Crystals, Symmetry and Tensors
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Lecture 6d
Volume of a Crystallographic Unit Cell

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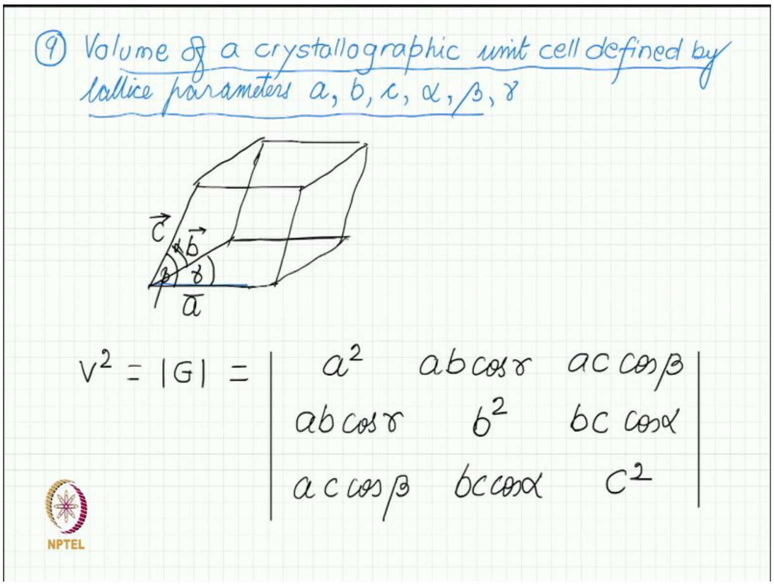

Now, Volume of a Crystallographic Unit Cell defined by lattice parameter, let us look at this. How do you find this volume, because this looks like a complicated formula, although simple means there is not much advanced mathematics in it, but still, you have six lattice parameters means three distances and three angles. And so, the final volume will be a function of all these three quantities.

So, the parallel pipette which you will form out of a, b and c with an angle of gamma, beta and alpha. So, what is this volume, many times you require this volume for your calculation. We can use some of the relationship which we have derived to find this volume one of that is that v square is nothing but determinant of G the metric tensor and metric tensor is easily written in terms of a square, because a dot a, then a dot b ab cos gamma by symmetry ab cos gamma comes here also b dot a then a dot c is ac cos beta by symmetry it again comes here also.

Then, this is b dot b b square b dot c, bc cos alpha and bc cos alpha by symmetry and finally, this is c square. So, all you have to do however complicated it may appear, but finally, all you have to do is to find the determinant of this matrix and you have a formula for a general unit cell volume.

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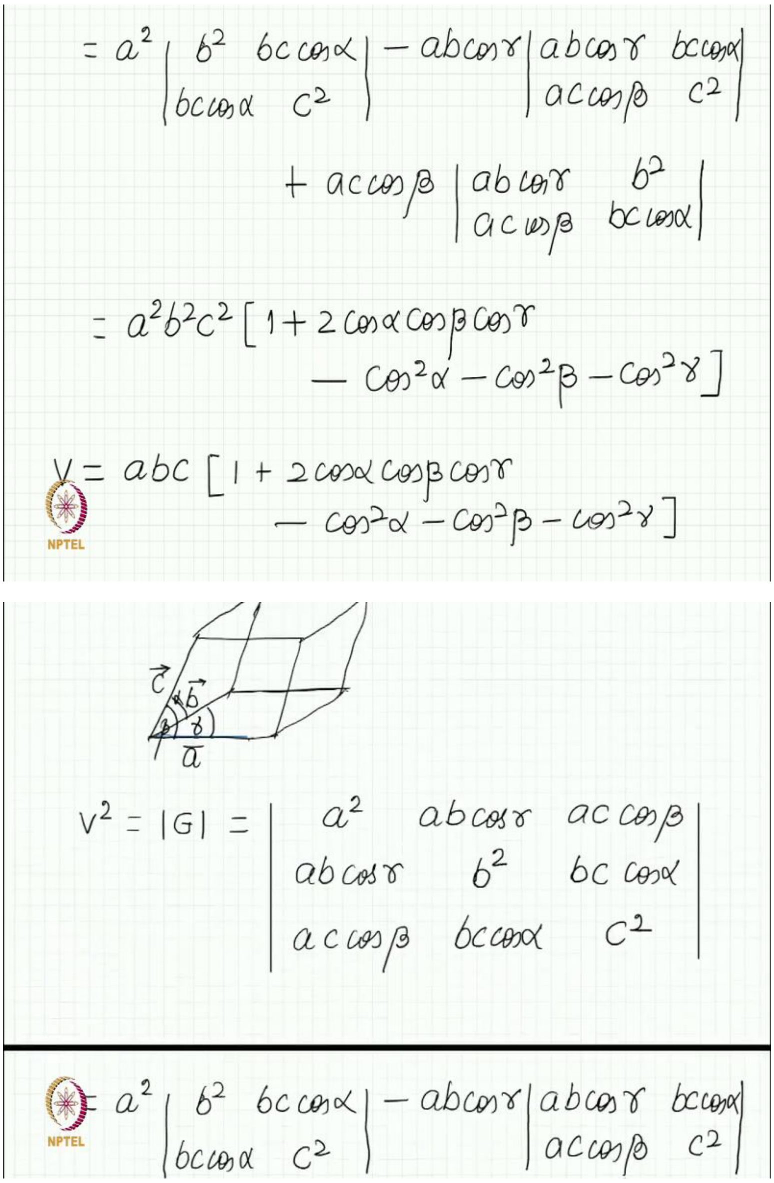

So, you can expand it so, maybe if you expand it by your first row, let us say then you have a square, b square, bc cos alpha bc cos alpha c square minus ab cos gamma ab cos gamma. So, you have ab cos gamma, bc cos alpha, ac cos beta, c square plus ac cos beta, ab cos gamma, b square, ac cos beta, bc cos alpha it looks messy, but finally, when you will work out it will all simplify to give you a square b square c square into 1 minus 2 cos alpha cos beta cos gamma minus cos square alpha cos square beta cos square gamma. You have to check my plus or minus sign whether I am making any mistake, this one is plus.

So, in the end it the formula does not turn out to be all that bad. So, but this was the square of the volume, remember, this was the square of the volume, because this was a determinant of the metric tensor. And we have shown that determinant of the metric tensor is the square of the volume. So, you just have to take the square root, then you get abc 1 beta minus and that is why the orthogonal unit cells are so nice, you can see all the cosine terms will vanish. As soon as these angles are 90 degree, all the cosine terms will vanish and will give you a nice formula for volume.

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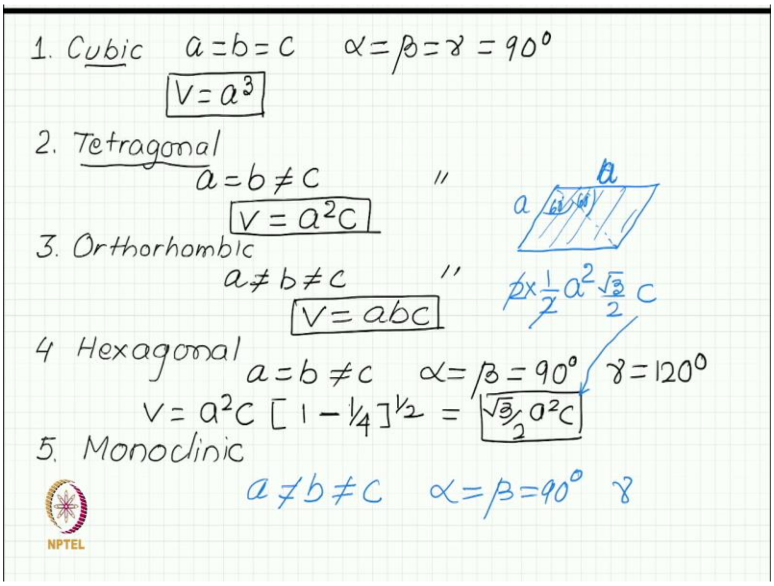

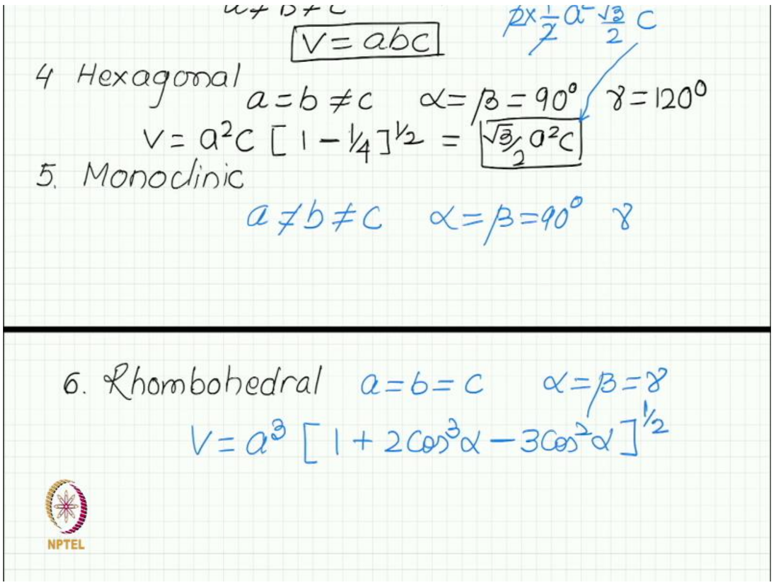

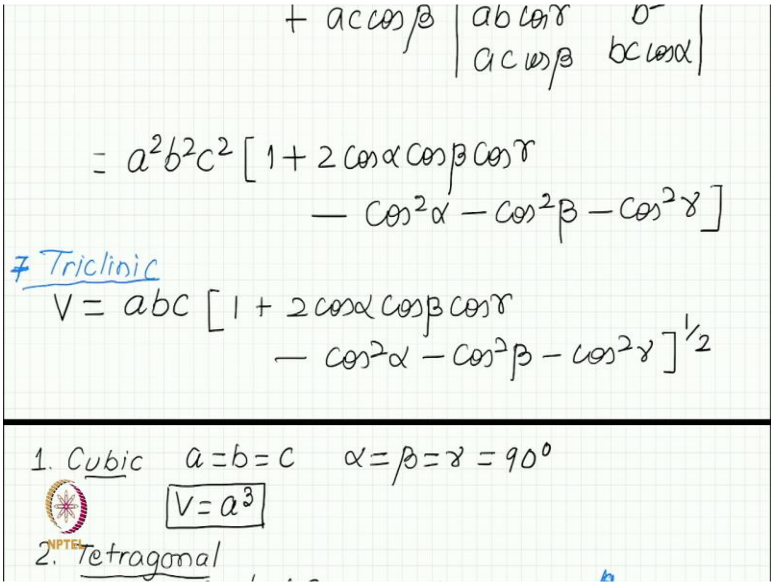

So, let us see one by one the application of this formula to different crystal systems. So, for cubic, we have a equals b equals c and alpha equal beta equal gamma. So, if we use this alpha, beta, gamma is 90 degree everything in that square bracket drops and abc becomes equal. So, V is a cube, you are not required to use that formula, but at least we are convinced that the formula works for this a special case. So, nothing is seriously wrong with that formula.

For tetragonal is the same thing angles are still 90 degree two sides are equal, third side is not equal and angles are 90 degree. So, now, you have V is equal to a square c. Orthorhombic none of the sides are equal. All angles are still 90 degree V becomes just the product of ab and c.

Hexagonal is the next simplest case, where a is equal to b but not equal to c, two angles are still 90 degree. So, life is not that bad, but one angle becomes 120 degree gamma is 120 degree. So apply it to your formula. So, V will become a square c 1 plus cos alpha cos beta cos gamma will disappear cos square alpha will disappear cos square beta will disappear, but minus cos squared gamma will remain. So, we will have 1 minus cos 120 degree is cos 60 degree, cos 60 degrees half. So, that means 1 by 4 and then a square root on top also. So, this becomes 3 by 4 and a square root of that root 3 by 4, root 3 by 2 a square c.

Let us see whether it is justified from our normal because hexagonal also we are not really required to use such complicated formula we could have done it with our school geometry. So, it is actually two equal lateral triangles which is the base. So, the area of the triangle is half ab which is equal so a square half ab sin 120, so, sin 120 is root 3 by 2. So, that is the area of one triangle, because there are two triangles involved. So, I will multiply it by 2. And this is the area of the base height is c. So, I multiplied with c. So root 3 by 2, a square c, happily, as given by the formula.

So formula seems to be working monoclinic also we can find monoclinic is also not that bad. It is like hexagonal, but the none of the sides are equal, two angles are again 90 degree. So, that is the good thing about it, only thing is that gamma is now arbitrary. So, you will find the volume as a function of gamma.

Rhombohedral, rhomboidal three sides are equal, three angles are also equal, but they do not have nice value like 90 degree or 120 degree. So, if we apply the formula you will get V is equal to a cube 1 plus 2 cos cube alpha minus 3 cos square alpha square root. So, all the seven crystals systems we have found the formula for volume starting with the most general case, which will be applicable for triclinic, because triclinic there is no relation. So, what we have found the general formula itself is for triclinic.

So, these are the conventional unit cell of seven crystal systems with which you are familiar, but tomorrow's tutorial exercise will try to make you familiar with these from a slightly different and more correct point of view. We will show you that these are okay from unit cell size and shape point of view, but these are not the definition these are not the definition of the crystal systems, cubic crystal system does not mean a equal b equals c alpha beta gamma equal to 90 degree, I can give you a crystal satisfying these properties but is not cubic?

So, the question is what is cub city? What defines cubic crystal, three fold symmetry. So, the symmetry is important. So, symmetry defines the crystal system. So, let us write this as a moral for tomorrow's tutorial as well as the forthcoming lectures also. So, now we are finishing, I think I took maybe two more lectures more than what I as per as announced in my program on these topics. So, does not matter. It is nice to go slowly. And now, we will change the topic from next class.

So, from next week, we will start on the central topic of this course, that is the symmetry and we will find that symmetry is very, very important and central to crystallography, central to all science in a way symmetry is very very important, but we will look at it from a more restricted perspective of crystallography. And in particular, we will see that these crystal systems are defined in terms of symmetry and not in terms of these lattice parameter relations.

So, for example, in hexagonal crystal you can very easily find and orthorhombic c unit cell that does not make it orthorhombic c, or in cubic crystal you can very easily fine rhombohedral or trigonal unit cell that does not make it rhombohedral or trigonal. So, thank you very much.