**X-ray Crystallography**
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**Lecture - 23**
**Qualitative Phase Analysis**

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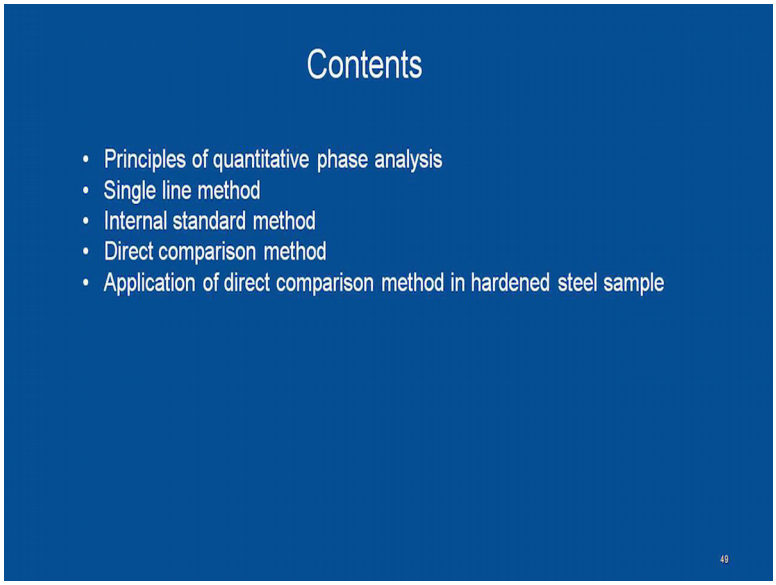


We have seen that every substance whether an element a solid solution or a compound has got it is characteristic x ray diffraction pattern. Thus x ray diffraction pattern of a phase is very much characteristic of that phase alone. In a sense an x ray diffraction pattern of a substance or a phase is just like the fingerprint of a human being do just as by distinguishing between the fingerprints 2 persons can be distinguished. In a similar manner by distinguishing between the powder patterns or powder x ray diffraction patterns of 2 substances or phases that 2 phases can be distinguished. Now let us suppose that we have got a phase mixture of a and b.

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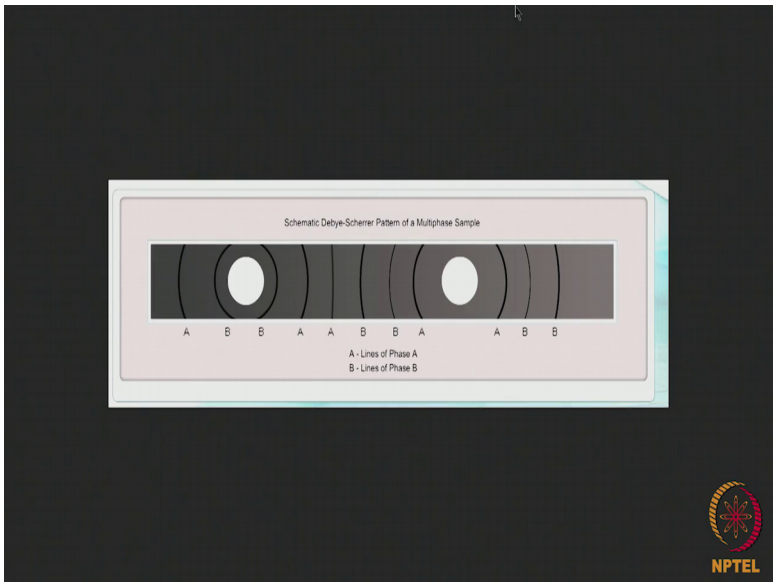


Now, here you see a number or diffraction lines the lines due to the phase A have been marked and the lines due to phase B have also been marked in this powder pattern.

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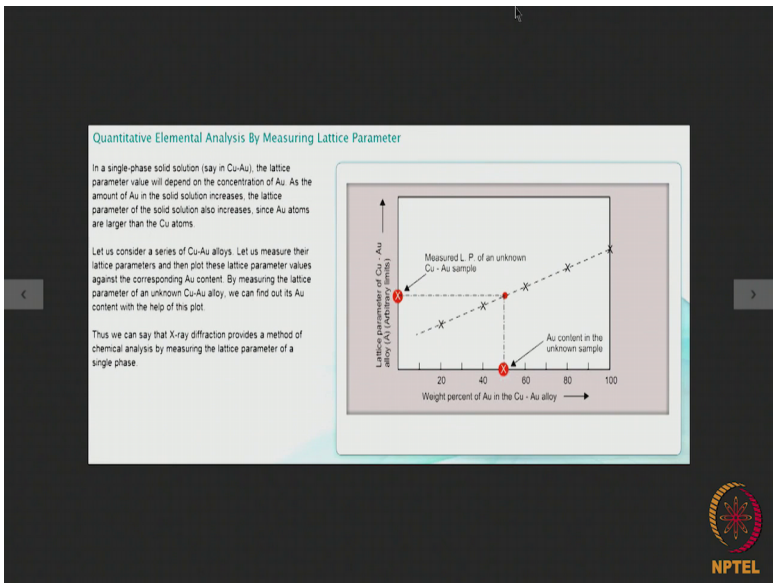


Now before going to the topic of quantitative phase analysis I would like to say a few words about the quantitative elemental analysis that can be performed by the measurement of the lattice parameter of a phase or phases in a mixture. Say for example, we have got a single phase solid solution of gold in copper. The lattice parameter value would depend on the concentration of mould in the alloy. As amount of gold in the solid

solution Increases in expect that the lattice parameter of the solid solution will also increase.

Since the gold atoms are larger than the copper atoms. Let us consider a series of copper gold alloys. Let us measure the lattice parameters and then plot this lattice parameter values against the corresponding gold content. This is shown in the right hand side of the figure. By measuring the lattice parameter of an unknown copper gold alloy we can find out it is gold content with the help of this plot. So, in this plot the lattice parameter of the solid solution has been plotted along the y axis and the Wight percent gold has been plotted along the x axis. So, this dotted line passing through these points shows how the lattice parameter of this solid solution changes as among to gold in the solid solution changes.

So, if we have got an alloy and an unknown alloy, we can simply have to measure the lattice parameter. Once we do that we put the lattice parameter value over here and find out the corresponding gold content of the alloy.

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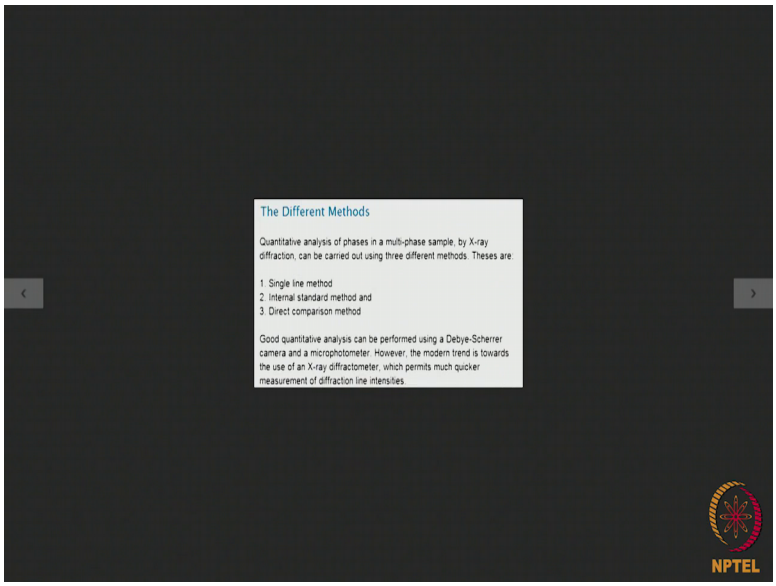


So, in this manner you can find out from the lattice parameter the quantitative chemical analysis in case of a solid solution. There are 3 different methods available for quantitative phase analysis by x ray diffraction. The first one is what is known as the single line method. The second one is known as the internal standard method. And the third one is known as the direct comparison method.

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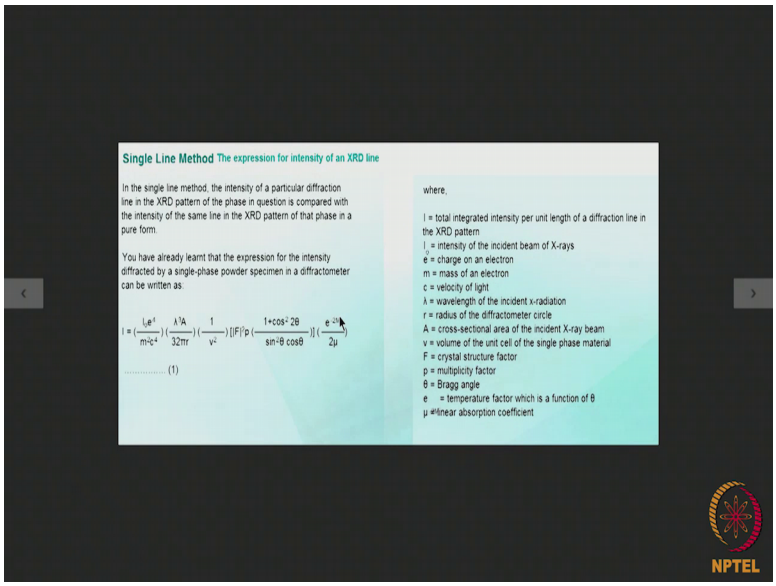


Now, I will describe all the 3 methods for mixtures easy and x ray diffractometer. First of all we deal with the single line method now as we are all aware in a diffractometer the expression for intensity of an exciting line is given by the equation 1, this is written on the board also.

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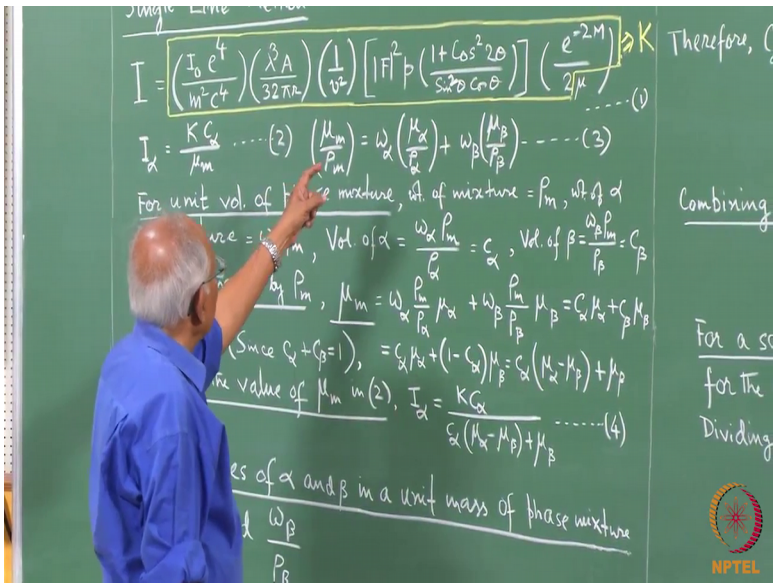


So, I is equal to I 0 e to the power 4 divided by m square C 4 lambda cube A by 32 pi R into 1 by v square into F square p into 1 plus cosine square 2 theta divided by sin square theta cosine theta into e to the power minus 2 m by 2 mu. Now we know that I is a total

integrated intensity per unit length of a diffraction line in the XRD pattern I 0 is a intensity of the incident beam of x rays.

E is a charge on an electron. M is a mass of an electron. C is the velocity of light. Lambda the wavelength of the incident x radiation, R is a radius of the diffractometer circle. A is a cross sectional area of the incident x ray beam, V the volume of the unit cell of the single phase material. F is equal to crystal structure factor. P is a multiplicity factor. Theta is a bragg angle. E to the power minus 2 m is a temperature factor which is a function of theta and mu is a linear absorption co efficient. So, this expression is valid for pure phases align of the pure phase. While we have a phase mixture of say 2 phases alpha and beta then there will be slight change in the expression.

For example, if we measure the intensity of the same line of a phase when it is in a pure form that intensity will be much higher compare to when this phase is present only as a small fraction of A phase mixture. So, when we are dealing with a phase mixture align of a particular phase, intensity of Align of a particular phase the expression for that must be multiplied by W alpha, the Wight fraction or C alpha, the volume fraction of the particular phase.

Say for example, this I here this is the intensity of A particular line in their pure phase. The moment this phase say is a alpha phase is present in the mixture containing the 2 phases alpha and beta then the intensity of that particular line In the phase mixture for alpha will be rectify, multiply this expression by C alpha and changing the value of mu the linear absorption co efficient of alpha as mu m, because we must write down the linear absorption coefficient of the mixture.

Now in this expression the whole term we shown by this yellow chalk is a constant for that particular line.

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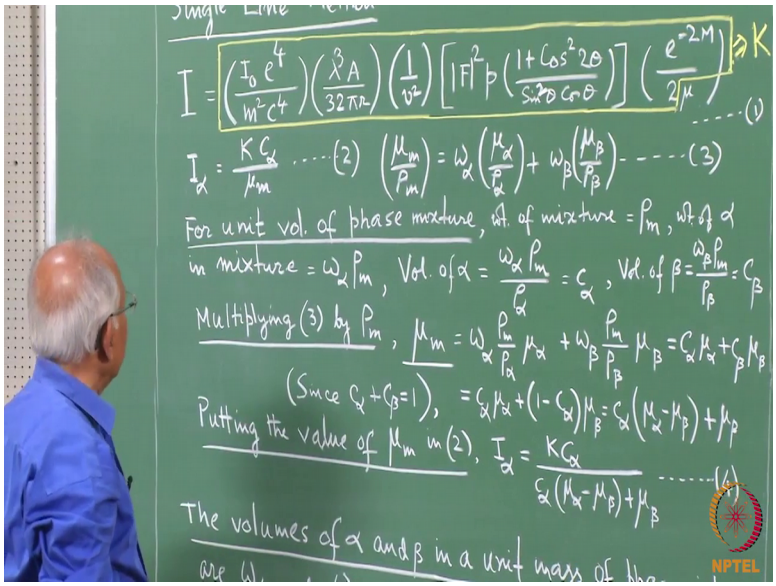


Therefore we can write it as a K a constant and this will be multiplied by C alpha by mu m. So, this is the dual expression for the integrated intensity of A particular line in a pure phase, and when that phase is present as part of a mixture of 2 phases then the intensity of the same line will be written as k.

Though thus particular term to see alpha which is the volume fraction of the alpha phase in the mixture divided by instead of mu we write mu m the linear absorption co efficient of the mixture. Now we know that when we are dealing with the mixture containing 2 phases alpha and beta, then the mass absorption coefficient of the mixture mu m by rho m can be written as W alpha into mu alpha by rho alpha plus W beta multiplied by mu beta by rho beta. So, W alpha is a Wight fraction of the alpha phase in the mixture that may beta is a Wight fraction of the beta phase in the mixture mu alpha.

And mu beta are the linear absorption coefficients of the alpha and beta phases in the mixture, rho alpha and rho beta are the densities of the alpha and the beta phase respectively. Now if we consider a unit volume of the phase mixture then the Wight of the mixture will be simply equal to rho m the density of the mixture. So, Wight of alpha in the mixture will be equal to W alpha to rho m similarly, volume of alpha will be equal to W alpha rho m divided by the density of the alpha phase rho alpha. And we know that the volume can be simply written as C alpha and the volume of the beta phase will be W

beta rho m by rho B and this can be simply as C beta, because we know the how it will talking about is for unit volume of the phase mixture.

Now, multiplying equation 3 by rho m, this equation 3 by rho m we get mu m equal to W alpha rho m by rho alpha into mu alpha plus W beta to rho m by rho beta into mu beta, and this can be written as C alpha mu alpha and this can be written as C beta mu beta. Since C alpha plus C beta; that means, the volume fraction of Alpha the volume fraction of beta in the mixture is equal to 1, then this can be written as C alpha mu alpha plus 1 minus C alpha into mu beta equal to C alpha in the mu alpha minus mu beta plus mu beta. Now if we put this value of mu m in equation 2 over here, we get I alpha equal to K C alpha divided by C alpha into mu alpha minus mu beta plus mu beta, this is our equation 4.

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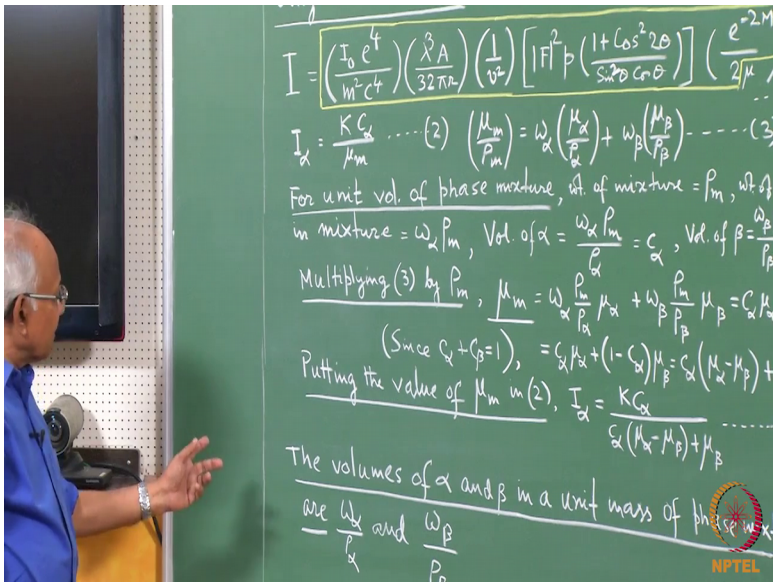


Now, when we consider the volumes of the 2 phases alpha and beta in a unit mass of the phase mixture, these are W alpha by rho alpha and W beta by rho beta respectively.

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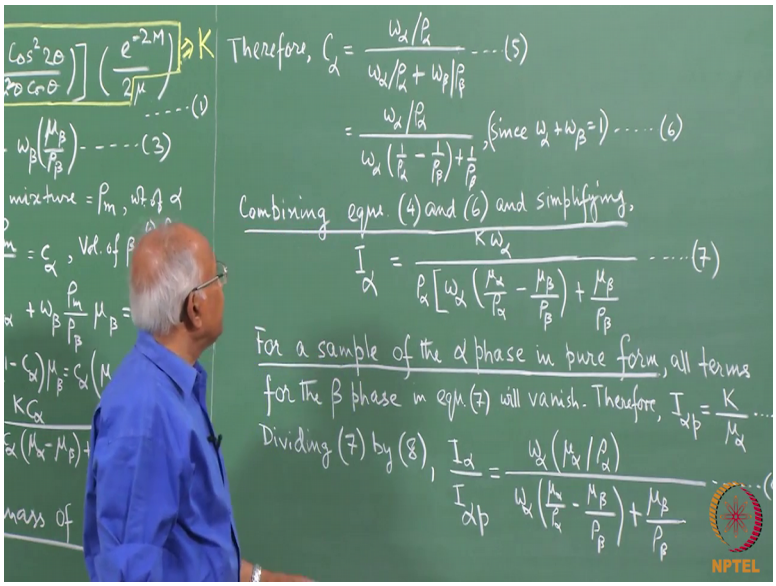


Therefore now, we can write C alpha will be equal to W alpha by rho alpha divided by W alpha by rho alpha plus W beta by rho beta, our equation number 5. Since W alpha plus W beta equal to 1, this equation can be written as W alpha by rho alpha divided by W alpha into 1 by rho alpha minus 1 by rho beta plus 1 by rho beta. Now if we combine the equation 4 over here if we combine equation 4 and equation 6 over here and simplify we can write down, I alpha equal to K W alpha divided by rho alpha into W alpha into mu alpha by rho alpha minus mu beta by rho beta plus mu beta by rho beta. For a sample of the alpha phase in a pure form if we get a sample of alpha phase in a pure form, then all the terms for the beta phase in this equation is simply vanish.

And therefore for the pure phase I can write down I alpha p for the for the pure form will be simply equal to K divided by mu alpha. Now if we divide equation 7 by equation 8 we can write down I alpha divided by I alpha p will be equal to W alpha into mu alpha by rho alpha divided by W alpha if the mu alpha by rho alpha minus mu beta by rho beta plus mu beta by rho beta. So, what we can see here, that if we get a phase mixture of alpha and beta, and if we concentrate on a particular line of alpha in the diffraction pattern for the phase mixture.

And if at the same time we look at the intensity of the same line in a pure form of alpha then divide them to intensity the first and the second one we get an expression like this. And here, if we look the values of mu alpha mu beta which are the linear absorption

coefficients of the alpha and beta phases and rho alpha and rho beta the densities of the alpha and beta phases they simply form the ratio of align of alpha phase in the mixture and the same line of the alpha phase in a pure form, this from this ratio knowing the value of mu alpha mu beta rho alpha rho beta, it is possible to find out the value of W alpha the Wight fraction of Alpha in the mixture.

And once you know the Wight fraction of Alpha in the mixture, and if the mixture contains only the 2 phases alpha and beta the Wight fraction of beta can also be found out. Now this method is known as the single line method because here we compare the intensity of A particular line of the alpha phase in the mixture with the intensity of the same line of the alpha phase in a pure form. So, from this single line method knowing the values of the linear absorption coefficients and densities of the constituent phases it is possible to find out the Wight fraction of the 2 phases alpha and beta; quantitative phase analysis by x ray diffraction namely the internal standard method. Say for example, we have got a mixture of 3 phases A B and C.

Let us suppose that we want to find out the volume fraction or the Wight fraction of A in the phase mixture. So, in the internal standard method what we do is we mix a known amount of a standard phase for which all the parameters are known and mix it with the given sample and make a composite sample.

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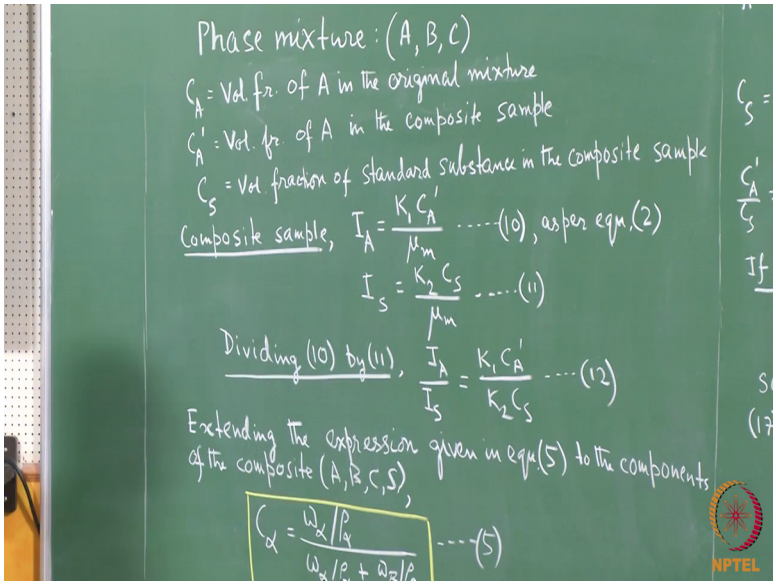

Say for example, when we make the composite sample say C A this is a volume fraction of the phase A in the original mixture and suppose C A, prime is a volume fraction of A in the composite sample and C S is the volume fraction of the standard substance in the composite sample. Then what we do? Then we take an x ray diffraction pattern of the composite sample in a diffractometer.

So, now for the composite sample using the expression for equation 2 we can write I A, the intensity of A particular line for the phase A in the composite sample is equal to K 1 C A prime by mu m, where mu m is the linear absorption coefficient of the mixture; the whole of the composite sample.

Now simultaneously if we concentrate on a particular line of the standard the diffraction pattern of which will also appear in the same XRD pattern for all the other components A B and C, then I S can be written as a constant K 2 into C S divided by mu m. Now if we divide equation 10 by 11 we can write down I A by I S is equal to K 1 C A prime divided by K 2 C S. Now we have already seen in equation 5, how to find out the volume fraction of A phase in a 2 phase mixture? This is the expression for equation 5; now, extending this expression to the components of the composite which we have made up of A B C and S.

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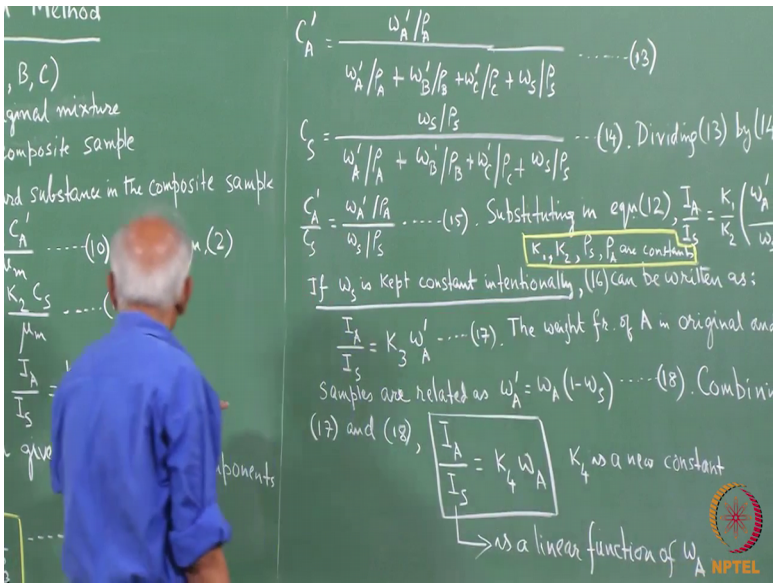


We can write down C A prime will be equal to W A prime by rho a divided by W A prime by rho a plus W B prime by rho B plus W C prime by rho C plus W S by rho S. This is

our equation 13. In a similar manner we can find out the expression for C S also which is equal to W S by rho S divided by the whole thing over here. So, this is our equation number 14. Now if we divide 13 by 14, we can write down C A prime divided by C S will be equal to W A prime by rho a divided by W S by rho S, this is all equation 15. Now if we substitute in equation 12, this is our equation 12.

Now, if we substitute in equation 12 we can write down I A by I S is equal to K 1 by K 2 multiplied by W A prime by rho a divided by W S by rho S, this is our equation 16. Now here K 1 K 2 rho S rho a are all constants. Now if while making the composite by adding the standard material if the Wight fraction is kept constant intentionally then equation 16 can be written as I A by I S is equal to K 3 W A prime, K 3 is a new constant incorporating the various parameters. Now the Wight fraction of A in the original and the composite samples are related in this manner, W A prime is equal to W A into 1 minus W S. Now if we combine the expressions 7 teen and 18, we can write down I A by I S is equal to K 4 which is a new constant into W A.

So, you see that if we concentrate on a particular line of A, and a particular line of the standard material in the composite that we have made and if we divide the intensity of A by the intensity of S, then this expression will be a linear function of W A the Wight fraction of A in the phase mixture. So, this gives us a method by which we can find out the Wight fraction of the different phases A B and C in a phase mixture of A B C. Now I come to the third method of quantitative phase analysis using x ray diffraction this is known as the direct comparison method.

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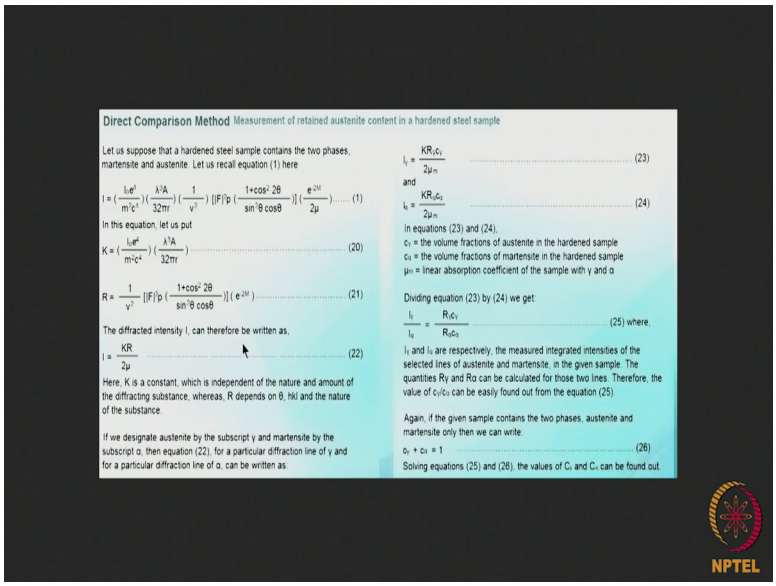


You see in the first 2 methods there are certain problems for example, in the single line method it is essential to have S you know a pure material one of the phases must be available in a pure form in order that the fraction of that phase in the phase mixture can be determined. And sometimes it may be very difficult to get a phase in a pure form. And in the second method the internal standard method also there may be a problem in getting a suitable standard. So, in this method we really do not need to have the phases to be present in pure form you know to be compared with or some internal standard to be found out for making a composite. So, in this method say for example.

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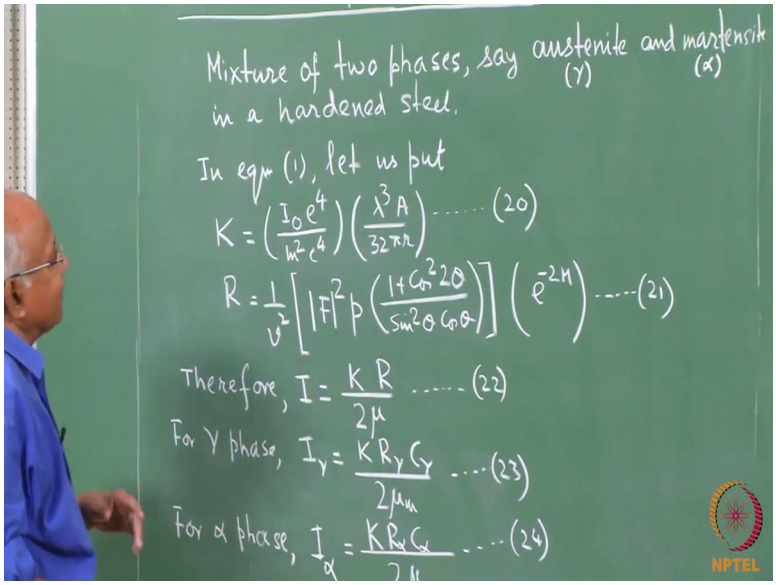

If we take a practical example in hardened steels very often we find that there are 2 phases. So, a hardened steel is a mixture of 2 phases namely FCC austenite phase gamma and BCT martensite phase alpha although martensite is body centered tetragonal, the tetragonality if it is not that high it can be considered simply as BCC alpha. So, we have a phase mixture of FCC austenite and BCC martensite. Now what we do in this method? We choose 2 lines one from each phase. So, we take we consider a particular XRD line from the austenite phase and a particular XRD line from the martensite phase in the x ray diffraction pattern of the mixture.

And then compare the intensities of those 2 lines and as I will show readily that a comparison of the intensities of the 2 chosen lines From the 2 phases it is possible to find out the volume fraction of individual phases. Now from equation 1 what we do you know if you remember the equation 1 we put K a constant equal to I 0 e to the power 4 by m square C 4 to lambda cube A by 32 pi r. Now this expression is the same for all the diffraction lines in the pattern. So, this is the same for all the diffraction lines in the pattern, we put it K, k is a constant for all lines diffraction pattern. And then the remaining part for example, 1 by B square F square p to 1 plus cosine square 2 theta by sin square theta cosine theta e to the minus 2 m we write as r. So, what is there in this expression as we remember v is the volume of the unit cell, F is a crystal structure factor, p is a multiplicity factor this expression here is the Lorentz polarization factor.

And this is the temperature factor. And naturally the value of R for the 2 chosen lines will be different, although, the value of K for the 2 chosen lines will be the same. So, in that case we can write down the expression for I equal to integrated intensity of A line is equal to K R by 2 mu the mu, is a linear absorption coefficient of a material as we know this is our this was our equation 1. So, this equation 1 can be written down in this simpler form by putting K is equal to this much R is equal to this much. But when we are talking about a mixture we have to make some changes. For example, this is valid for a pure phase, a line of a pure phase.

But when we have a phase mixture say, when we talk about the gamma phase then the intensity of A line in the gamma phase there I have to put K instead of R it will be R gamma you know R gamma for that line multiplied by C gamma the volume fraction of gamma in the mixture. If the whole thing is gamma then the intensity of A line a particular line will be very high, but if you know it is present only as a fraction then

intensity will automatically come down. So, intensity of the chosen line in the gamma phase can be written as K R gamma multiplied by C gamma C gamma is a volume fraction of the gamma phase in the mixture and instead of writing mu the linear absorption.

Coefficient for a pure phase now we have to write down twice mu m of the mixture. Similarly, for the alpha phase

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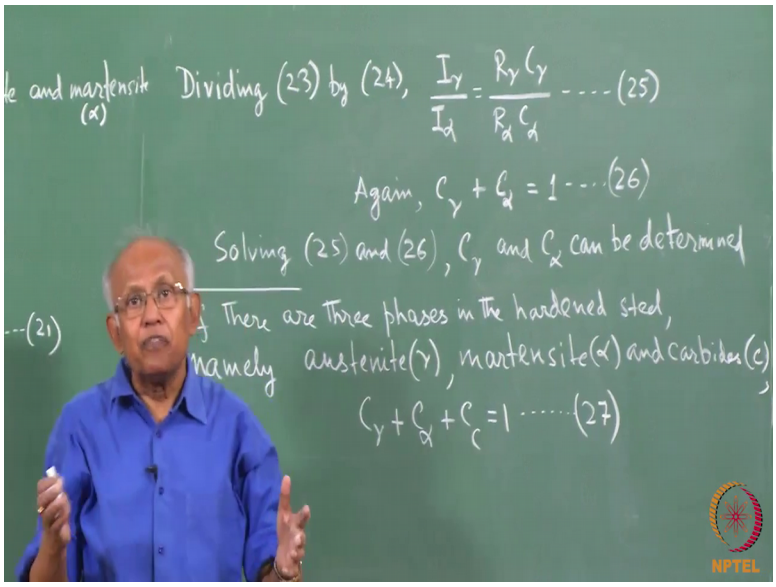


We can write down I alpha is equal to K R alpha C alpha C alpha is a volume fraction of the alpha phase in the mixture by 2 mu m. Now if we divide 23 by 24, we can write down I gamma by I alpha is equal to R gamma C gamma divided by R alpha C alpha. Again you know that if it is a 2 phase mixture of austenite and martensite only then C gamma plus C alpha equal to 1. Now if we solve these 2 equations then it is possible to determine the value of C gamma and C alpha.

But in order to do that we have to find out the values of R gamma and R alpha. So, once we can determine the values of R gamma and R alpha then by solving equations 25 and 26, it is possible to find out the volume fractions of the austenite and the martensite phase in the phase mixture of austenite and the martensite in hardened steel. Now if there are more than 2 phases. So, say for example, sometimes there are 3 phases present in the hardened steel namely austenite martensite and some carbides. There we can write down

the volume fraction of Austenite plus volume fraction of martensite plus volume fraction carbides equal to 1.

And following the same method as we have done for a 2 phase mixture it is possible to find out the volume fractions of all the 3 phases individually. The direct comparison method is unique in the sense it neither leaves the availability of any of the phases in a pure form nor it is necessary to mix a standard material with the phase mixture in order to determine the volume fractions of the individual phases in the mixture. So, in that way it has got an advantage over the previous 2 methods. Now for hardened steel you know it is sometimes very essential to find out the volume fraction of Austenite, because what happens if we make any tool out of that material, during service the amount of austenite gradually changes into martensite or some other phase.

And that may give rise to lot of internal stresses and dimensional instability. That is a reason why it is very much essential to find out the volume fraction of the retained austenite phase. Now this can be d1 by using the microscopic method also. In fact, the microscopic method is pretty good and rather accurate for you know an austenite contained about say 15 percent and above.

But when it is below 15 percent you know in that case the x ray diffraction method using the direct comparison method can be a better proposition. So, this is the reason why the direct comparison method is very useful in industrial practice. Now I will illustrate the use of the direct comparison method taking a practical example. Let us consider a high carbon steel sample.

Now, if this sample is taken to the austenitic range and then directly quenched in a bucket of water; we are going to get 2 phases martensite and some austenite. Now we now if we take the x ray diffraction pattern of the sample, then the pattern will show lines of both austenite and martensite.

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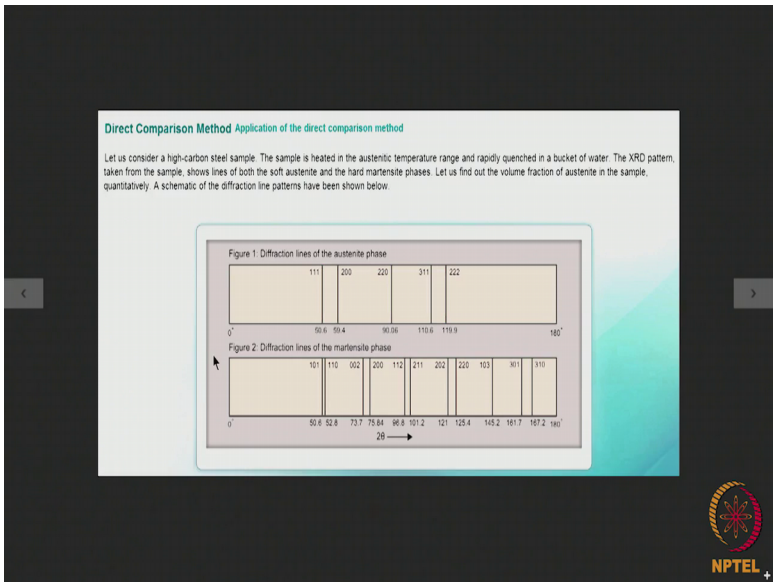


Now, this is a schematic of the line positions in the x ray diffraction pattern for the austenitic phase and also for the martensitic phase. So, in the direct comparison method if we want to find out say, the volume fraction or the Wight fraction of Austenite in the hardened steel we have to compare the intensities of one line from each phase.

For example in this particular case we choose the 2 0 0 line of martensite and 2 2 0 line of the austenite. Now 2 0 0 line for martensite we can see that the 2 theta is 75.84 degrees, and for 2 2 0 line of austenite the 2 theta is 90.06 degrees. What happens essentially is when we talk about martensite the lines 1 0 1 and 1 1 0 this should be shown as separate lines very close to each other. Similarly 0 0 2 2 0 0 these 2 lines should be seen very close to each other.

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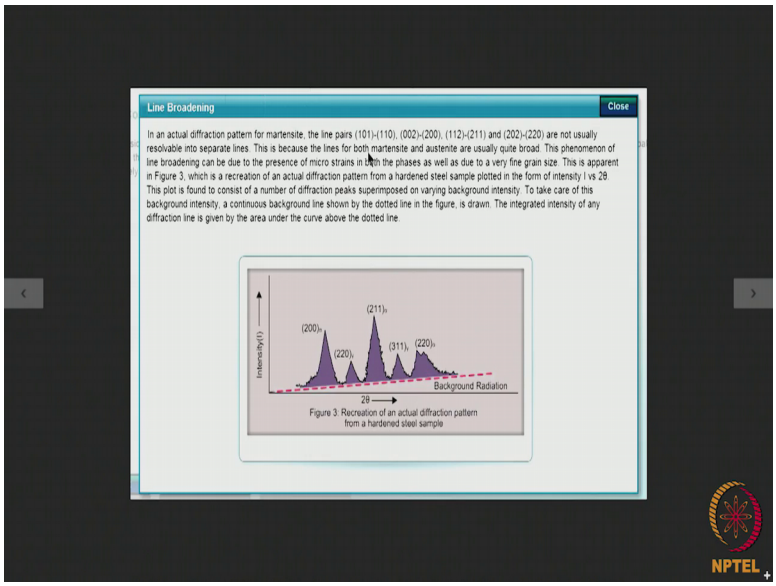


And 1 1 2 2 1 1 and 2 0 2 2 2 0 these are to be shown very close to each other, but you see the resolving power should be very high in order to see these as very distinct lines, but it is normally not possible. Moreover the reason for this is because of the presence of micro strain, and also because of the fineness of the grains you know, the lines show some broadening. As a result these 2 doublet So to say lines will appear as one these 2 will appear as one these 2 will appear as one these 2 will appear as one; so if we take a practical example and draw the intensity versus 2 theta plot for a composite of martensite and austenite phases.

We see that this is say the 2 0 0 alpha peak, this is the 2 2 0 gamma peak, this is the 2 1 1 alpha, this is the 3 1 1 gamma, this is the 2 2 0 alpha etcetera, etcetera. Now as we know the background varies from 2 theta 0 to 2 theta 180 degree and the background goes up as 2 theta increases. Say this is the background radiation here.

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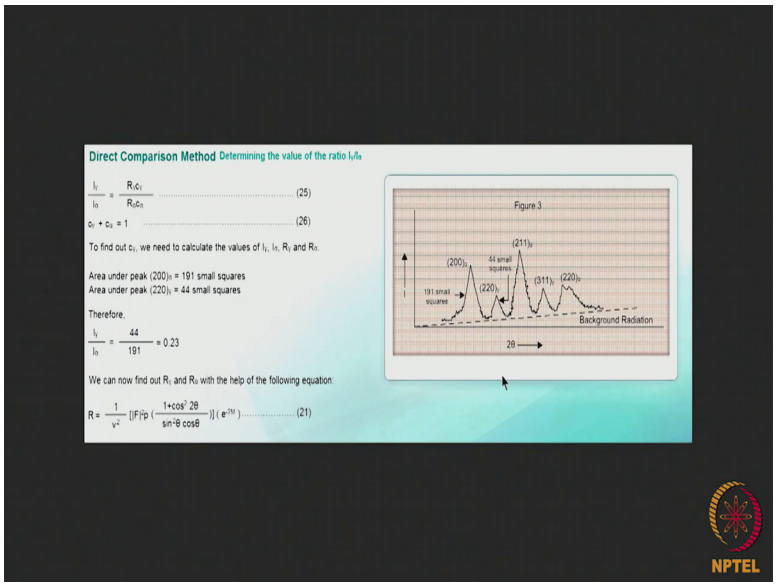


Now we are going to use the direct comparison method in order to determine the values of the volume fractions or the Wight fractions of austenite and martensite in the hardened sample, as we have seen already.

If we choose a particular line of gamma and a particular line of alpha, we can write down I gamma by I alpha is equal to R gamma C gamma divided by R alpha C alpha. So, I gamma and I alpha these are the integrated intensities of the chosen gamma and the alpha lines. Now if we want to find out C gamma we need to calculate the values of I gamma I alpha, from the pattern and also R gamma and R alpha. Now if we put a transparent graph paper on top of the I versus 2 theta plot as we obtained from a diffractometer, we find that the area the integrated intensity which is proportional to the area under the line. So, here for the 2 0 0 alpha there are 191 small squares of the graph paper within this region.

And if we compare it with the 2 to 0 gamma peak you know the number of small squares is 44 therefore, we can write down I gamma by I alpha is equal to 44 by 191 which is equal to 0.23. So, this much can be calculated from the plot of I versus 2 theta straight away. Now we have to find out the values of R gamma and R alpha with the help of the following equation, as we already seen.

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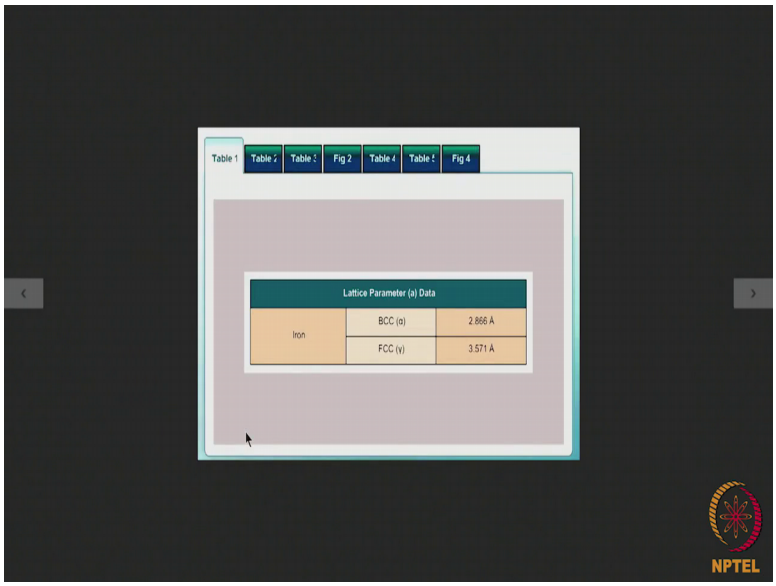


So, this is the equation for R. Now, how to determine these values? In order to do that we need to have a number of tables showing the values of different parameters: for example, for measuring the value of v the volume of the unit cell in the 2 phases.

We need to have the lattice parameter data. Say for example, for BCC alpha this is the lattice parameter 2.866 and for FCC gamma this is the lattice parameter 3.571.

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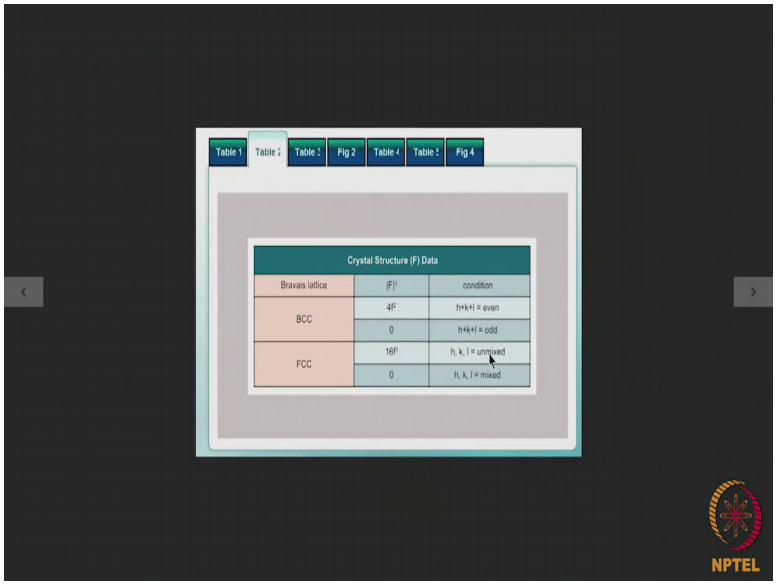


Now we need to have the crystal structure factor data. So, for BCC we know that F square is equal to 4 small f square, small f is atomic scattering factor and when this is

possible this is possible when h plus K plus l is an even quantity. And it will be 0 when h plus K plus l is an odd quantity, on the other hand for FCC bravais lattice, value of F square will be 16 small f square where f again is atomic scattering factor.

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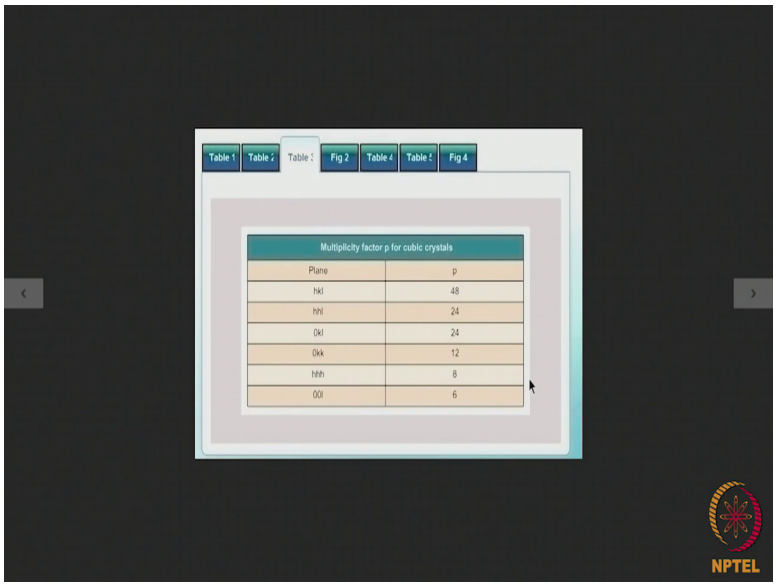


And this is true for h k l unmixed and it is equal to 0 when h k l are mixed then we get another table for multiplicity factors. So, on this side are shown the h k ls and on this side the value of the multiplicity factor. So, if the plane is h k l; that means, h k l all 3 are different, then multiplicity factor is 48 h h l multiplicity factor is 24 0 K l type of planes multiplicity factors 24, 0 k k type of planes multiplicity factor is 12 h h h type of planes it is 8 for example, 4 1 1 1 planes multiplicity factor is 8 0 0 l planes it is six. So, 1 0 0 plane it is 6 etcetera, etcetera; so using these tables.

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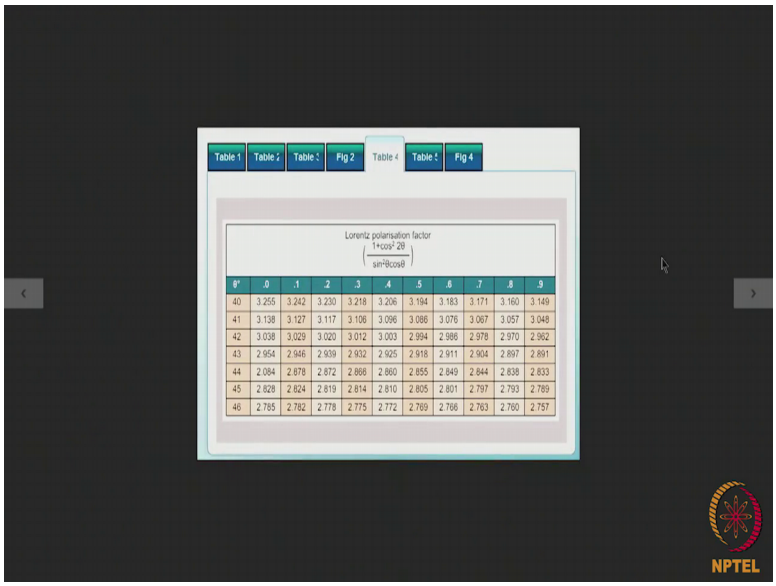

Lorentz polarisation factor $\left(\frac{1+\cos^2 2\theta}{\sin^2\theta\cos\theta}\right)$

| θ° | .0 | .1 | .2 | .3 | .4 | .5 | .6 | .7 | .8 | .9 |
|---|---|---|---|---|---|---|---|---|---|---|
| 40 | 3.255 | 3.242 | 3.230 | 3.218 | 3.206 | 3.194 | 3.183 | 3.171 | 3.160 | 3.149 |
| 41 | 3.138 | 3.127 | 3.117 | 3.106 | 3.096 | 3.086 | 3.076 | 3.067 | 3.057 | 3.048 |
| 42 | 3.038 | 3.029 | 3.020 | 3.012 | 3.003 | 2.994 | 2.986 | 2.978 | 2.970 | 2.962 |
| 43 | 2.954 | 2.946 | 2.939 | 2.932 | 2.925 | 2.918 | 2.911 | 2.904 | 2.897 | 2.891 |
| 44 | 2.084 | 2.878 | 2.872 | 2.866 | 2.860 | 2.855 | 2.849 | 2.844 | 2.838 | 2.833 |
| 45 | 2.828 | 2.824 | 2.819 | 2.814 | 2.810 | 2.805 | 2.801 | 2.797 | 2.793 | 2.789 |
| 46 | 2.785 | 2.782 | 2.778 | 2.775 | 2.772 | 2.769 | 2.766 | 2.763 | 2.760 | 2.757 |

We can calculate the value of F square we can calculate the value of p we can calculate the value of v etcetera, etcetera. Then comes the Lorentz polarization factor 1 plus cosine square 2 theta by sin square theta cosine theta. Here I have plotted only some definite values relevant to our problem. So, here it is theta in degrees from 40 to 46 then it is 0.1 0.2 0.2 0.3 0.4 etcetera, etcetera. 0.9 for example, you know if theta is 40 degrees then this is the value of the Lorentz polarization factor. If on the other hand theta is 40.1 degree then the Lorentz polarization factor is this. If it is a 42.5 degrees of theta then you have to find it out.

So, it will be 2, 0.994 if it is say 45.9 degrees a theta. So, it is 2.789 etcetera, etcetera. So, from this table we can find out the value of the necessary Lorentz polarization factor for the lines.

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We are using say a cobalt K alpha radiation in this particular case and the wavelength is 1.7901 angstrom. Now the value of sin theta by lambda is given here this is theta. So, we find out the value of sin theta in each case divided by the lambda that is used. So, these are the values of sin theta by lambda and here the temperature factor has been given as a function of sin theta by lambda.

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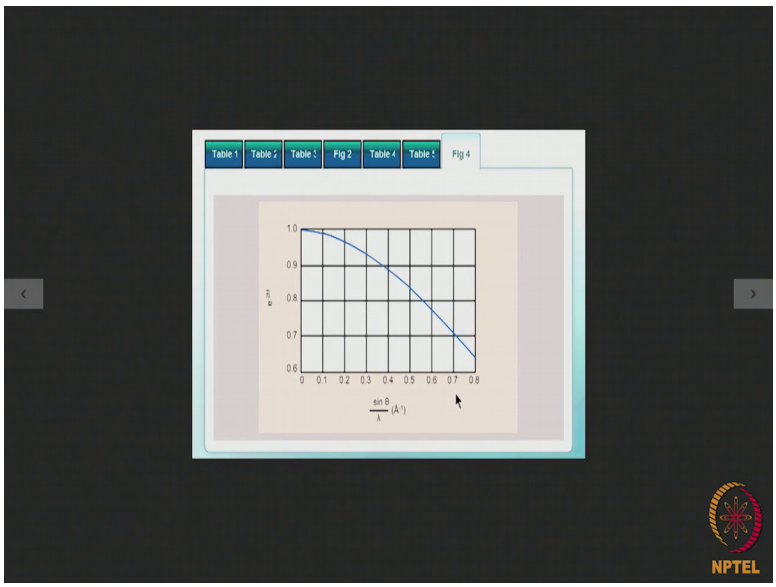


And naturally for any line we calculate first the sin theta for lambda and corresponding value of sin theta by lambda you can find out what should be the value of the

temperature factor. So, using all these different tables we can find out the value of R for the chosen lines from the martensite and the austenite phases.

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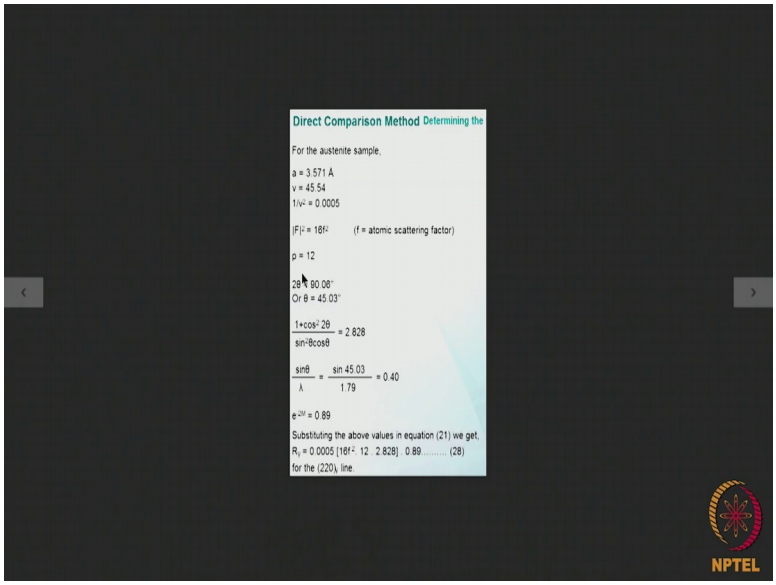


Now if we look at the austenite phase, we can write down a is 3.571 angstrom. So, v the volume of the unit cell is 45.54 1 by v square is 0.005 F square is 16 small f square small f is that mix catching factor p is equal to 12 now 2 theta for that austenite line.

Which we chose is ninety 0.06. So, that theta is 44.03 degree and using the table I shown earlier the Lorentz polarization factor is 2.828 sin theta by lambda, for that particular line is this equal to 0.40 corresponding to that we can find out what is the temperature factor which is 0.89. So, if we substitute the above values in the equation 21, what we find R gamma is equal to 0.0005 into 16 F square into 12 into 2.828 into 0.89. So, this is true for the 2 2 0 gamma line. In a similar method when you look at the chosen line from the martensitic sample.

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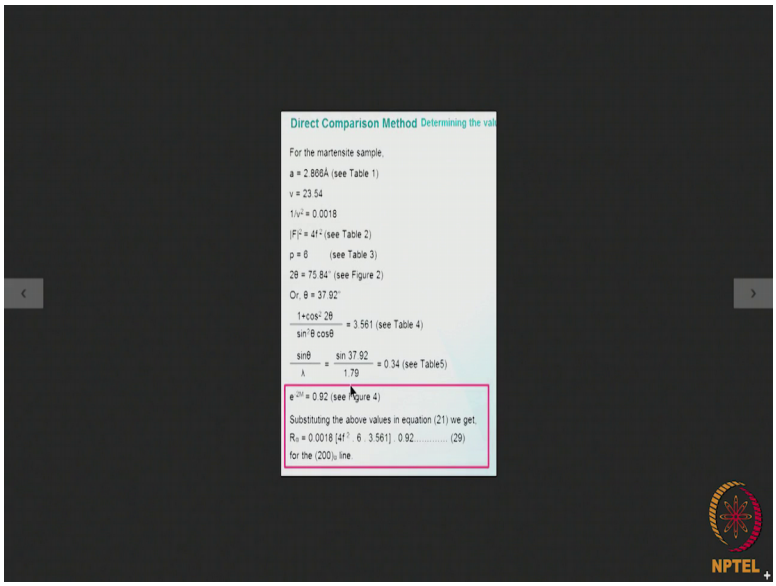


Which is a 2 0 0 martensite line a is 2.866 angstrom from the table which I have shown already. So, this is the value of volume v unit is of the unit cell 23.54 1 by v square is 0.0018 capital F square is 4 F square, this F stands for; that means, catching factor for this type of plane multiplicity factor is 6 from the table and for 6 is from this line 2 theta is 75.84 degree. So, theta is this much and the value of the Lorentz polarization factor can be read out from the table as 3.561 sin theta by lambda can be calculated to be 0.34 and using all those values and the temperature factor comes out to be 0.92.

Now, we can substitute our values and equation 21 and get R alpha is equal to 0.0018 into 4 F square into 6 into 3.561 into 0.92. So, now, we have found out the values of R gamma and R alpha for the chosen lines.

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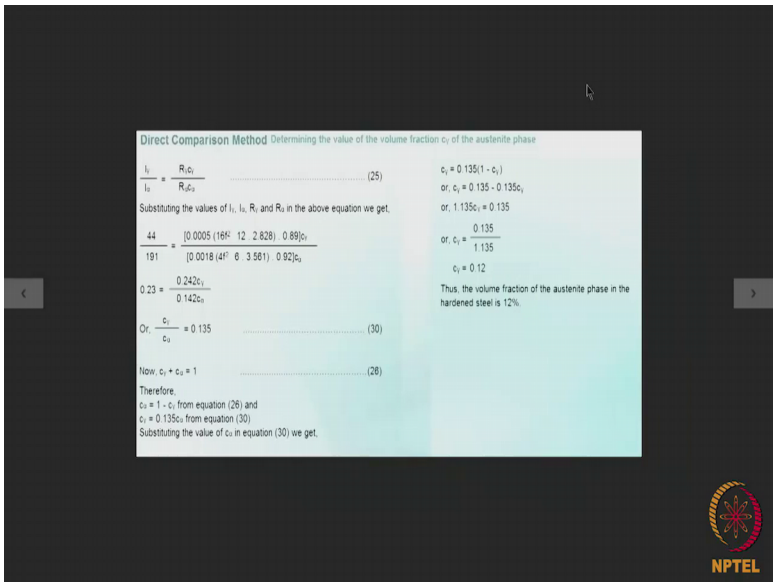


So, putting those values in this equation we have already seen I gamma by I alpha is 44 by 191 that is by direct measurement on the I versus 2 theta plot and then put the values of R gamma and R alpha and here multiplied by C gamma and C alpha. So, 0.023 is equal to 0.24 to C gamma by 0.0142 C alpha. So, C gamma by C alpha is 0.135, but since the material contains only 2 phases gamma.

And alpha we can write C gamma plus C alpha is equal to 1. So, you see that now we have got 2 important expressions one for C gamma by C alpha, and the other for C gamma plus C alpha. Now if we solve these 2 equations we find the value of C gamma is 0.12; that means, the volume fraction of Austenite phase in the hardened steel is 12 percent. So, this is really a very elegant method of determining the volume of volume fraction, the value of the volume fraction of the austenite phase in a sample of hardened steel. Of course, this method can be extended.

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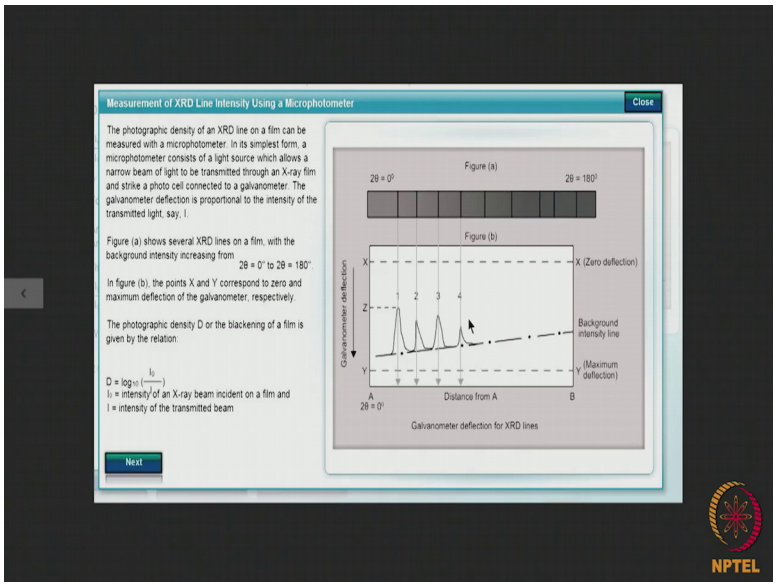


Ah in other systems also. You see till now I talked about the diffractometer method. Sometimes in some laboratories people use the old divisor and method to in order to find out the volume fraction the quantitative measurement of the volume fractions of different phases in a phase mixture. So, in that case how we determine the integrated intensity? Now the photographic density of an excited line on a film like this can be measured using a micro photometer. So, in it is simplest form.

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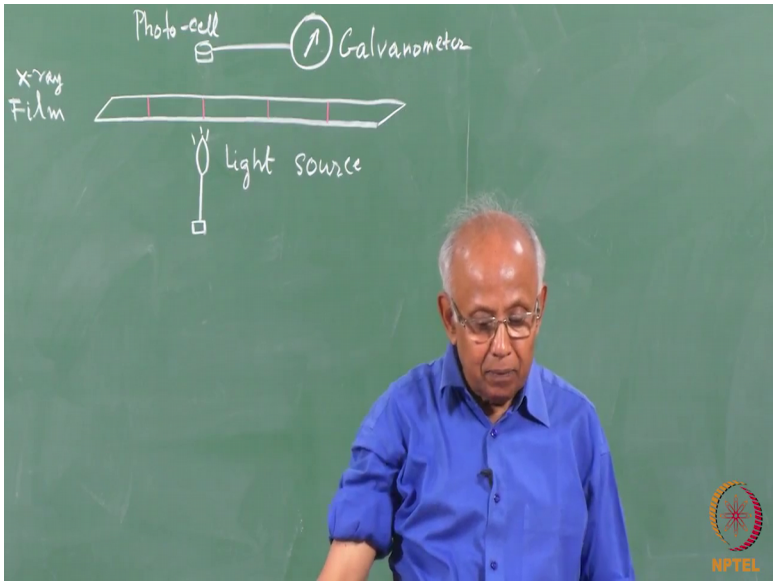

In it is simplest form a micro photometer consists of a light source which allows a narrow beam of light to be transmitted through an x ray film and strike a photocell connected to a galvanometer.

So, we have the x ray film say these are the x ray lines and naturally these are much darker as compared to the background, and we have a light source which can illuminate the x ray film from below above there is a photo cell which will record the transmitted, light intensity and this again connected to a galvanometer. The galvanometer deflection will be proportional to the intensity of the transmitted light we say I. Now in this figure several exciting lines have been shown on a film and the background as you can see changes from light to very dark as we move from 2 theta equals 0 to 2 theta, theta is equal to 180 degree. Now this is the figure b.

And here the point x corresponds to where the galvanometer shows 0 deflection. And y is the point where the galvanometer shows maximum deflection. Now for the lines 1 2 3 and 4 this is what we find the galvanometer deflection, this is what we get for the 4 lines according to their intensities. And the photographic density or the blackening of a line is given by the relation, D is equal to D is equal to log I 0 by I to the power 10 at the base to the base 10, I am sorry, D is equal to log I 0 by I to the base 10 I 0 is the intensity of the not the extra beam is wrong here I 0 is the intensity of the light incident on a film and I is intensity of the transmitted beam.

So, you say that you know if we have a photographic film which records the diffracted intensity from a phase mixture then, this is how we can find out the area under the curve and measure the integrated intensity, and use the same method as I have described already.