X-Ray Crystallography

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Lecture - 36
Tutorial 09
Tutorial problems
Effect of Crystallite Size on Diffracted X-Ray Intensity

Hello everyone. Welcome to this tutorial class of X-ray Crystallography course. I hope all of you are following the lectures on the phase diagrams and rain size calculations and so on. And you also must have studied about the scherrer formula how it is useful in calculating the grain size and so on, based on the line broadening of X-ray peaks. So, if you look at the line broadening effect of you know X-ray diffraction one can attribute this to several factors. I hope you have got some idea about this during this course. But one of the reasons is about the grain size right. So, the whole scherrer formula is based upon the line broadening of the X-ray diffraction peak.

I would like to solve couple of problems in the today, and also I will just do some work out from problem on the blackboard using the, how using the diffraction how to calculate the phase diagram how where it is applied something like for example, how to find out this always line of a inlaying so on. So, so what I will do is I will first to take up the simple problem on the grain size just to get (Refer Time: 01:43). You all must have studied about these grain size calculations using the ASTM standards and then it is very elementarily taught, how to calculate the grain size using the ASTM or reference chat and so on.

So, first we will take up some simple problem then we will move on to the scherrer formula and so on.

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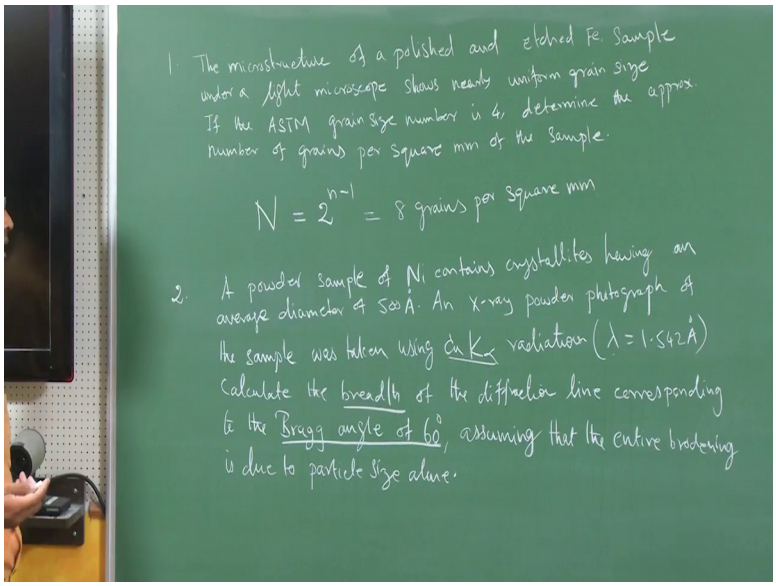

So, the question is the microstructure of a polished and etched iron sample under a light microscope shows there nearly uniform grain size. If the ASTM grain size number is 4 determine the approximate number of grains per square mm of the sample. So, this is done by simply this formula. So, where n is the small n is the ASTM grain size number then you simply use this and then it will be of 8 grains per square mm. So, this is very, very rough methods, but it is very fast method. If you look looking for an accuracy then it is a it is not an a advisory to use this method.

Generally researchers use a scherrer equation. I hope you have seem the formula scherrer formula derivation we will also post that I am the lecture of derivation of scherrer formula. And we will now take a one problem using the scherrer formula. So, the question is a power sample of nickel contains crystallites having an average diameter of 500 angstrom. And X-ray photograph power photograph of the sample was taken using copper k alpha with a lambda 1.542 angstrom. Calculate the breadth of the diffraction line corresponding to the Bragg angle 60 degree, assuming that the entire broadening is due to particle size alone.

So, here is the assumption the broadening is due to several factors, but if you assume that this broadening is purely because of the particle size alone, then the scherrer formula is valid. So, how to proceed with that?

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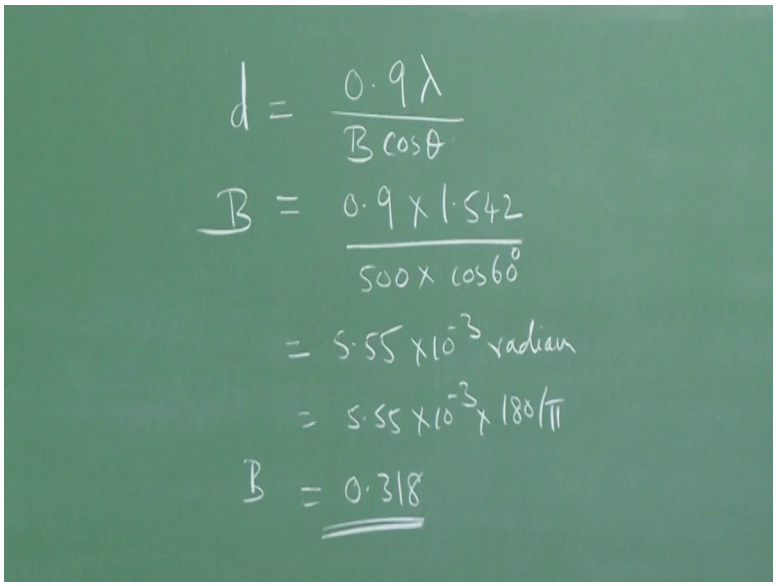

So, you have the formula scherrer formulas of this kind. So, you just simply substitute this into this equation 0.9 into 1.542 divided by 500 into cos 60. So, this is B. Simply you can re write this equation and then you are going to get something like that 5.55 into 10 to the power minus 3 radian. So, this is the breadth of this X-ray diffraction B.

So, you should also realize that this for much more accurate calculations there is something called Williamson hall plots are also being used. We will post that problems and then derivation of that and then you can look at those problems also in then another tutorial. So, where you will be able to appreciate the contribution of the stress I mean strain and particle size and so on. We have demonstrated were how to separate these effects using the you know contribution of each for example, strain and particle size on the X-ray line broadly. So, you can use that Williamson hall plot method also to find out accurately about the contribution of strain and particle size and so on.

So, now what we will I do is, I will just do one more problem on application of the X-ray diffraction techniques on the phase diagrams, simple problem.

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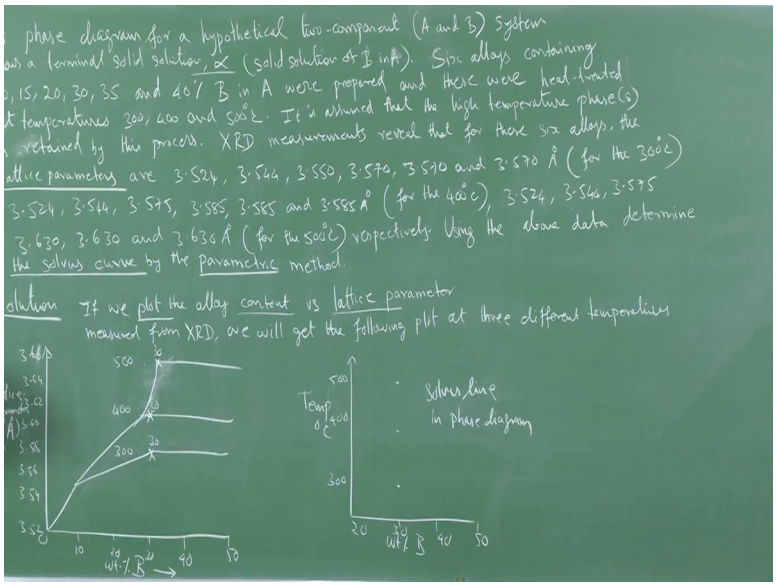

So, the problem is width long to read, but So, your phase diagram for a hypothetical 2 component system A B shows terminal solid solution alpha, that is solid solution of B in a/. So, you produce there are 6 alloys containing 10 percent, 15 percent, 20 thirty 35 and 40 percent of B in a were prepared and they were heat treated to temperatures at 300 400 and 500 degree centigrade right. Temperatures and it is assume that high temperature phase is retained by this process. And XRD measurements reveals for the 6 alloys the lattice parameters or 3.524, 3.544, 3.550, 3.57 3.57 and 3.57 and so on.

For 300 degrees centigrade, and then 3.524, 3.544, 3.575, 3.585, 585, 585 angstroms for 400 degree centigrade and 3.524 3.544 3.575 3.630, 0.630, 3.630 angstrom for 500 degrees respectively; so using this data determine the n solvus curve of the alloy system using parametric method. So, it is basically the application of X-ray diffraction in determining the phase diagrams. So, what you have seen in the lecture nodes how the parametric method is useful that has been explained. So, we will now try to use that where method again to identify the solvus curve for the alloy.

So, how do we proceed? So, if you plot the alloy content versus lattice parameter you obtained from the X-ray diffraction. We will get the plot for the different temperature. So, what is that we are going to do? It is basically lattice parameter versus alloy content. So, this is so, what we have done is if we actually use this data and you put it in a an excel plot. It will some it will appear something like this. So, I have drawn it has a

schematic, but then if you actually plot this values you will get a nice straight line kind of it may not be a straight line, but at least a linear segment you will see.

But what we all if you have to appreciate from this plot is see after particular composition irrespective of the temperature, the lattice parameter become constant. So, see as the temperature increases there is a variation the lattice parameter, but then at this particular composition after this lattice parameter becomes constant. So, that is something we can use this point, then we can re plot this. So, if you look at the inter section where this lattice parameter begin to remain constant and then if you plot temperature versus percentage of composition we will get the a solvus line of the alloy in the phase diagram.

So, that is something you can readily appreciate, how this lattice parameter constants are, I mean the X-ray measurements of the lattice parameters are useful to find out the solvus line of the alloy. So, the other problems involving the grain says calculation as I mentioned you see Williamsons and plots and so on, you can see it in the another video.

Thank you.