Condensed Matter Physics
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Diffraction Methods for Crystal Structure – Worked Examples

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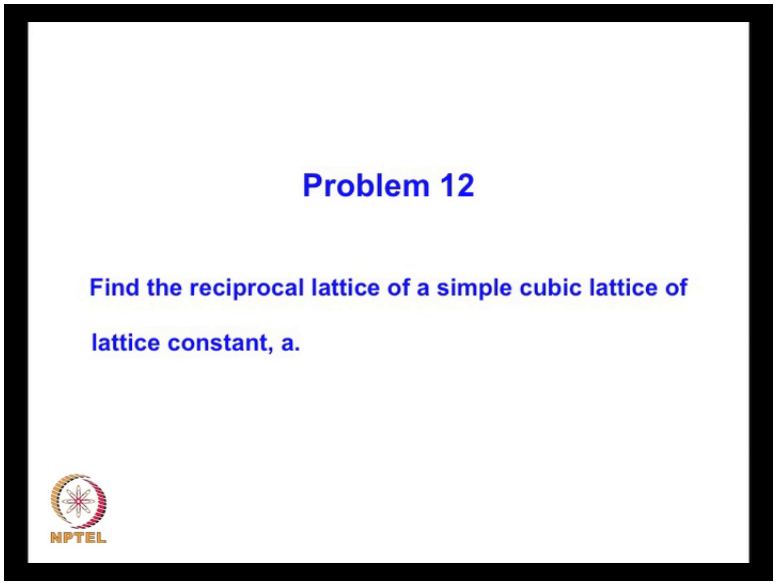

Next, we have to find the reciprocal lattice of a simple cubic lattice of lattice constant, a. So, we consider a simple cubic lattice, we have a simple cubic lattice.

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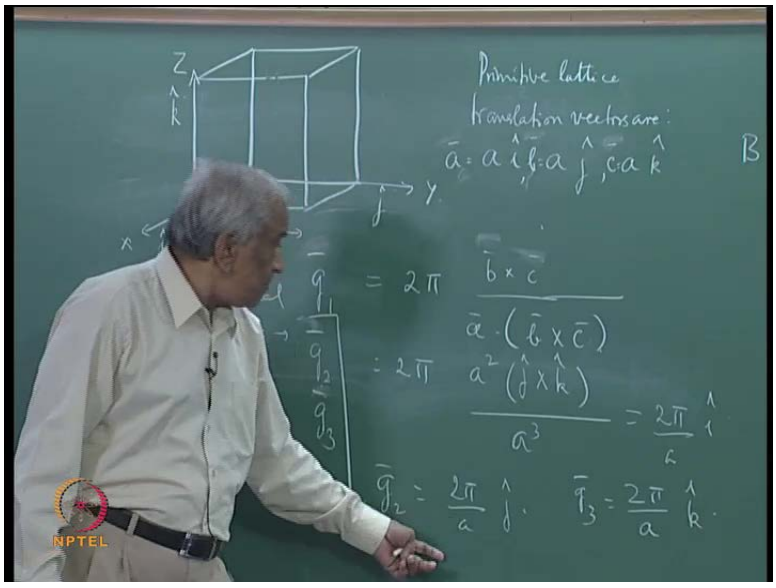

The lattice constant here is a, and it is a cube. Let us choose the x, y, z directions; this is x, this is y, and this is z and this is origin. So, we have unit vectors I along this, j along this, and k along this z axis.

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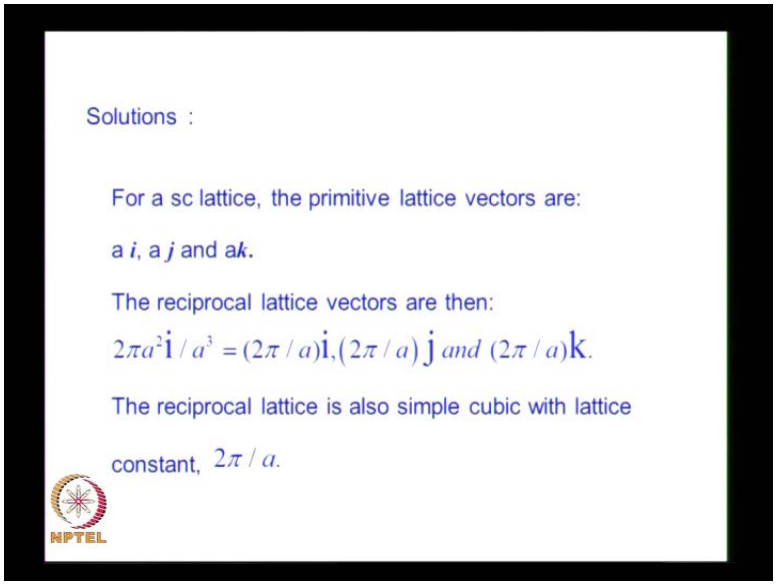

So, we have for this simple cubic lattice, the primitive lattice translation vectors are a i, a j, a k, these are the lattice translation vectors. Now we know the reciprocal lattice vectors g 1, g 2 and g 3; these are the reciprocal lattice vectors. They are given by the definition 2 pi time b cross c, where a, b, c - these are a equal to a 1, a equal to, this b equal to, this c equal to… So b cross c by a dot b cross c that is the definition. So, we have 2 pi times, 2 pi times b cross c is a square into j cross k by this will give me a cube.

So this will be 2 pi by a and j cross k is i. In this same way, we can show the g 2 is 2 pi by a times j; and g 3 is 2 pi by a into k. So there is reciprocal lattice is also a simple cubic lattice, because of side 2 pi by a in reciprocal space. So the lattice constant in reciprocal space is 2 pi by a.

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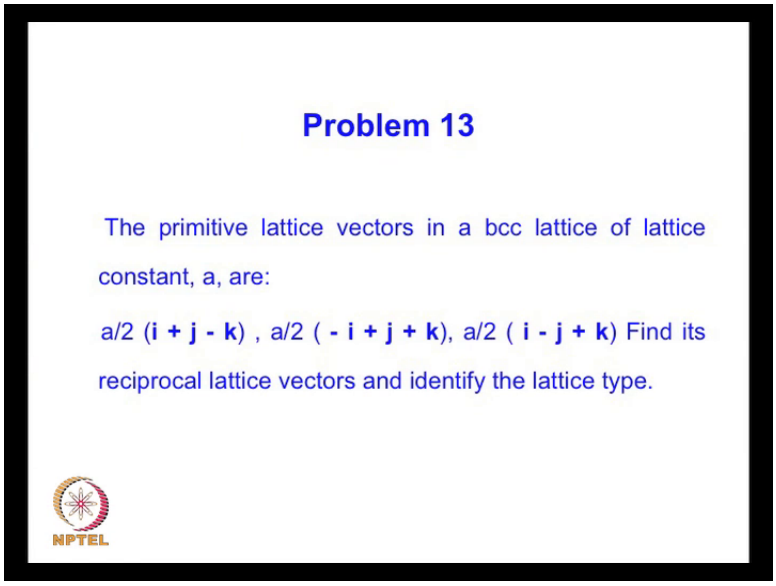

Next in a similar way, we discuss the reciprocal determine the reciprocal lattice vector for a b c c lattice. This is the simple cube.

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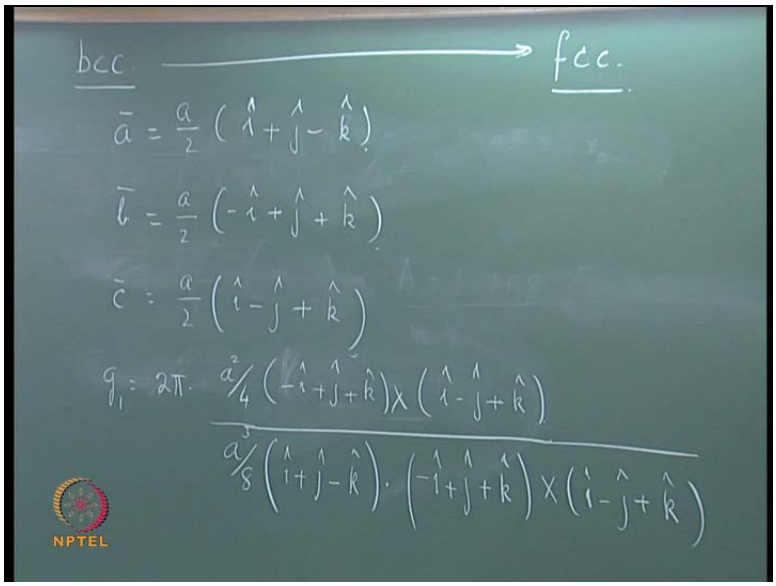

Now we go on to a b c c lattice, a body centered cubic lattice for which the primitive translation vectors are a by 2 time i plus j minus k; a by 2 times a cyclic permutation minus i plus j plus k and then 2 pi a by 2 times i minus j plus k. So again, doing the same thing, we find g 1 as a square 2 pi times a square by 4 minus i plus j plus k cross i minus j plus k divided by the k let

triple product of the all 3 together. So this will be ah these are a, b and c. So here, we will have a cube by 8 times i plus j minus k dot minus i plus j plus k cross i minus j plus k.

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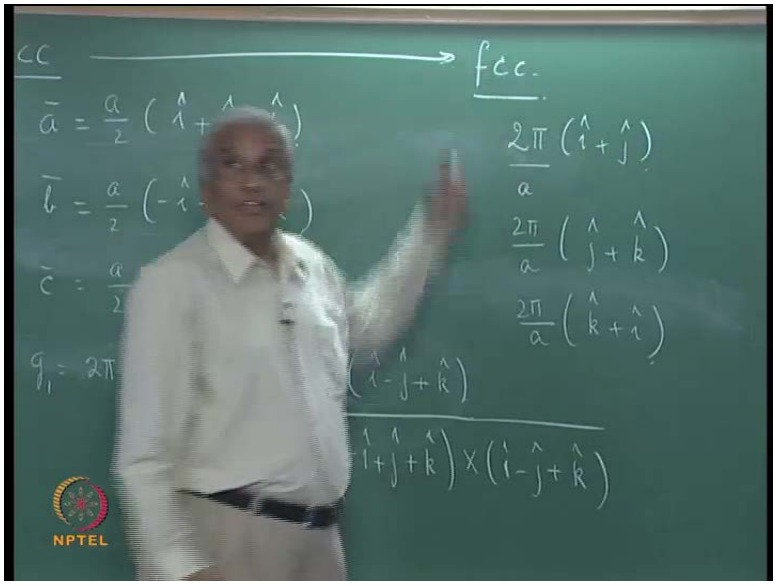

So simplifying, we get lattice translation vectors corresponding to a face centered cubic lattice. So the reciprocal lattice of the body centered cubic lattice will be face, the results will be 2 pi into i plus j by a of course. And 2 pi by a j plus k and 2 pi by a k plus i. These will be the reciprocal lattice translations vector and these correspond to a face centered cubic lattice.

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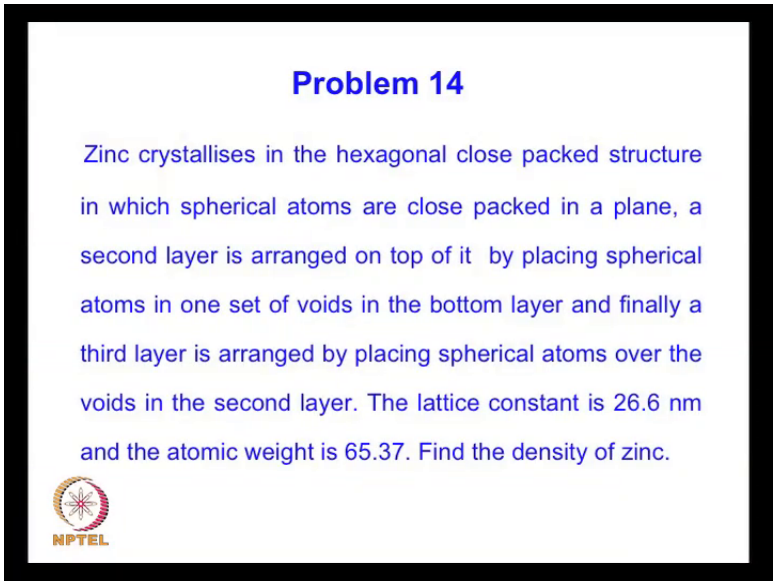

The next problem is about zinc which crystallizes in a hexagonal close packed structure.

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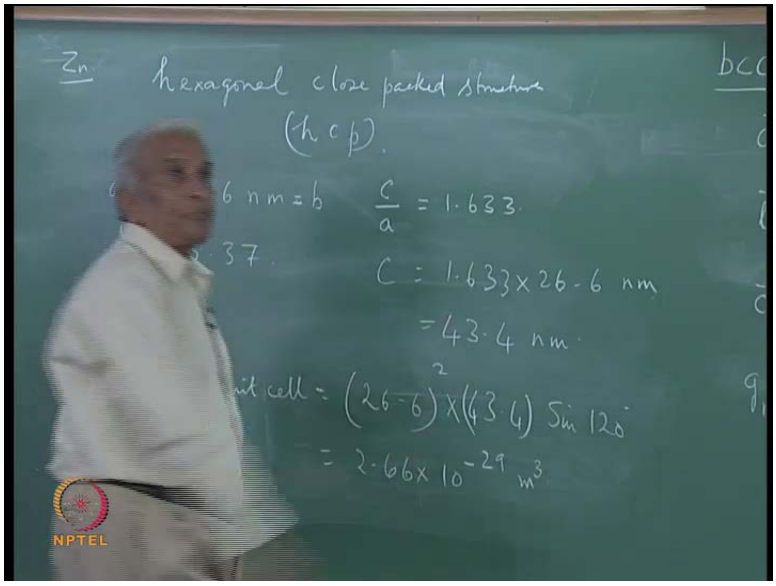

Problem concerns the element zinc, which has a hexagonal close packed structure, in short it is known as h c p. So the lattice constant is given to be 26.6 nano meters.

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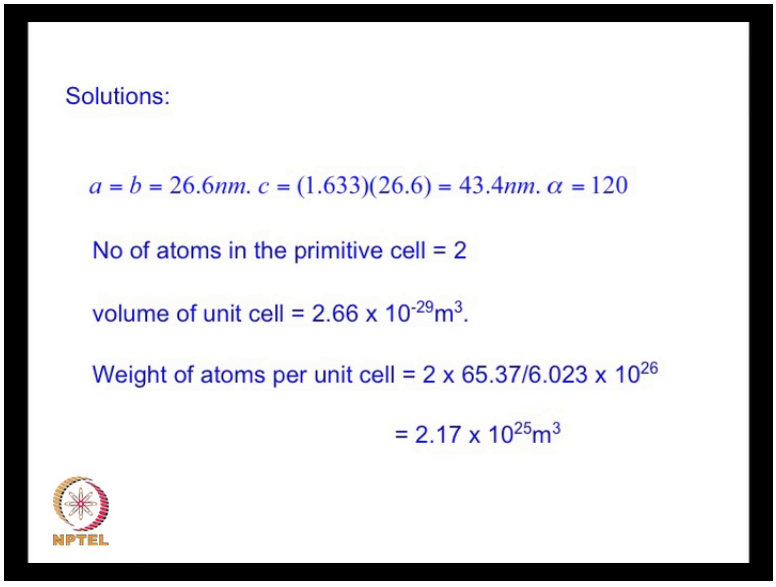

And the atomic weight is 65.37. Since it is given as a hexagonal close packed structure, in a previous problem, we found that the c by a ratio for structure structure is 1.633. So if a, this also equal to b in the plane perpendicular to the z axis. So this c will turn out to be 1.633 times 26.6 n

m – nano meter, and that is 43.43. So, the volume of the unit cell will be a b or a square, so 26.6 square times 43.4 times sin 120 which is the angle in the base cell plane. So that works out to be 2.66 into 10 to the power minus 29 meter cube. Now they are ask to find the density of zinc from this calculation, so we have to we know the volume of the unit cell, now we have to find the mass of the atoms in the unit cell.

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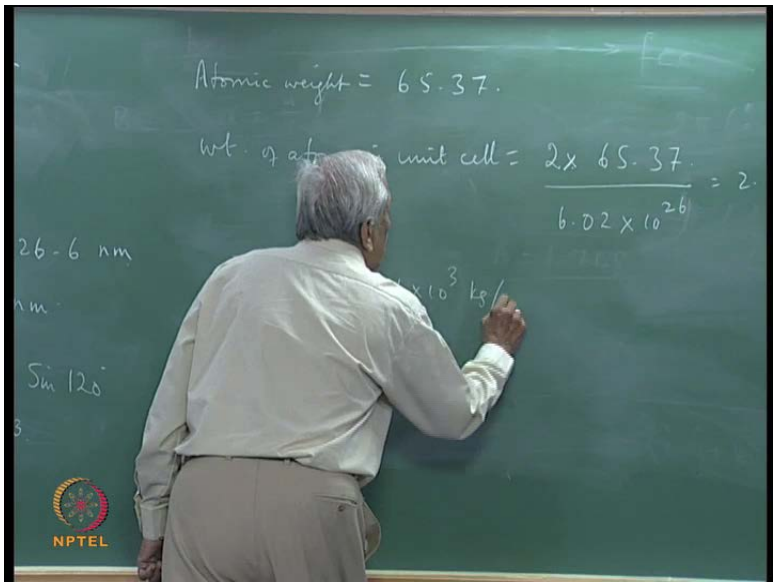

We are given that the atomic weight is 65.37, that means a mole of this material a gram atom base 65.37 grams. So weight of the atoms in the unit cells is we have 2 atoms in the unit cell for h c p structure. So this into 65.37 by the Avogadro number 6.02 into 10 to the power 26. So since we know the weight and the volume, the density is just the ratio of the weight to the volume which turns out to be 8.16 into 10 to the power 3 kilogram per meter cube.

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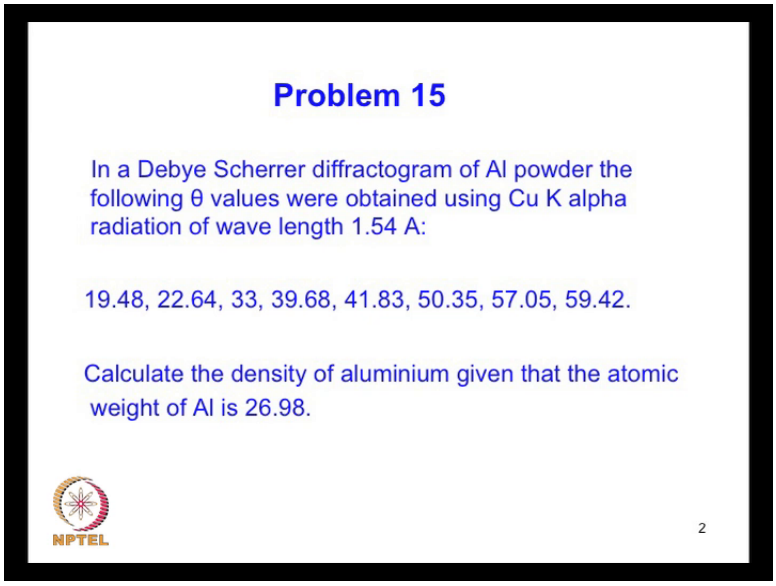

The next problem concerns the Debye Scherrer, we already discussed.

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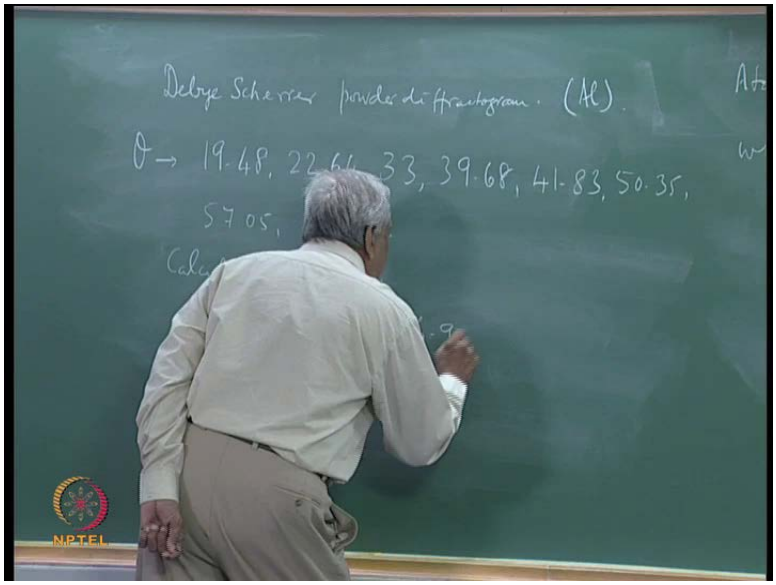

The next problem concerns the Debye Scherrer, we already discussed. The Debye Scherrer x-ray diffraction method, so powder diffractrogram of aluminum, aluminum powder. So we are given the various theta values obtained these are 19.48, 22.64 and 33., 33, 39.68, 41.83, and then 50.35, then 37.05, and 59.42– these are the theta values which were experimentally obtained. We ask to

calculate density, we are told that the atomic weight is 26.98. How do we go? This is the powder diffractogram, so in which we have the basic relationship, because aluminum has…

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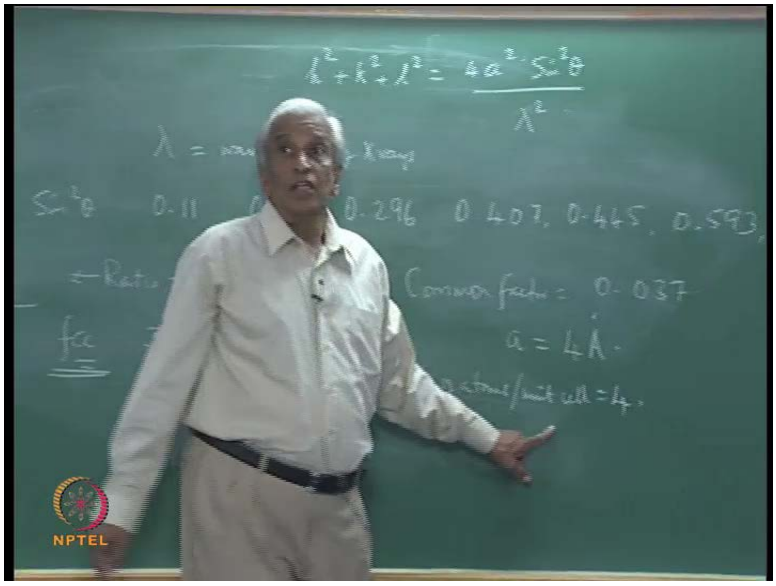

So I will first in the Bragg laws, we have to find sin square theta, and then we have the basic relationship for diffraction by a plane with miller indices h, k, l as h square plus k square plus l square is four a square sin square theta by lambda square, where lambda is the wavelength of x-rays. So from the theta values, we go to the sin square theta values, so the sin square theta values are as follows for these angles 0.11, 0.14, 0.296, 0.407, 0.445, 0.593, and 0.704, 0.74, so these are the sin square theta values. So obviously, we can look at the ratios, it is not the ratio is not 1 is to 2 is to three etcetera, obviously. So, we try the other one for an f c c structure, this is the value for a simple cubic structure and the body centered cubic structure. So it is neither simple cubic nor body centered cubic, so we try f c c - face centered cubic for which the ratio should be 3 is to 4 is to 8 is to 11 etcetera and that is the case. The case, so it is a face centered cubic structure.

So this is the first information we get from the given theta values. The common factor for all these, if I take the common factor, it is 0.137. Because if I divide 0.11 by 3, 0.14 by… 4 etcetera. So that is equal to that is given by the common factors here, so four a square by lambda square.

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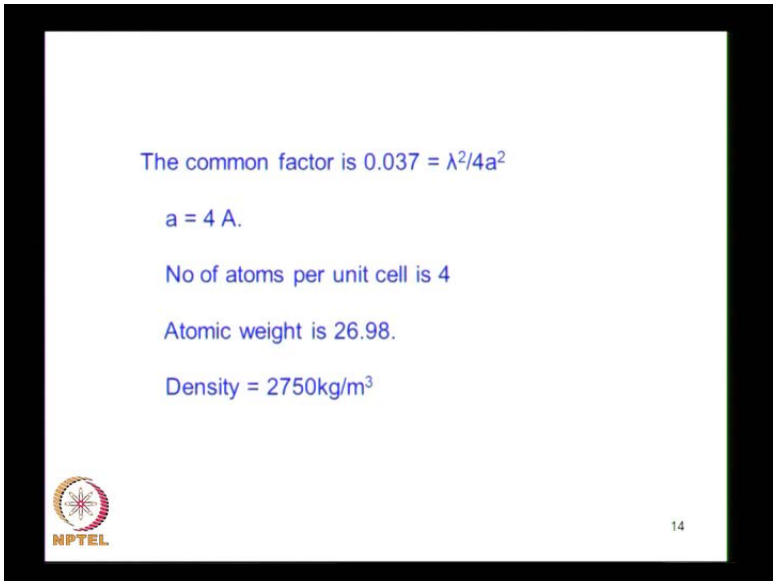

And therefore, from that knowing the wavelength here of the x-rays, we can arrive at a value for a, which turns out to be 4 Angstrom. And since it is a face centered cubic structure, number of atoms in the unit cell is 4. And since we are given the atomic weight here, we know the mass of each atom, and now we know that there are 4 atoms in the unit cell, so we know the mass of the all the atoms in the unit cell. And we have the volume of the unit cell which is simply a cube, therefore the density is got which is required answer it turns out to be 2750 –2750 kilogram per meter cube. So this is how knowing the atomic parameters, the lattice constant and the type of structure, we can calculate the theoretical density of any given material.

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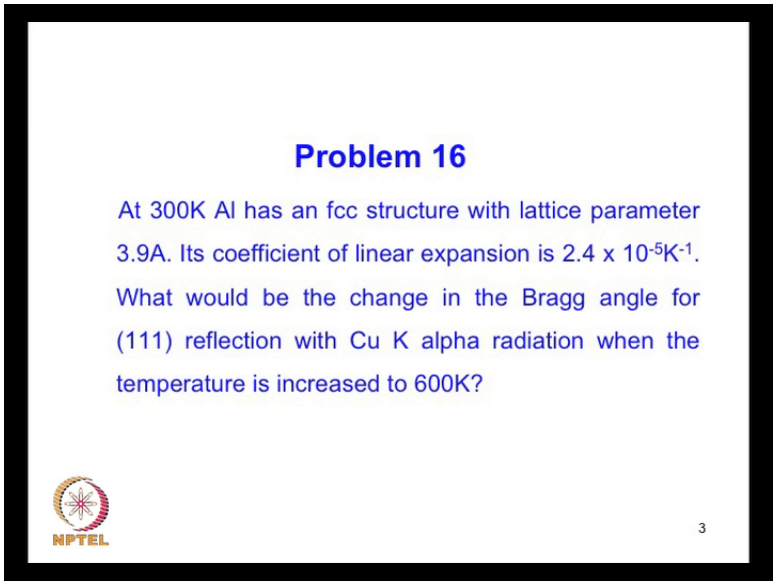

The next question is also about aluminum, which has we have seen as the f c c structure with lattice parameter, which in this problem is given a three point Angstrom at three hundred k. So the coefficient of linear expansion is also given. Therefore, we are ask to calculate the change in the Bragg angle.

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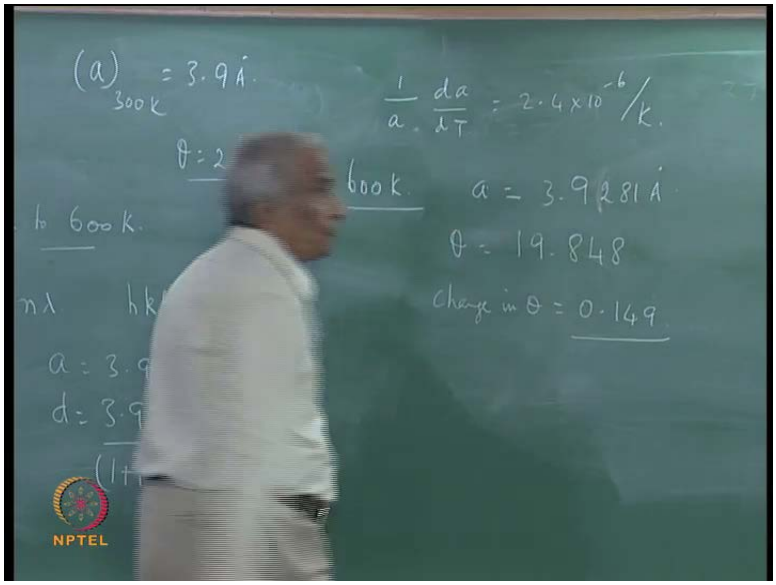

So the problem is to calculate the change in the Bragg angle theta for 1 1 1 reflection, when we have irradiation from copper k alpha radiation. And the temperature is increased, increase from

300 k to 600 k. So the powder is warmed up. So the lattice constant to start with is given to be 3.9 Angstrom. So how do we do this?

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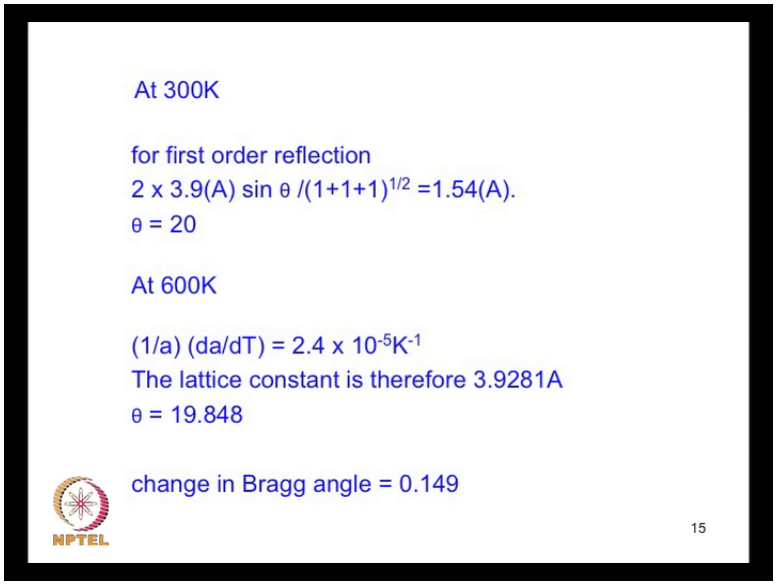

Again we go by the same procedure using the starting from the Bragg reflection condition which gives me 2 d sin theta equal to n lambda, for first order n is 1. And d for, d h k l and h k l is given to be 1 1 1. So the corresponding from the lattice constant which is given as 3.9 Angstroms, so we can calculate d 3.9 into by 1 plus 1 plus 1 h square plus k square plus l square to the power half, so 3.9 by root three in Angstroms. So substituting the values, we get the theta as 20 degree from the given values at 300 k.

Now we are also given the coefficient of expansion – thermal expansion, so the lattice constant a changes and the thermal expansion coefficient is defined as 1 by a d a by d T and that is given as 2.4 into 10 to the power minus 6 per k. Therefore the new lattice constant at 600 k lattice constant will go to, using this value, we get 3.4.94, 9281 Angstrom. Therefore, the corresponding theta calculated in the same way turns out to be 19.848. Therefore, the change in Bragg angle, change is 0.149.