Condensed Matter Physics
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Lecture – 38
Point Defects in Solids – Worked Examples

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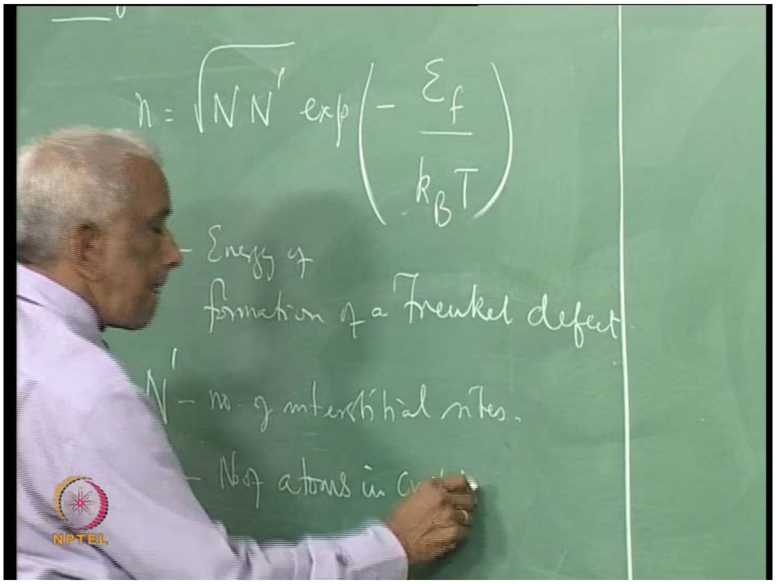

Today we are going to work some problems on the topic of point defects in solids.

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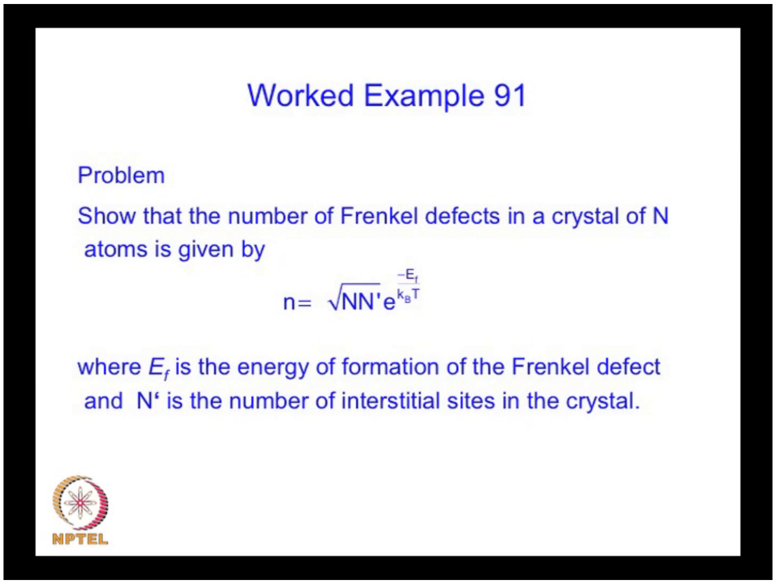

The first problem, we are required to show that the number of Frenkel defects in a crystal of N atoms is given by… this is root of… Here E f is the energy of formation of a Frenkel defect, and N prime is the number of interstitial sites while N is the number of atoms in crystal.

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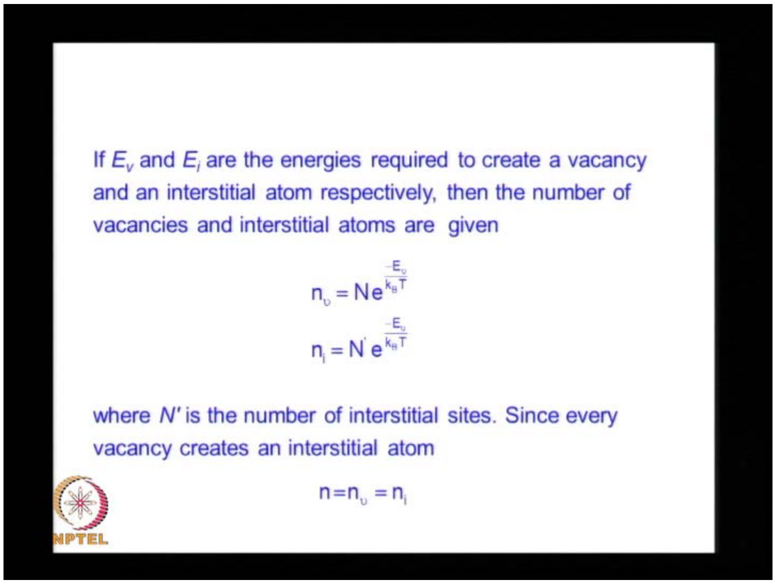

We do this by writing the energy for the formation of a vacancy.

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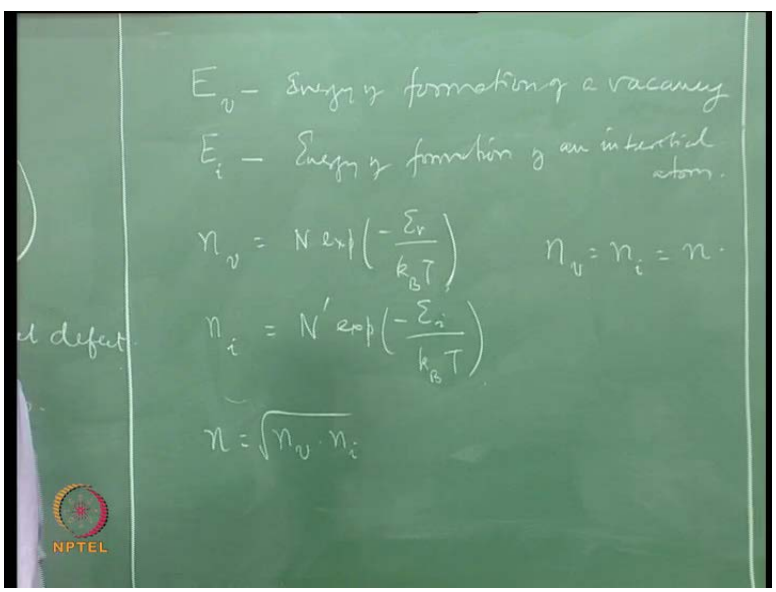

And E i is the energy of formation of an interstitial atom. Once these are given, the number of vacancy as we have already seen is just N exponential minus e v by k B T; and by the similar argument, the number of interstitial is N prime exponential minus e i by k B T. And by definition the number of vacancies and the number of interstitial should be equal, so let us call it n.

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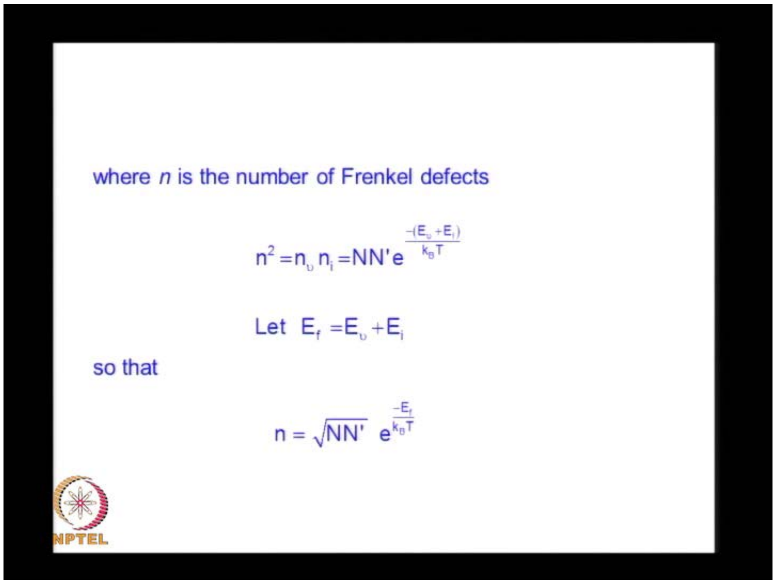

So that n – the number of Frenkel defects is just n v times n i square root. So this will be N, N prime square root is exponential minus e v plus e i by k B T.

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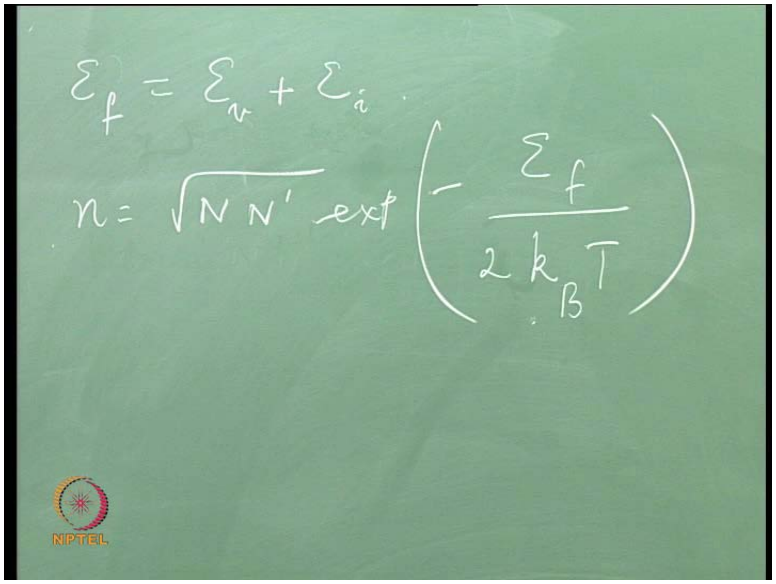

So we define the Frenkel energy for the formation of a Frenkel defects as sum of the energy required for forming a vacancy and the energy required for forming a interstitial atom. So defining like this, we get the result…

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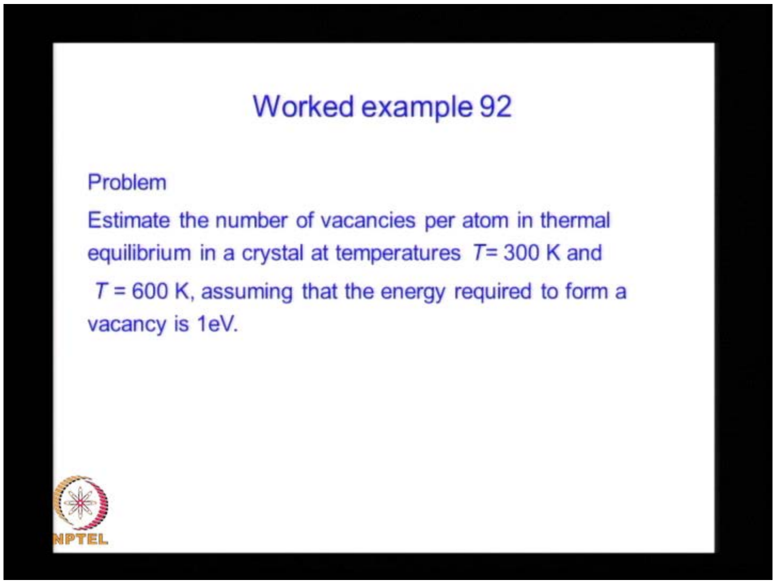

Next, we required to estimate the number of vacancies per atom in thermal equilibrium at temperatures T equal to 300 K.

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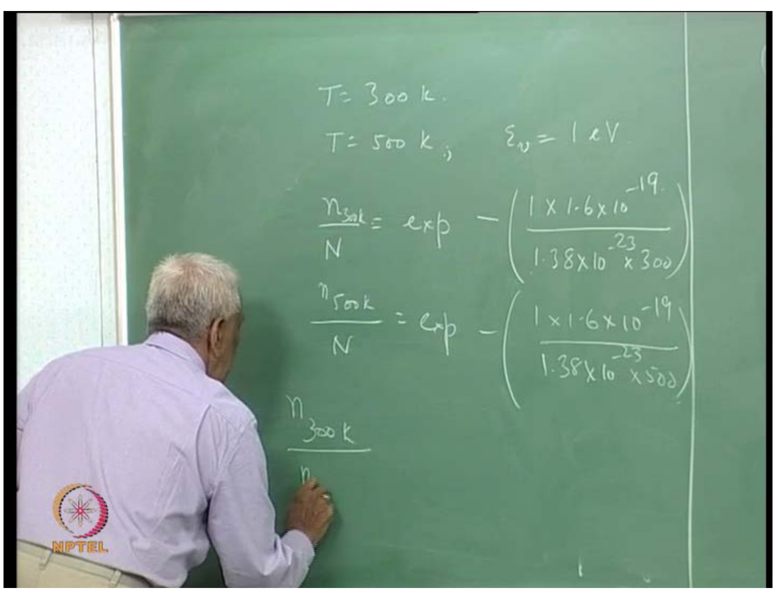

And T equal to 500 K if the activation energy, the energy for the formation of a vacancy is one electron volt.

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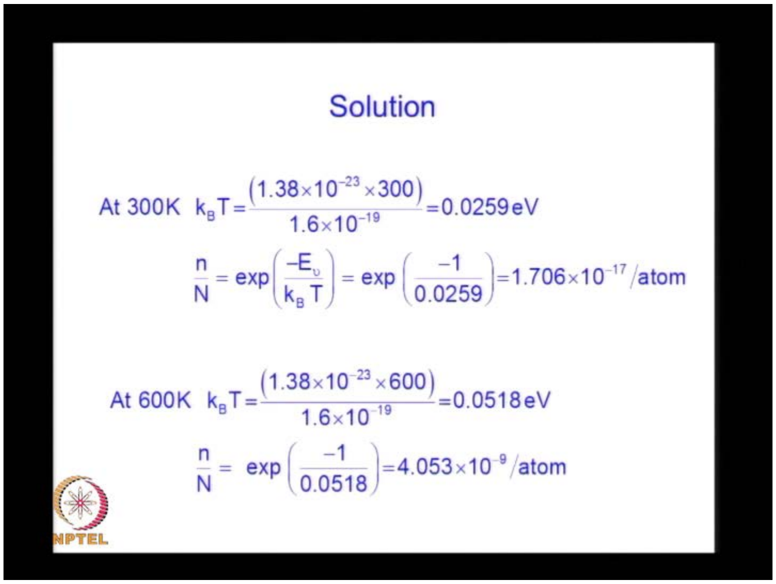

So it is a simple substitutional problem, so we have n by N – the number of vacancies by the number of atoms is just exponential minus 1 electron volt which is 1.6 into 10 to the power minus 19 by k B T which is 1.38 into 10 to the power minus 23 into 300 at 300 K. Similarly, n 500 K by N is exponential minus 1 electron volt, which is 1.6 into 10 to the power minus 19 by 1.38 into 10 to the power minus 23 into 500. So the ratio n 300 K by n 500 K, no we are ask to find these at 600 K, so this is also 600.

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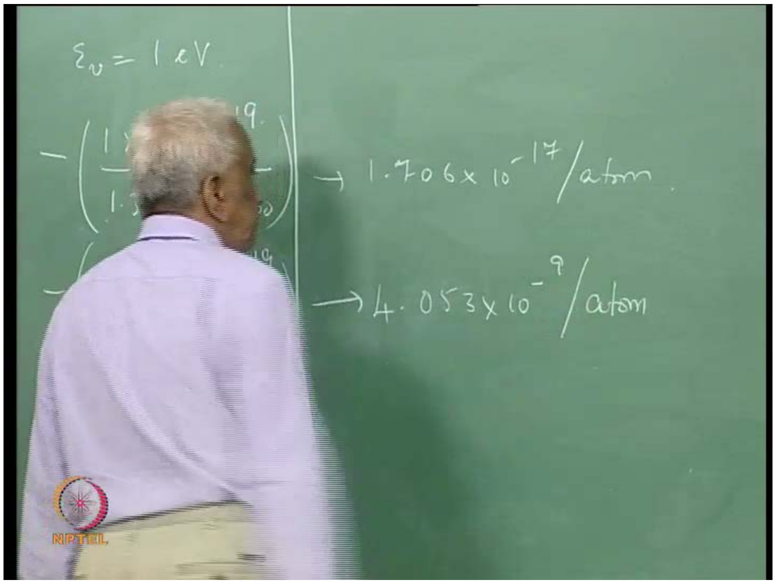

So it is simply a question of a finding this, so you get 1.706 10 to the power 17 per atom, and this works out to be 4.053 into 10 to the power minus 9 per atom. So by just heating it to 600 k from 300 k, you get an enhancement of the vacancy concentration by 8 orders of magnitude.

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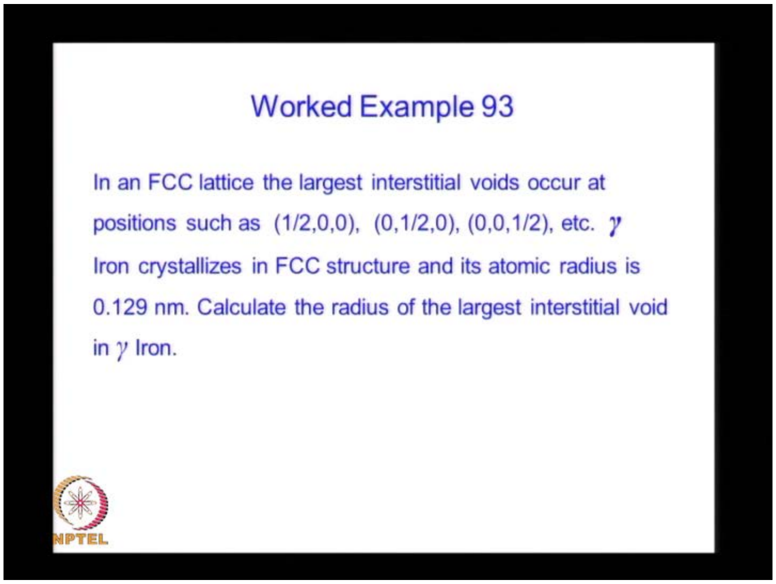

So, this is a very remarkable result. Next, we move on to consider, an FCC lattice in which the largest interstitial voids occur at positions.

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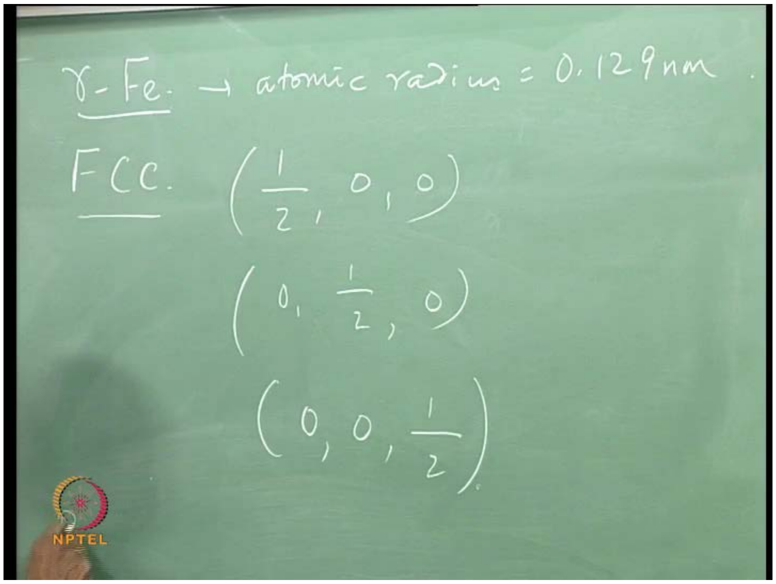

Such as half, 0, 0, these are the coordinates; 0, half, 0, and 0, 0, half centers and the edges. And this is the structure of gamma iron, which has an atomic radius of 0.129 nano meters. So we are ask to find the large radius, the largest interstitial voids the radius of… that is the question.

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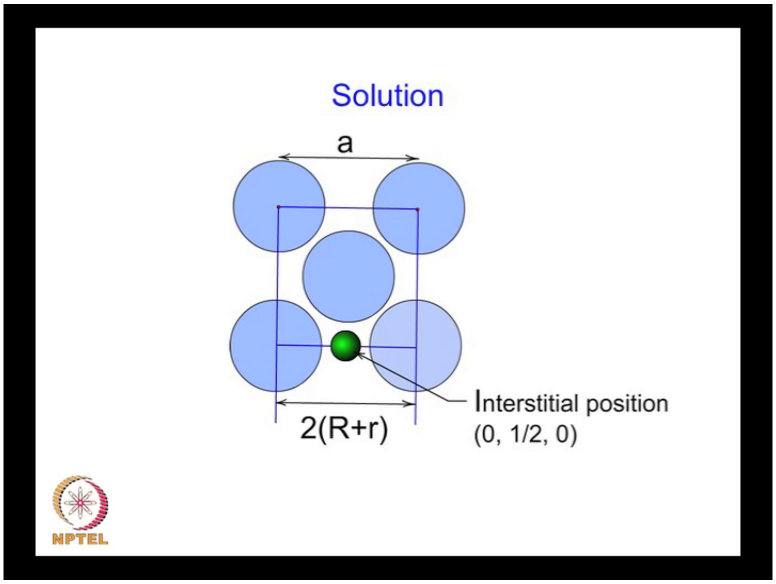

So to do this, again we are given the sides, so the figure shows how it is. You got the square phase and the interstitial position occurs at the center of the cube edge and if the radius of these the interstitial atoms is r - small r and the radius of the iron atom is capital R then.

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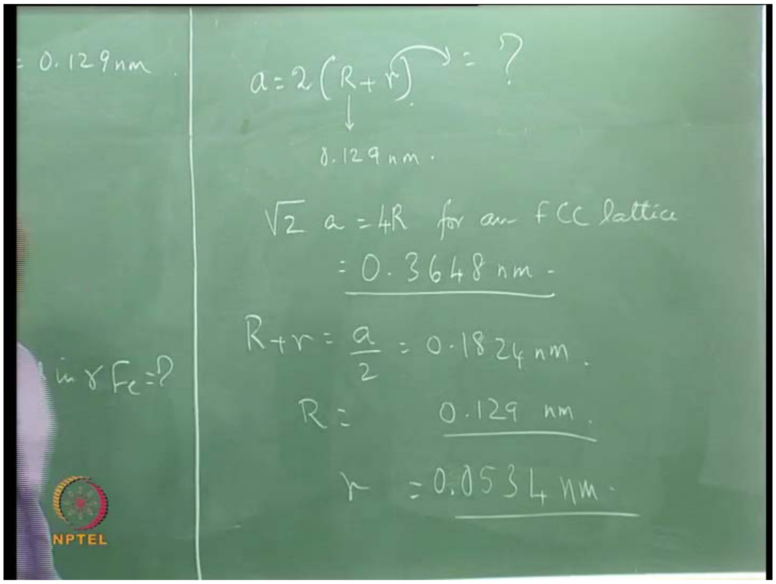

The distance is the side of the cube is 2 into R plus r.

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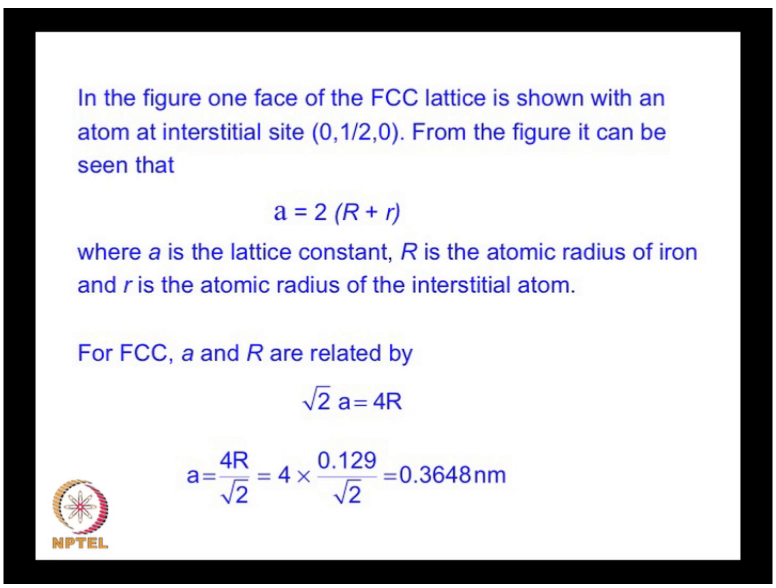

So that is the lattice constant. And R is the atomic radius given as the 0.129 nano meters. And we are ask to find this. Now a and R are related by root 2 a equal to for an FCC values – the face centered lattice, so that means so a will be 0.3648, so that is the lattice constant.

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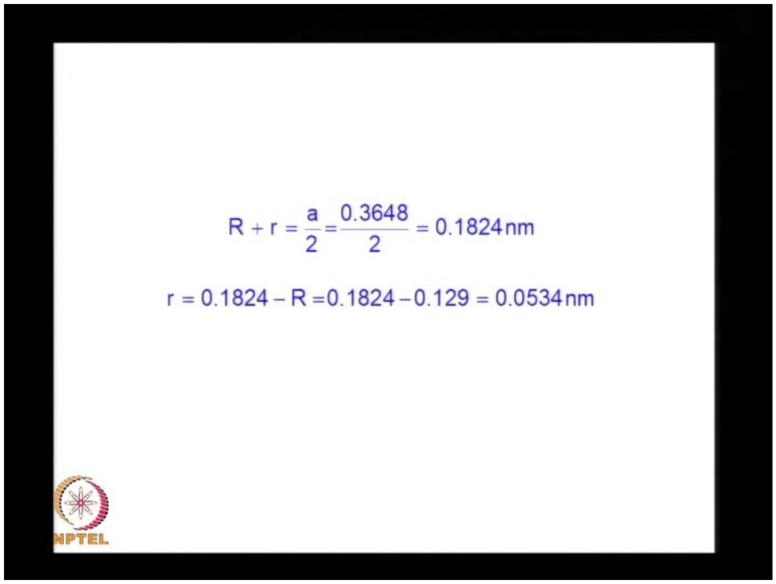

And R plus r is simply a by 2, which is naught 0.1824, and R is 0.129. Therefore, r is difference between these two that is the radius of the largest interstitial.

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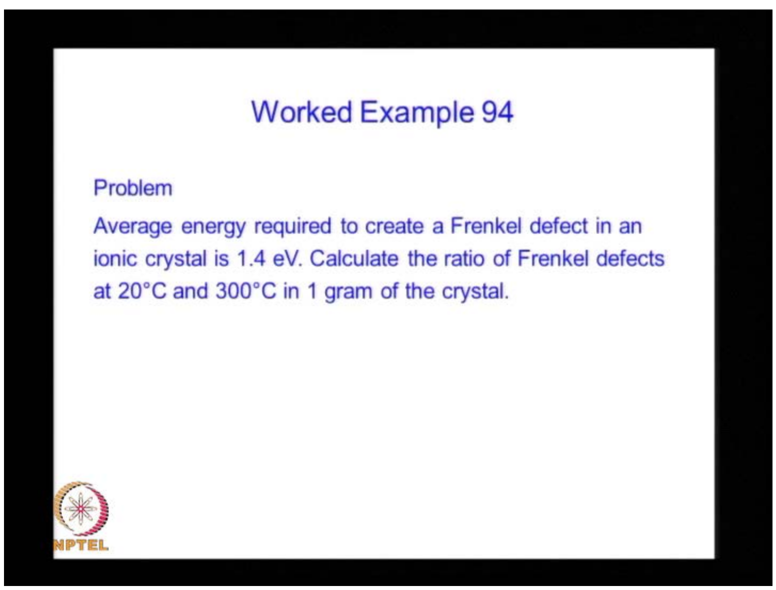

Next we are told that the average energy required to create a Frenkel defect is given to be 1.4 electron volt in ironic crystal.

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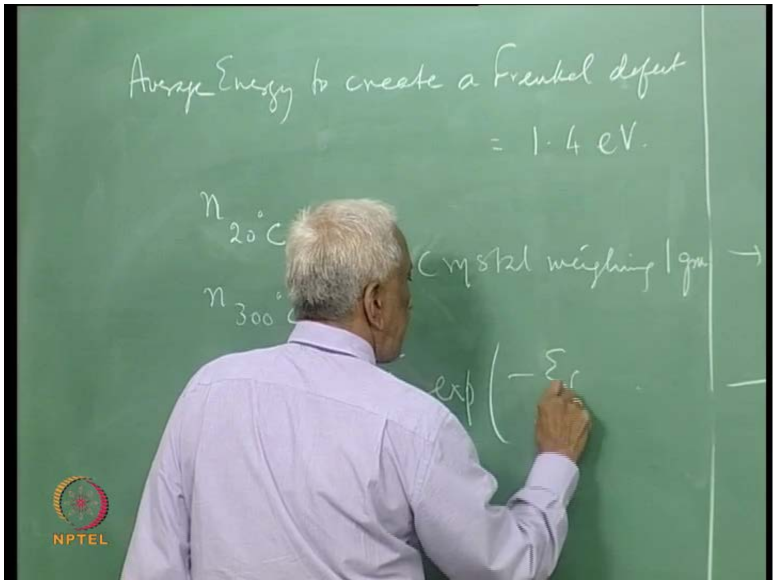

So we are ask to calculate the ratio of Frenkel defects at 20 Celsius and 300 Celsius, in a crystal being one gram. So we know the expression for the number of Frenkel defects, we have already done this.

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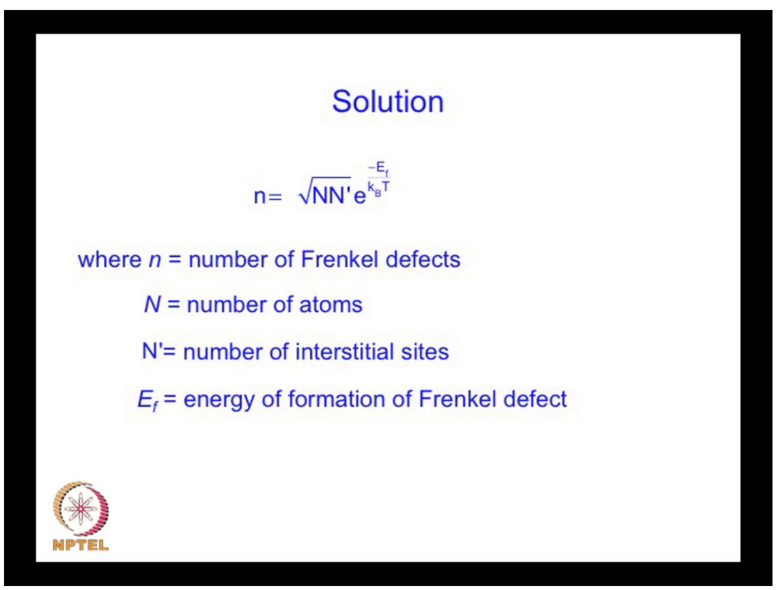

Where E f is 1.4, N is the number of atoms, and we just take the ratio.

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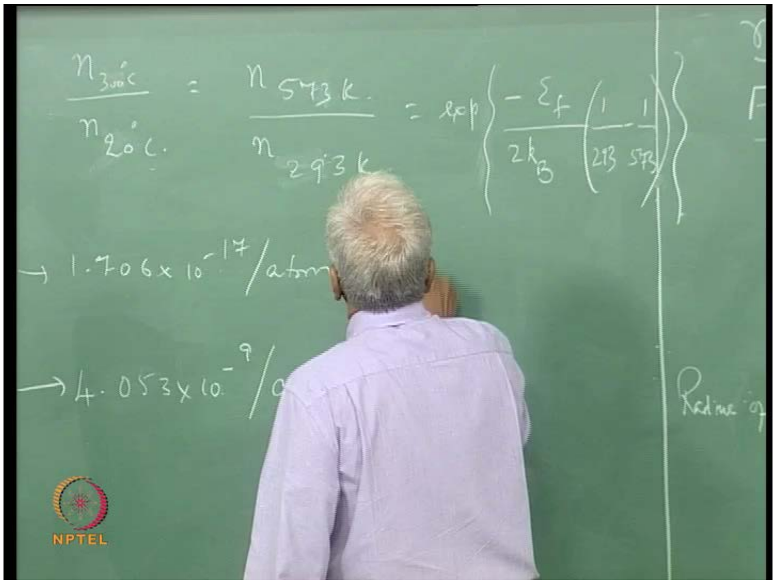

So n 20 Celsius by n 300 Celsius. So that is the same as 293 K and this is 573 K.

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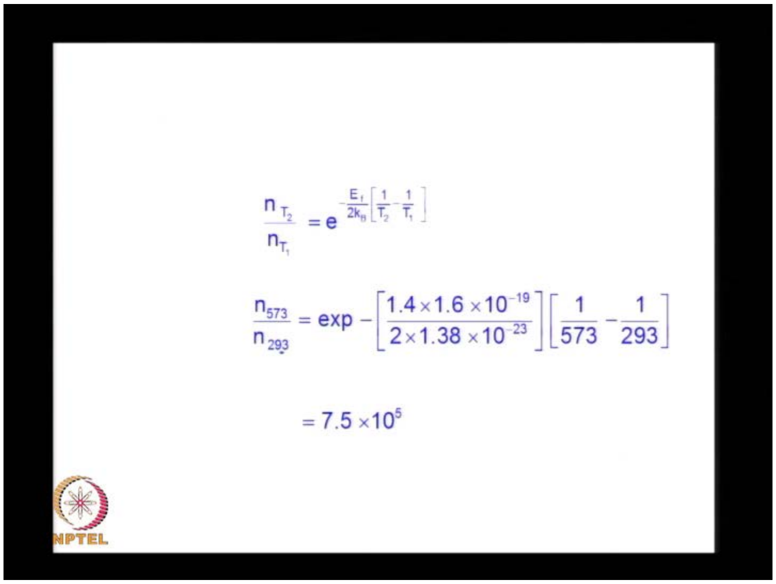

So the ratio will be N and prime will cancel, so you will have exponential minus E f by 2 k B into 1 by 293 that is works out well it is the other way about it may write 300 k and 20 here. So this becomes 573 and this becomes 293, so that this will be this ratio works out to be 7.5 into 10 to the power 5. So the number of Frenkel defects by simply heating it from 20 Celsius to 300 Celsius increases by 5 orders of magnitude.

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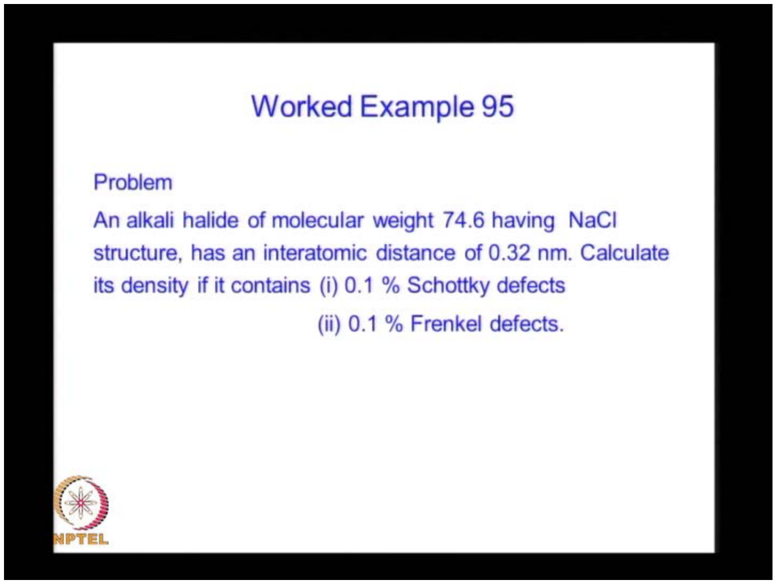

Next we are told that an alkali halide.

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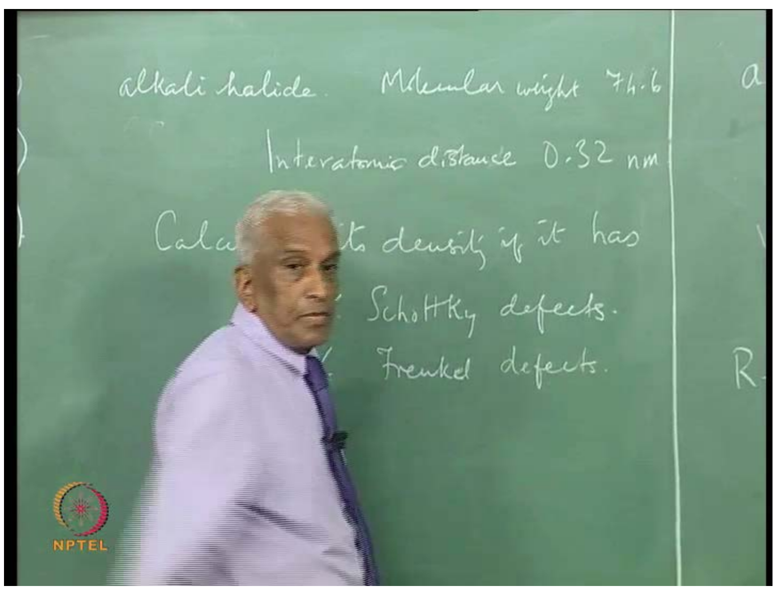

Such as a sodium chloride has a molecular weight of 74.6, inter atomic distance is given to be 0.32 nano meter. So we are ask to calculate density if it has 0.1 percent Schottky defect or 0.1 percent Frenkel defect. So the presence of defects of Schottky or Frenkel both will change the density of the crystal.

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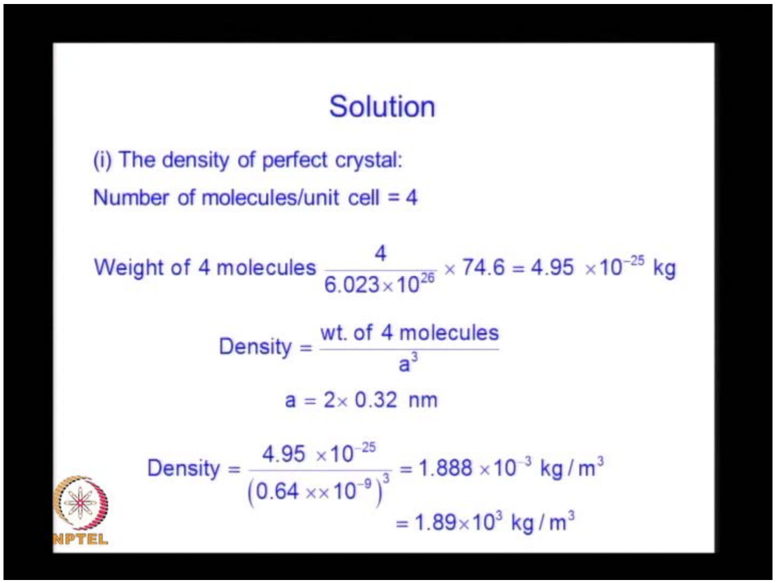

So we are ask to find this. Now in order to know this, we first calculate the density of the perfect crystal in the usual way.

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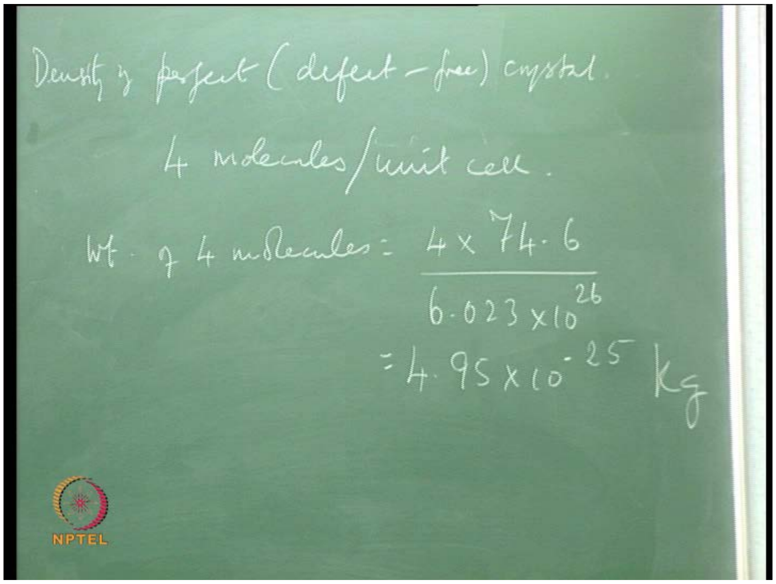

Perfect means defect free for which we are given the molecular weight and this is the sodium chloride structure, so the number of molecules per unit cell is 4. So the weight of 4 molecules which occupy the unit cell is 4 times 74.6 divided by… That is works out to be 4.95 into 10 to the power minus 25 kilograms.

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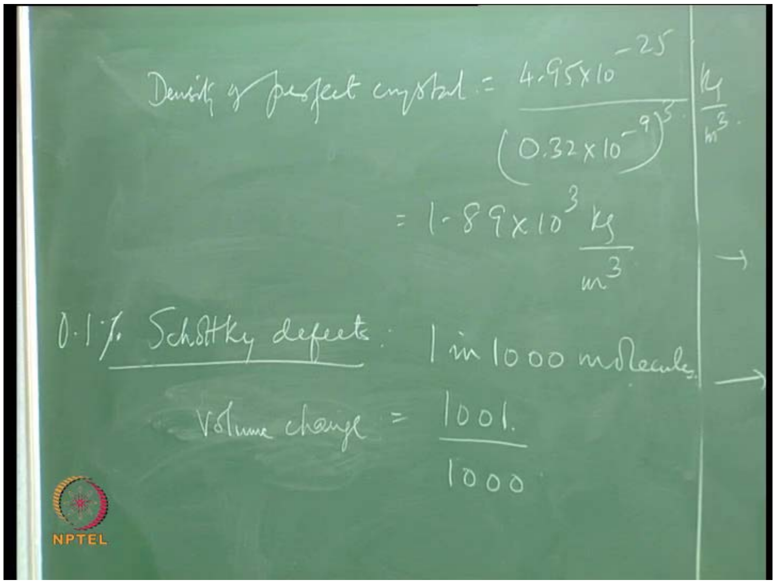

So this is the density and volume of the unit cell is just a cube, where a is given to be, so the density of the perfect crystal is just ratio of these two and that will be 1.89.

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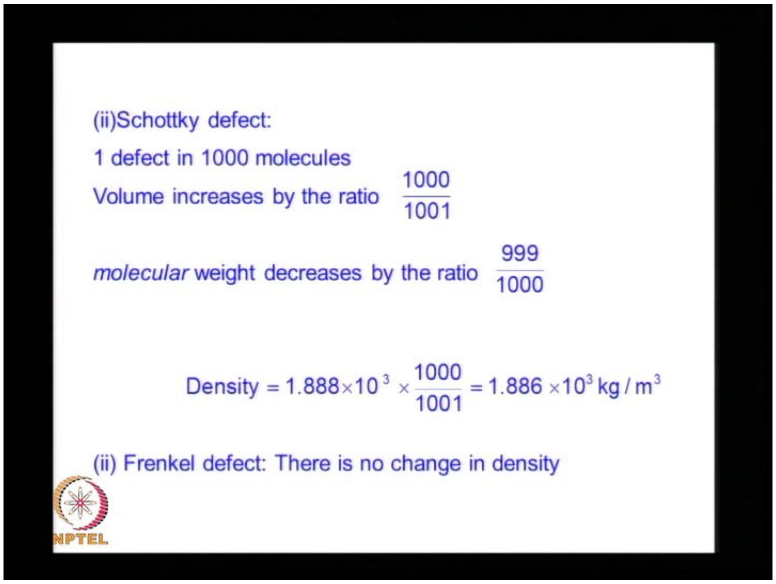

Now if we have Schottky defect 1 percent then what happens, you have 0.1 percent. Yes, so this is 1 in 1000 molecules, so the number of Schottky defect is just the number of molecules divided by 1000.

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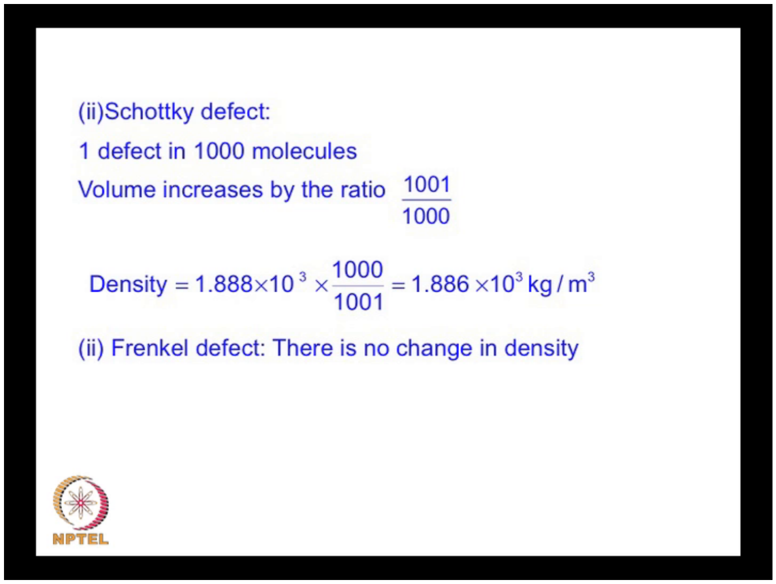

And therefore, the volume change, we are interested in the density change, so volume. So if I have 1000 molecules, now the volume due to the Schottky defect increases by the factor 1001 by 1000, because there is one Schottky defect. Whereas, in the case of Frenkel defect, since it is a vacancy plus an interstitial, therefore, whatever be the concentration, there is no change in density. And in this case, since the volume changes by this, decreases by a factor.

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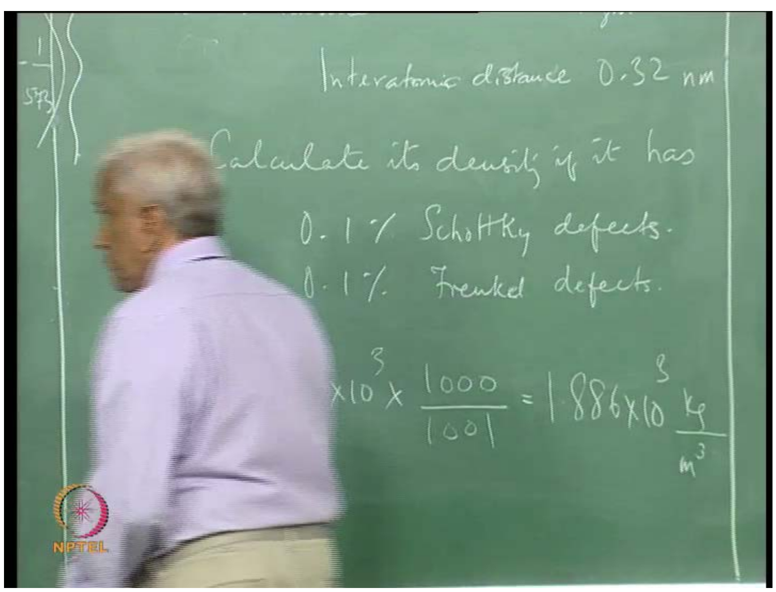

Therefore the density is, go the density there 1.89 into 10 to the power 3 into this factor 1000 by 1001, and that would be 1.886…

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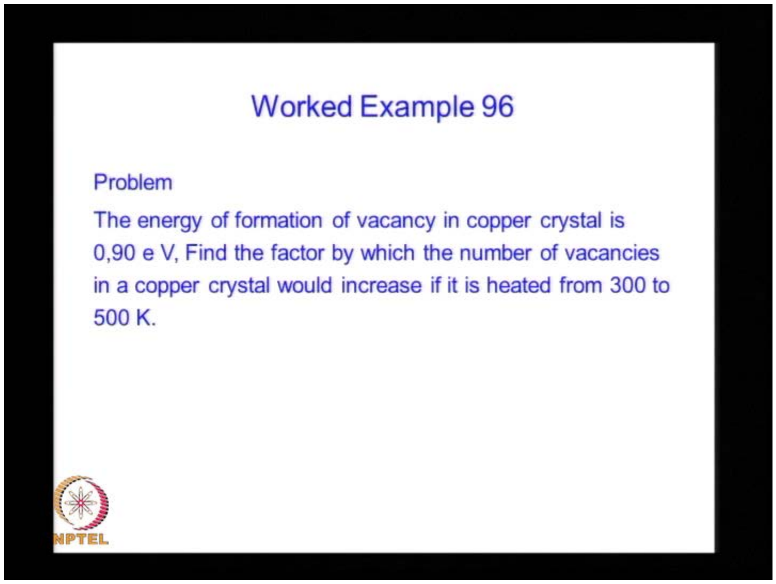

Next we are told the crystal of copper.

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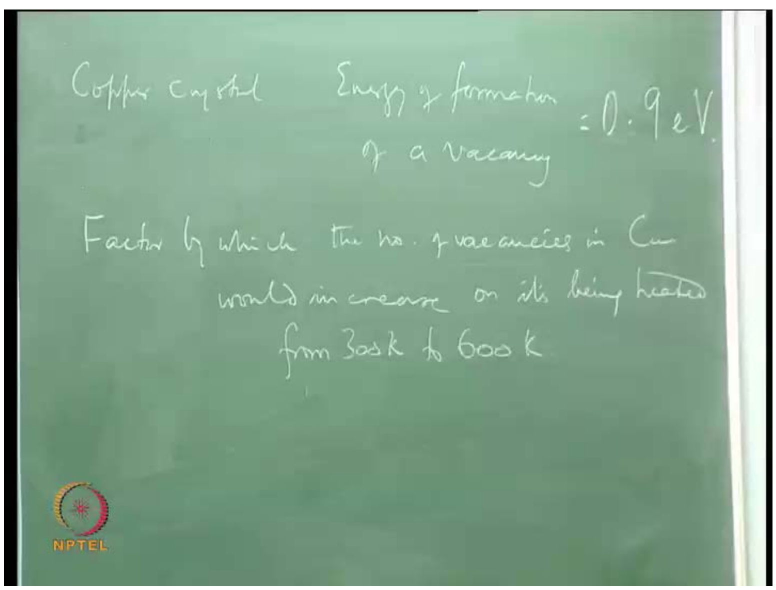

In which the energy of formation of a vacancy is given to be 0.9 electron volts. Find the factor by which the number of vacancies in copper would increase if it is heated from 300 300 K to 600 K, again relatively a straightforward, question to answer.

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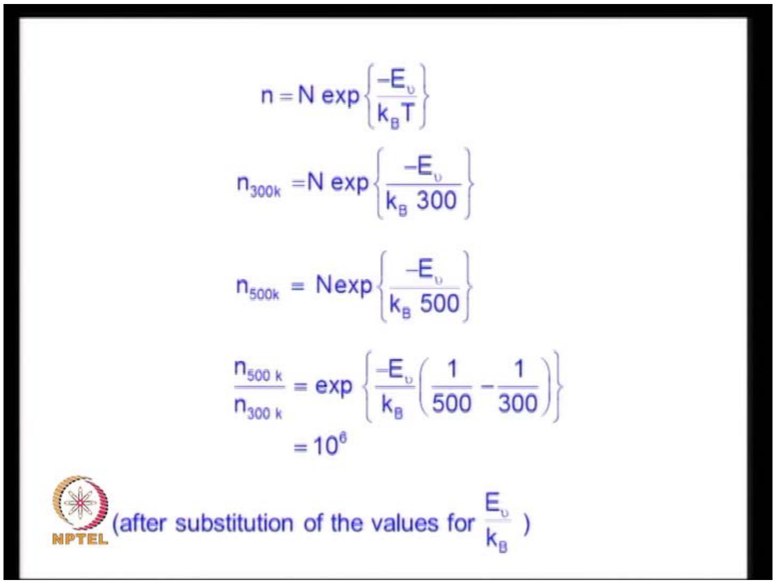

Use this standard expression, the number of vacancies.

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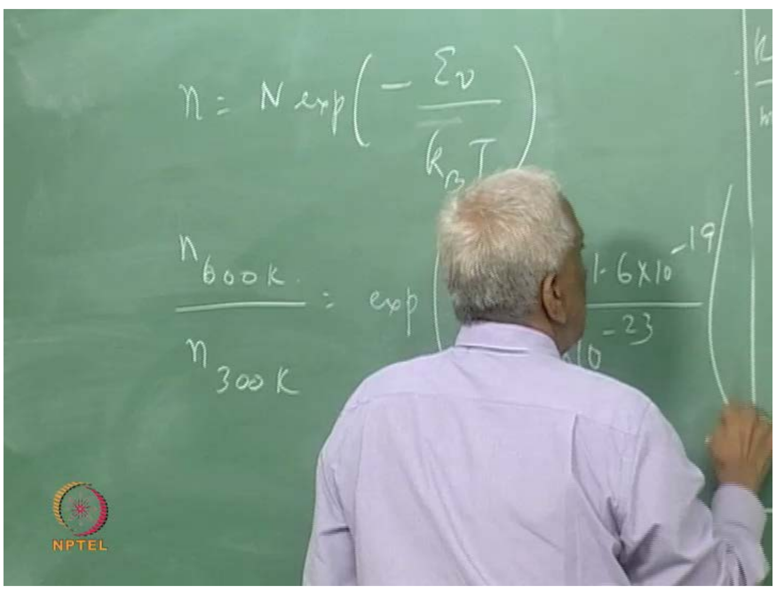

So we have n 600 K by n 300 K. That will be the ratio will simply the exponential minus 0.91.6 into 10 to the power minus 19 by 1.38 into 10 to the power minus 23 into 1 by… So if you calculate this that works out to be 10 to the power 6.

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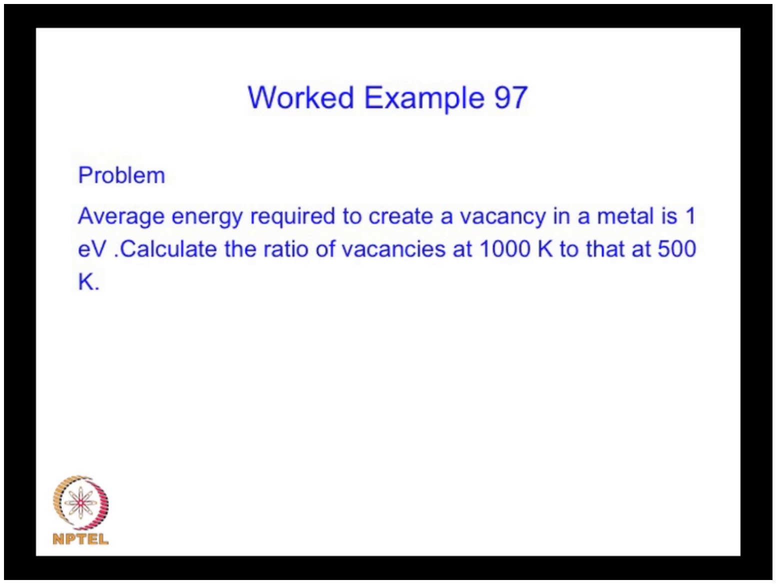

We are told that in a metal the average energy.

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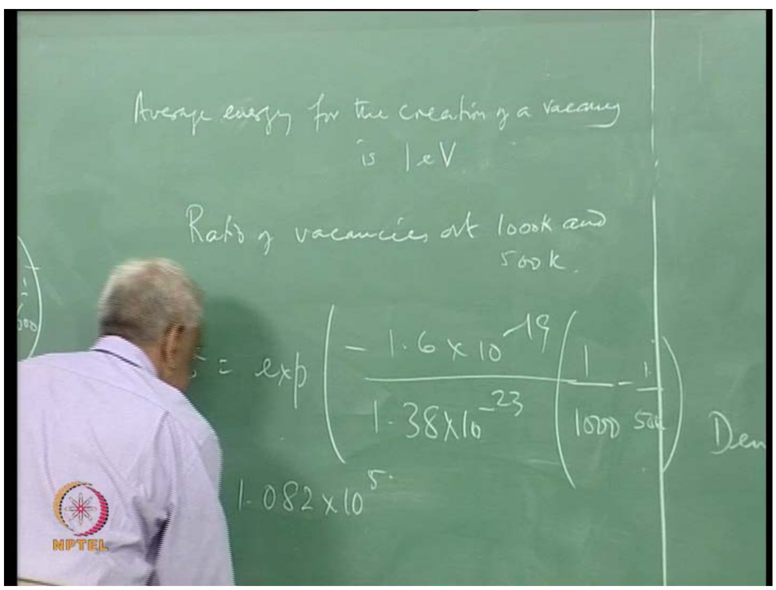

Needed for the creation of a vacancy in a metal is one electron volt. So calculate the ratio of vacancies at 1000 k and 500 K. Again a very simple question, n 1000 K by n 500 K is exponential minus… That is again comes to 1.082 into 10 to the power 5. These are all just to give you an order of magnitude idea about the relative concentration of vacancies and other defects when one heats the metal as we go to higher temperature.

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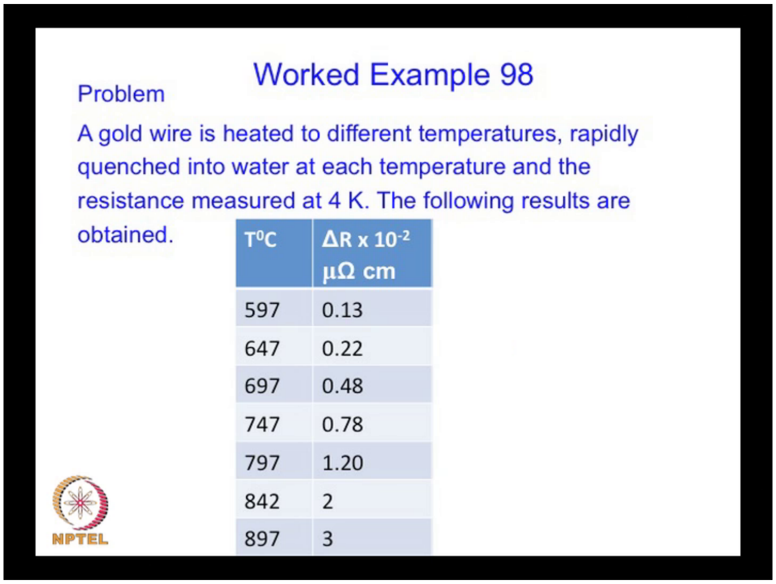

Next we have data concerning a resistance.

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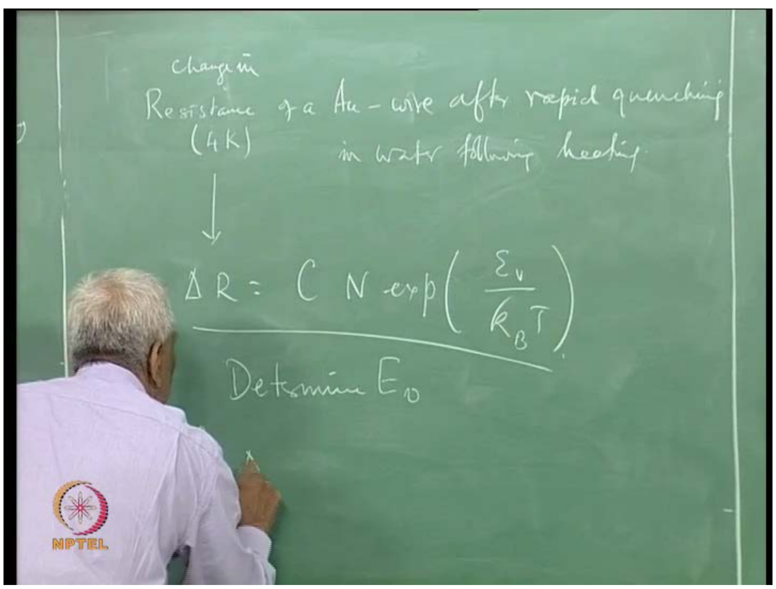

The change in resistance of a gold wire is given at different temperature, the gold wire is heated to different temperature and then rapidly quenched into water at each temperature and the resistance is measured at four K, after rapid quenching in water following heating. So the temperatures to which, there heated are all given in tabular form.

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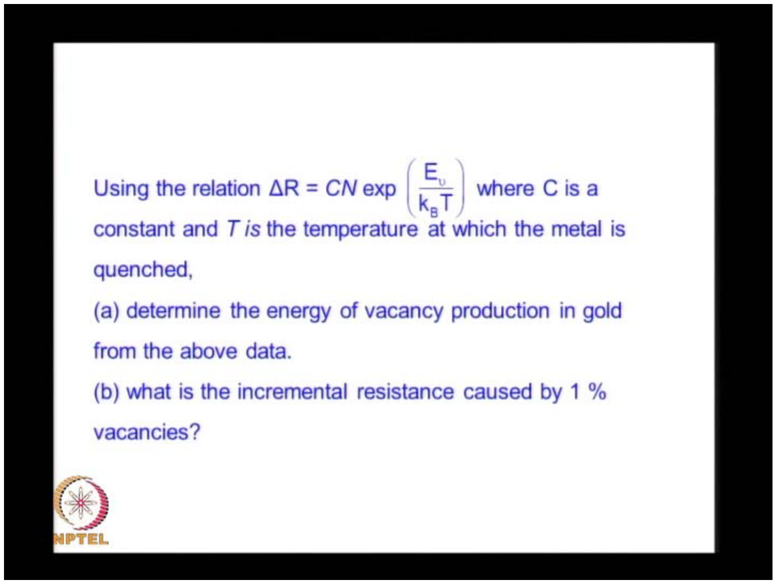

And we are given the relation delta R, the change in resistance is some constant C times N exponential minus E v. C is a constant and T is the temperature at which, to which it is heated. So we are ask to determine the energy of vacancy production, determine E v. In order to do that from this relation we can that log delta R is log C plus log N plus E v by k B T.

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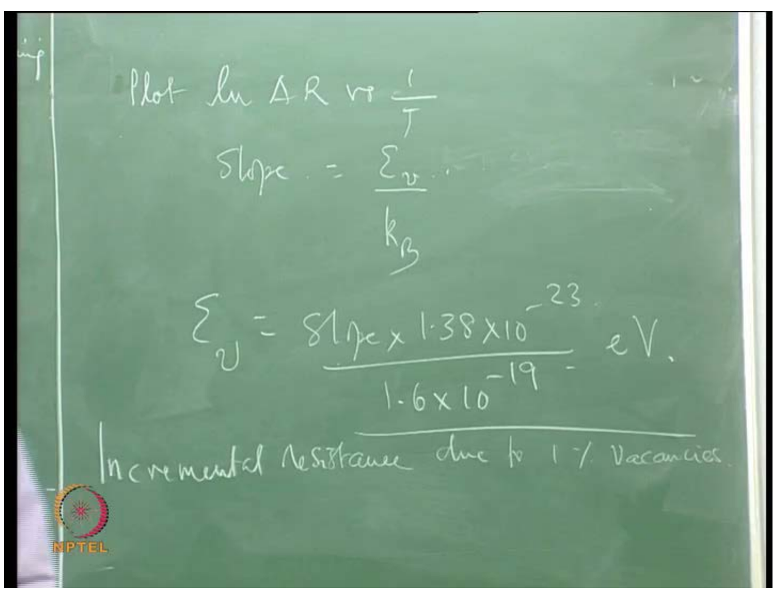

So if one plots log delta R from the given data as the function of versus one by T. The slope gives the energy of the vacancy.

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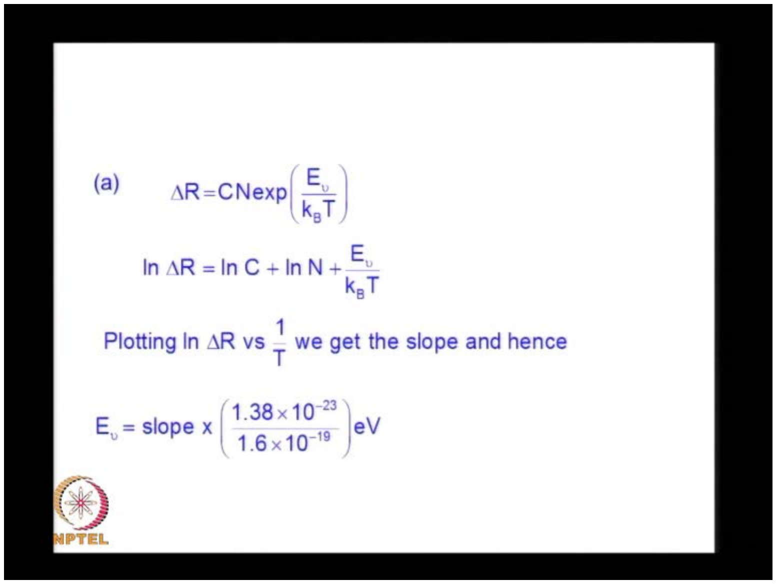

So this is the slope, so E v will be slope times the Boltzmann constant and if you want to find it in electron volt divide by 10 to the power minus 19, that would give it in… Since this involves plotting this is simply given as a expression, one can do this and see. And we are also ask to calculate the incremental resistance caused by 1 percent vacancies.

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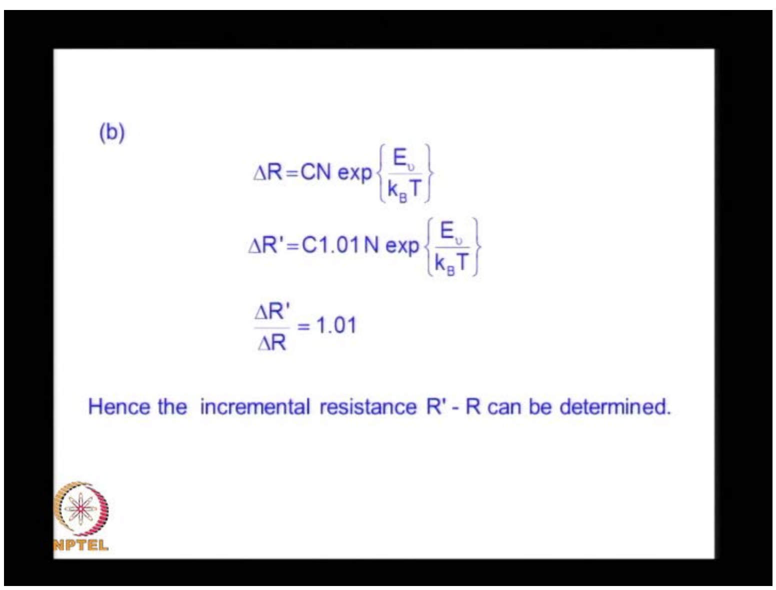

Again one uses the data, and find delta R from this data, so it will be 1 percent increase in vacancy.

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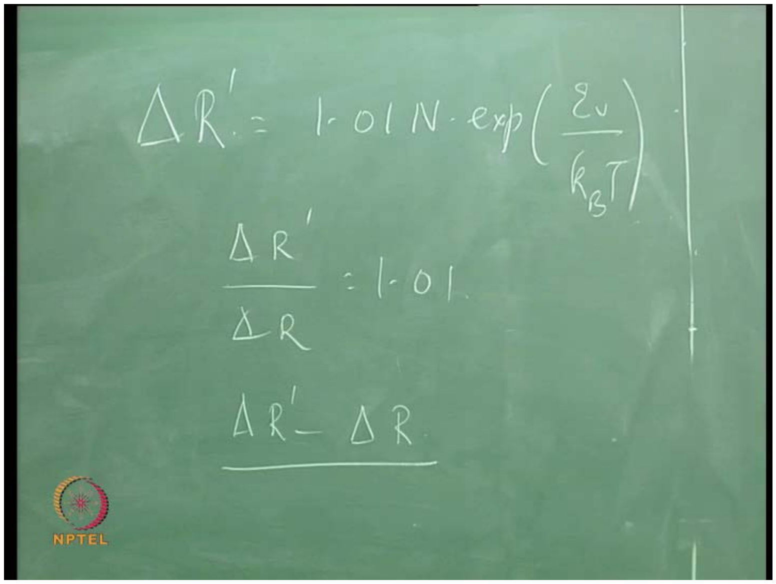

So 1.01 N exponential, so that is out modified. So this is delta R prime, so delta R prime by delta R just 1 point naught one. So one can find the delta R prime minus delta R, that is the incremental resistance.

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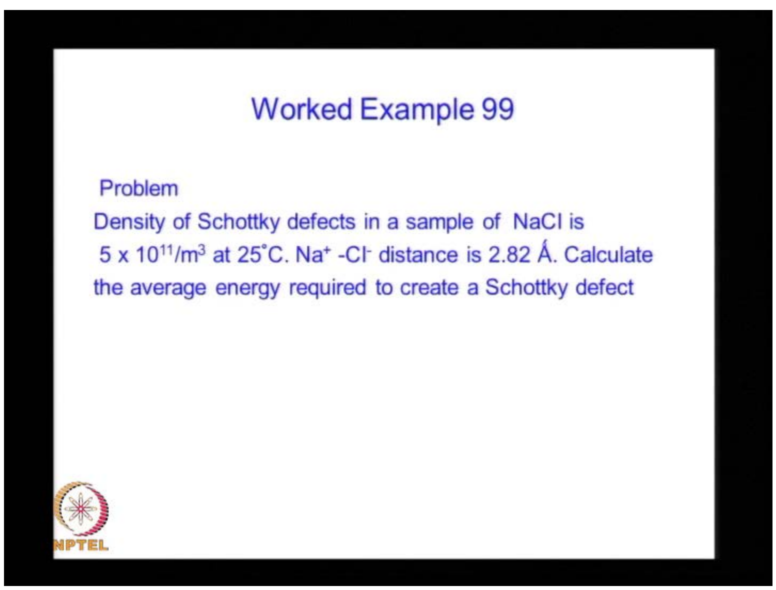

The last problem concern, the density of Schottky defects.

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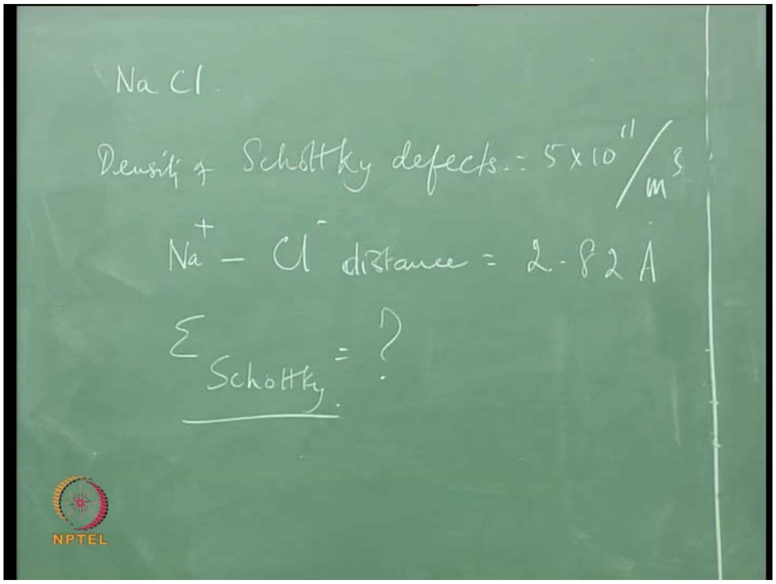

Which is given in a sample of sodium chloride, density means concentration that is given as 5 into 10 to the power 11 per meter cube. And the distance of the sodium plus to the chlorine minus iron distance, the sodium chloride is also given to be 2.82 angstrom unit. So we are ask to calculate the average energy for the creation of Schottky defect that is the question.

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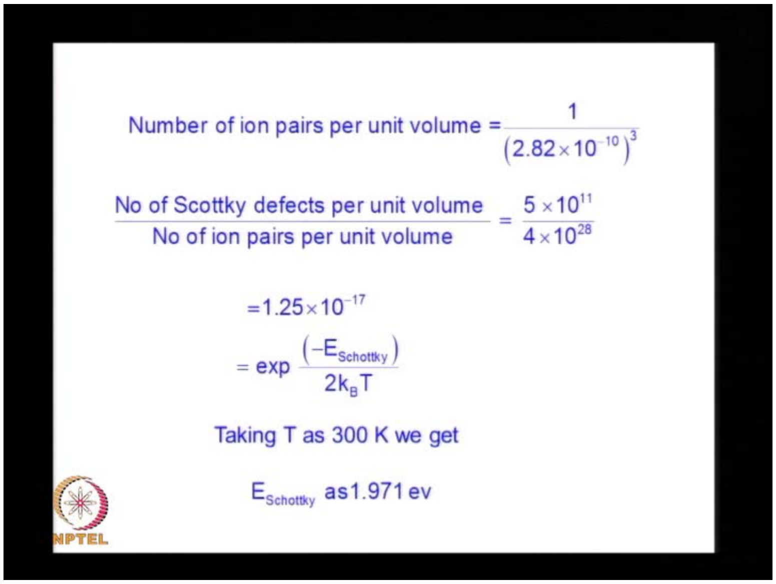

So in order to do this, since see Schottky defect involves vacancies in both the anion and cation sites simultaneously, so we must find the number of iron pairs in the given data.

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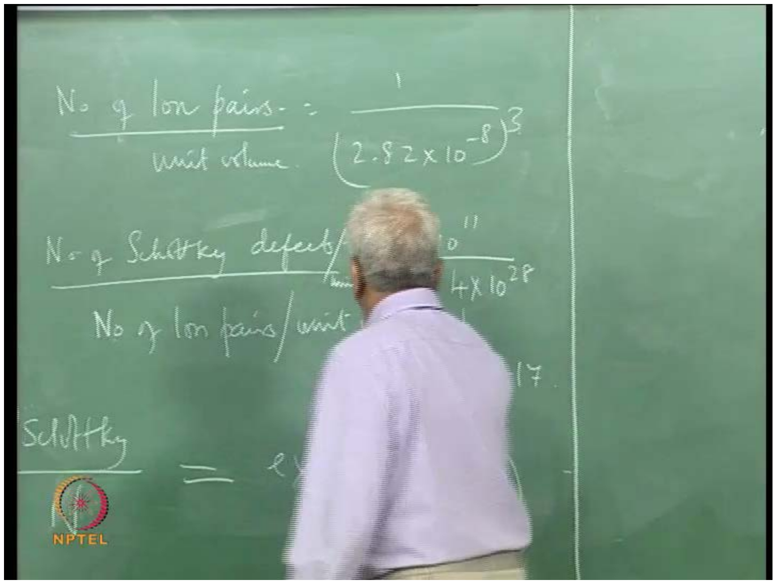

So that will be 1 by 2.82 into 10 to the power minus 8 cube, that is the lattice volume per unit volume. And number of Schottky defects, in order to calculate this, we have 5 into 10 to the power 11 is given. So that divided by the number of ion pairs both per unit volume. We take the ratio of these 2 this works out to be 4 into 10 to the power 28, so that will give me 1.25 into 10 to power minus 17. And that is the ratio of N by and that is given to be exponential minus E Schottky by 2 k B T. So since this is known to be equal to this.

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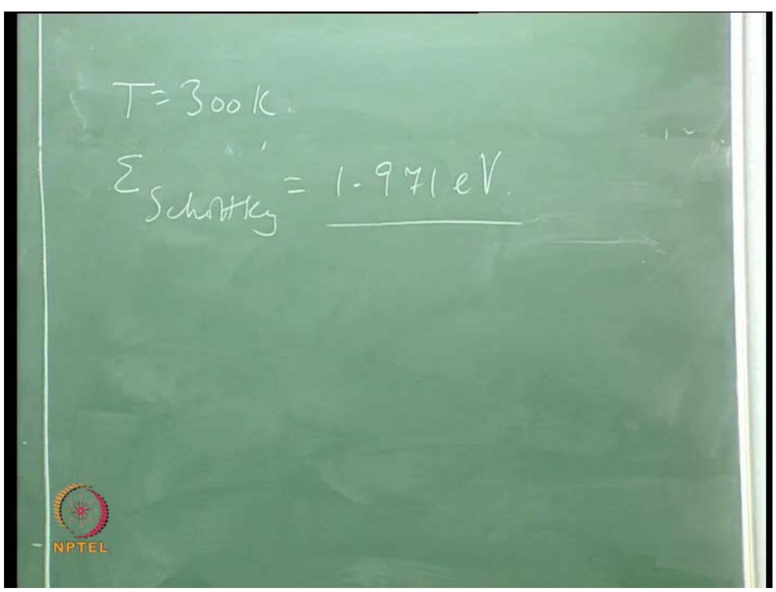

Therefore, we can the temperature as 300 K and get the energy of Schottky pair as 1.971 electron volts.