structured factor is 0. Now u, v, w for the corner atoms are right and for the atoms atom which is at the center of the unit, the cell is half of the unit cell size.

So, it is half, half, half that is u, v and w are half, half, half, consider the structure factor F for the 100 planes and then if we consider that then it is equal to atomic scattering factor small f times exponential 2 pi i for the atoms which are present at the corners 000 and that is equal to h 1 multiplied by 0 plus k 0 into 0 plus l 0 into 0 exponential 2 pi i right one times half plus 0 into half plus 0 into half right. So, if we calculate this then this is f exponential 2 pi i 0 that is 0 and then exponential 2 pi i times right. So, this becomes equal to exponential 0 plus exponential pi i right and then this becomes e to the power exponential to the power 0 is 1 and then exponential to the power pi i is basically minus 1 right. So, this becomes equal to 0.

So, the structure factor for the 100 is 0, and therefore it is a missing reflection or missing diffraction.

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Let us consider the case for the structure factor 110 and then how it will be? f times exponential, 2 pi i times 1 into 0 plus 1 into 0 plus 0 into 0 plus exponential 2 pi i times 1 into half plus 1 into half plus 0 right.

Now, that gives this becomes equal to 1 and this becomes equal to 2 pi i right, because half plus half is 1 and therefore, this becomes 2 times f. And therefore 110 is present in the case of the body-centered cubic material. Let us take a 111 so f equal to capital F equal to atomic scattering factor small f times exponential 2 pi i and 1 into 0 plus 1 into 0 plus 1 into 0 right times exponential 2 pi i times 1 into half plus 1 into half plus 1 into half. And therefore is atomic scattering factor times 1 plus e exponential. 2 pi i times 3 by 2 which is exponential 3 pi i and this is basically equal to minus 1 right and therefore this becomes equal to 1 minus 1 is equal to 0. So, we can understand that why 100 and 111 are missing diffractions right. Now let me rub it and then let me go for the FCC.

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So, if we go for the face-centered cubic crystals we will find out that there are as usual atoms present at the corner right and then there are atoms present at the faces right. So, all the faces have 1 atom present. So, if we consider u, v, w of this equation then these are 000 for the corner atoms, these are half, half, 0 for the atom present in the face center of the x y plane right this is half, 0, 0 present in the z x plane x z plane and this present in the y z plane right.

Now, if we calculate the structure factor for 100 in this case, then this becomes equal to function exponential 2 pi i times 1 time 0 plus 0 times 0 plus 0 times 0 and it becomes plus; if i make it whole bracket exponential 2 pi i times 1 into half plus 1 into sorry 0 into half plus 0 into 0. And then if you can keep on adding like that 2 pi i time 1 into half 1 into half plus 0 into 0 plus 0 into half and then and this is for this one and then exponential times 2 pi i 1 into 0 plus 0 into half plus 0 into half right. And then if we look into it then this becomes 1 and e to the power pi i becomes minus 1 and here also e to the power pi i this one becomes minus 1 and this one becomes e to the power 0 becomes 1. So now, if we look into this what we will find out that the structure factor becomes equal to 0 and therefore, we have 100 as a missing diffraction.

Now, if we consider 110 the same equation with exponential 2 pi i times 1 into 0 plus 1 into 0 right then for the 000 positions and then exponential 2 pi i times 1 into half plus 1 into half right for the for this position and plus exponential 2 pi i times 1 into half plus 0 sorry 1 into 0

right and then exponential 2 pi i again and 1 into 0 plus 1 into half right plus 0 into half right this is the thing.

And then this becomes equal to 1 and then this becomes equal to 2 pi i into 1 and therefore this becomes 1, whereas this equation becomes minus 1 and this becomes minus 1, so you have 0 structure factor. Let us take another case F 111is a function of atomic factor times exponential 2 pi i times 1 into 0 plus1 into 0 plus 1 into 0 plus exponential 2 pi i times 1 into half plus 1 into half plus 1 into 0 right plus exponential 2 pi i times 1 into half plus 1 into 0 plus 1 into half right plus exponential 2 pi i times 1 into 0 plus 1 into half plus ` into half right.

Now atomic factor this becomes equal to atomic factor times 1 plus this is 2 pi i so it becomes 1 and then this is also 2 pi i and then it becomes 1 and this is also 2 pi i and then it becomes 1. So, this is 4 of atomic scattering factor f. So, the 111 planes of the FCC is having constructive diffraction considering the structure factor.

Now, if we do this for all the other planes then we can find out what is the structure factor that can be obtained for each and every plane corresponding to the Cubic unit cell, Body-centered unit cell, and Face-centered unit cell right.

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So, let us go to the next slide and see that the diffraction extension criteria are controlled by the structure factor for the hkl planes, for the diffraction condition satisfied planes that are

Braggs law satisfied planes all the planes will have a certain angle theta to satisfy its Braggs angle right. And then there are diffraction extension criteria according to the structure factor for all the materials.

And we have been observing these different cubic structures; Simple cubic, Body-centered cubic and Face centered cubic because these are most of the metallic materials that we use steel aluminum etcetera nickels all are having this crystal structure mostly body-centered cubic and face-centered cubic. The diffraction condition is satisfied for simple cubic for all the hkl planes 100, 110, 111, 200, 210 each and every scale plane.

In the case of body-centered cubic, it was observed that the diffraction conditions are only satisfied if the h plus k plus l is even and for the face-centered cubic material the diffraction condition is satisfied if h k and l are unmixed ok. The absent diffractions are for the body-centered cubic if h plus k plus l is odd in the case of FCC hkl if it is mixed, then the diffraction is absent. So, in the case of body-centered cubic material, the extension criteria show that the diffraction can be obtained from 110, 200, 211, 220. And we see that if we add them 1 plus 1 plus 0 is an even number 2, 2 plus 0 plus 0 is even number 2, 2 plus 1 plus 1 is 4 which is again an even number, 2 plus 2 plus 0 is again 4 which is an even number. On the other hand, if we look into the FCC 111, 200, 220 and you can see that each of these planes have unmixed h k l. So, 111 have all odd numbers 200, and 220 have all even numbers.

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The intensity peaks obtained by X-rays are usually broadened and therefore it is important to understand that why the X-ray peak broadens. If we consider a uniform crystallite microstructure or a polycrystalline material if annealed to a large extent there could be a possibility, though it is an ideal situation where grain is equivalent to a crystallite.

So, if the grain is equivalent to a crystallite when there is no defect present in it, defect in terms of dislocation in terms of statistically stored dislocations or geometrically necessary dislocation arrays forming geometrically necessary boundaries. Then if there is no misorientation within the grains the peak coming from the diffracted X-ray beam should be a concentrated peak and it should not have any broadening.

But in real-life scenarios even an annealed material will a grain in annealed material will contain some kind of substructure, at least it will contain some kind of cell or subgrain which is formed inside it. So, there will be always some amount of statistically stored dislocation present in it. So, there will be some kind of misorientation boundaries present within the grains and therefore the grain will be formed by the various amount of crystallites.

So, and this crystallite will always they will have a misorientation between each other and that is the reality. Under such a situation a strong intensity beam coming from a diffracted X-ray is have a broadening and the broadening that occurs we can calculate from it the full-width half maxima that is FWHM which is also known as the integral breadth.

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The integral breadth can be used to calculate the crystallite size and we have learned in the previous lectures that crystallite size is basically a uniform agglomeration of crystal that possesses the same reflection pattern. So, using the Scherrer formula one can observe the relationship between the crystallite size and the full width at half maxima the Scherrer formula is given by this.
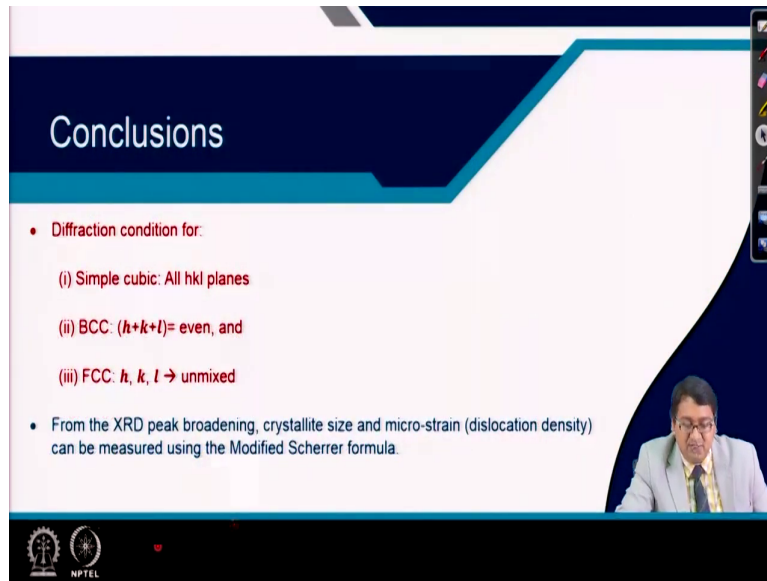
And this is the modified Scherrer formula where beta is the full-width half maxima or the integral breadth times the cos theta by lambda; lambda which is the wavelength of the incident x-ray beam equal to k times D v, where k is a constant depending upon the crystallite shape which is usually 0.89 for equiaxed crystallites and D v is the volume-weighted average crystallite size plus 4 times e which is the microstrain times sin theta by lambda.

We all know that theta here is the Braggs angle theta which is for a particular hkl plane, one can use this formula and the modified version of these versions of this formula to calculate both D v which is crystallite size, and e which is microstrain and from e one can calculate the dislocation density of the material.

There are limitations of this way of calculating dislocation density and crystallized size from the material and these are limitations of the Scherrer equation. These are the crystallite size of the order of thousand Armstrong or less than that can only be measured using this method, greater than that it cannot be measured. An error of greater than 20 percent usually occurs during the measurement of crystallite size using X-ray diffraction.

A peak broadening apart from the crystallite size and the microstrain is contributed from other factors like the instrumentation broadening and the that is the broadening due to the instrument.

Coming to the conclusion of this lecture is that diffraction conditions for Simple cubic say that all hkl planes will diffract. In the case of Body-centered cubic, the h plus k plus l will be even then only the diffraction condition will be satisfied. In the case of Face-centered cubic h, k, l are all unmixed right, then only the diffraction is satisfied. From the XRD peak broadening one can observe crystallite size microstrain that is dislocation density it with the help of the modified Scherrer formula.

Thank you.