Texture in Materials
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Module - 03
X-ray diffraction phenomena
Lecture - 07
Structure Factor and Diffraction Extinction Criteria

Good day to everyone. This is the 7th lecture and it is on X-ray diffraction phenomena, module 3. So, the lecture is all about the Structure Factor and the Diffraction Extension Criteria.

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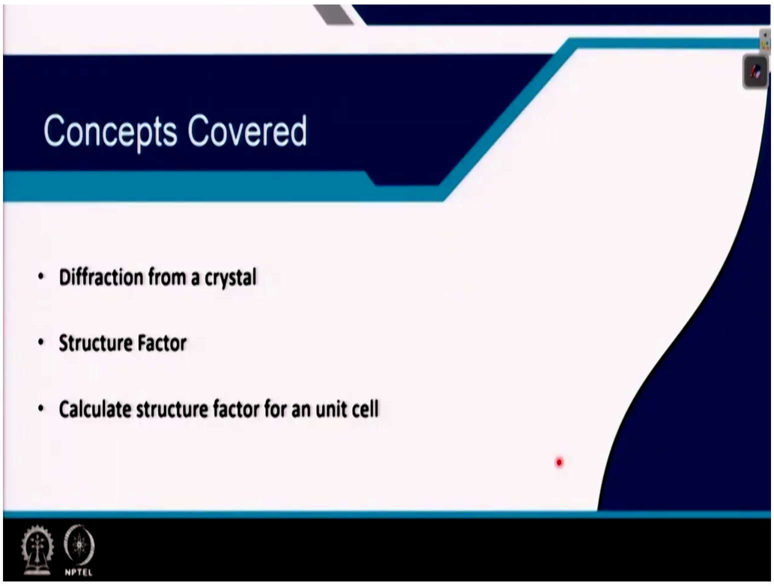

The concepts that will be covered in this lecture are diffraction from a crystal, structure factor, and how to calculate structure factor for a unit cell.

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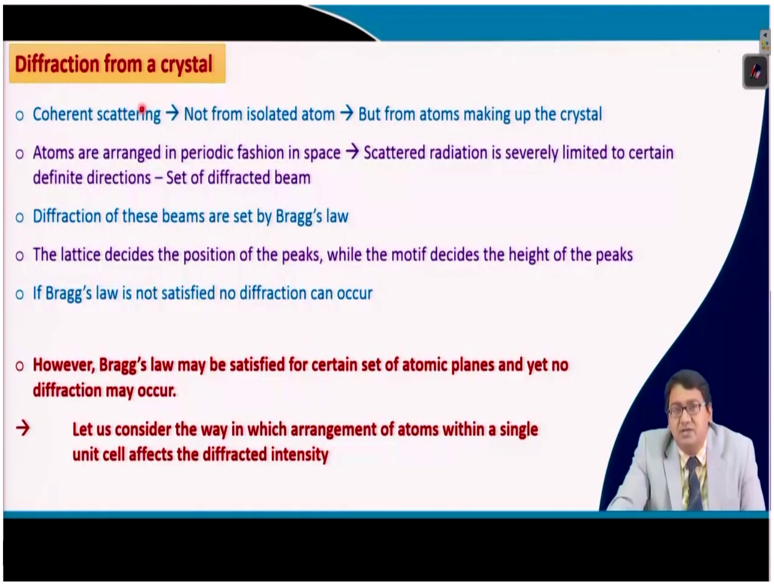

, diffraction from a crystal occurs when coherent scattering occurs not from an isolated atom, but from atoms that make up the full crystal. Now, in a crystal, the atoms are arranged in a periodic fashion in space and therefore, the scattered radiation has severely limited options to a certain direction, limited to a certain direction. So that it can come out as a set of a diffracted beam.

So, the diffraction of these beams is set by Bragg's law that we learned in the previous lecture. The lattice decides the position of the peaks, while the motif decides the height of the peak. That means, that if at different positions of the crystal structure if different motif are present; that means, different atoms or different molecules are present then it will decide the diffraction heights coming from the X-ray beam. So, if Bragg's law is not satisfied no diffraction can occur. However, even if Bragg's law is satisfied for a certain set of atomic planes, yet it is found out that there is no diffraction taking place. And in this lecture, let us consider the way in which the arrangement of atoms within a single crystal or a single unit cell affects the diffraction ability or the diffracted intensity.

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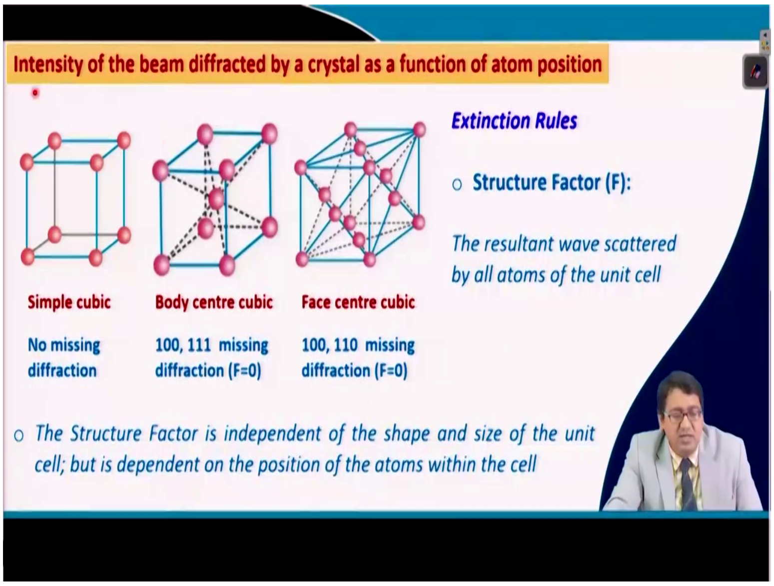

So, the intensity of a beam diffracted by a crystal is as a function of atom position is very important. for a unit cell, the atom positions are only at the corners of the unit cell, and therefore, there is no missing diffraction. On the other hand, there is an atom sitting at the center of the unit cell for the body-centered cubic crystal along with the atoms present in the corner of the unit cell. And in this case, we will see that there are some missing diffraction that is 100, 111 poles are missing or intensities are missing. In case of face-centered cubic, there are atoms present at the 6 faces along with the atoms present at the corner. So, in the face-centered cubic crystals too, 100, 110 intensity spots are missing.

Now, this is based on the extinction rule decided by a factor which is known as the structure factor. A structure factor is the resultant wave scattered by all the atom of the unit cell. So, if structure factor which is F is 0 for certain hkl planes, then there will be no diffraction even if the Bragg's law is satisfied. Now, the structure factor is independent of the shape sorry shape, and size of the unit cell, but it is dependent on the position of the atom within the cell.

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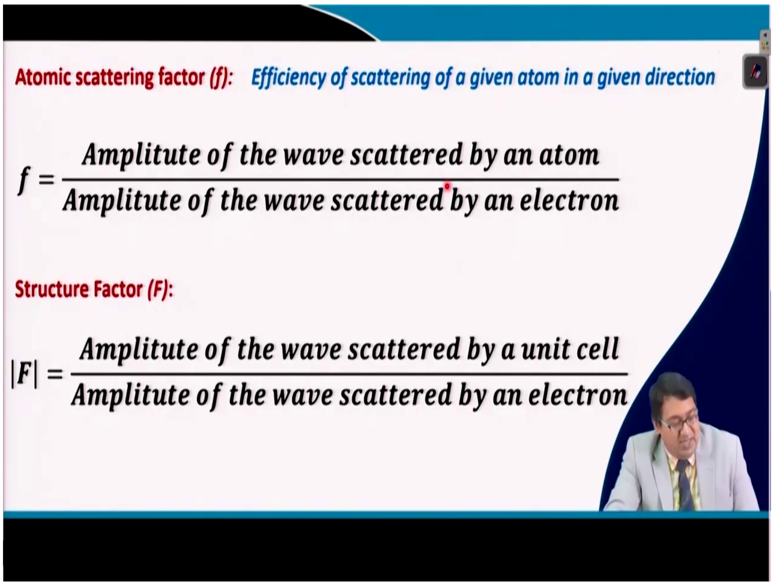

So, before we understand the structure factor let us define what is atomic scattering factor. See, atomic scattering factor is the efficiency of scattering of a given atom in a given direction. That means, atomic scattering factor given by a small f is equal to amplitude of the wave scattered by an atom by amplitude of the wave scattered by an electron. Now, what is structure factor then? Structure factor then becomes efficiency of scattering of a given unit cell in a particular direction, right. That means, capital F structure factor is equal to amplitude of the wave scattered by unit cell divided by amplitude of the wave scattered by an electron.

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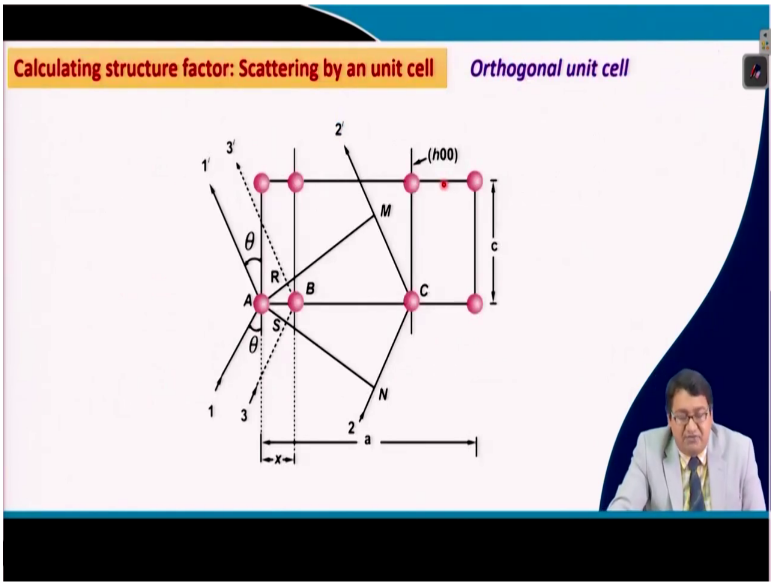

In order to calculate the structure factor, we should consider scattering of a unit cell. in order to do that we usually consider an orthonormal unit cell. The orthonormal unit cell has a lattice parameter which is a, and the positions of the atoms in the orthonormal unit cell at the corners, right. And if there are atom present at a certain position for a particular plane say, for example, an hkl plane in this case that we have taken h00 plane. So, for simplicity what we have done is that we have considered a two-dimension plane, the simplest two-dimension plane of an orthogonal unit cell, right. Now, that the X-ray beam is falling incidenting on the atom from this direction to this corner atom A and it is diffracted at an angle theta, right. Now, if we are considering a plane in this two-dimension unit cell a plane is h00. Then it consists of atoms at this plane and then another incident beam, 2, is falling on this atom and is diffracting here, right.

So, now let us find out that what is the phase difference, of an atom diffracting for a certain hkl plane and if we put another atom B at a parallel to this h00 plane in this unit cell.

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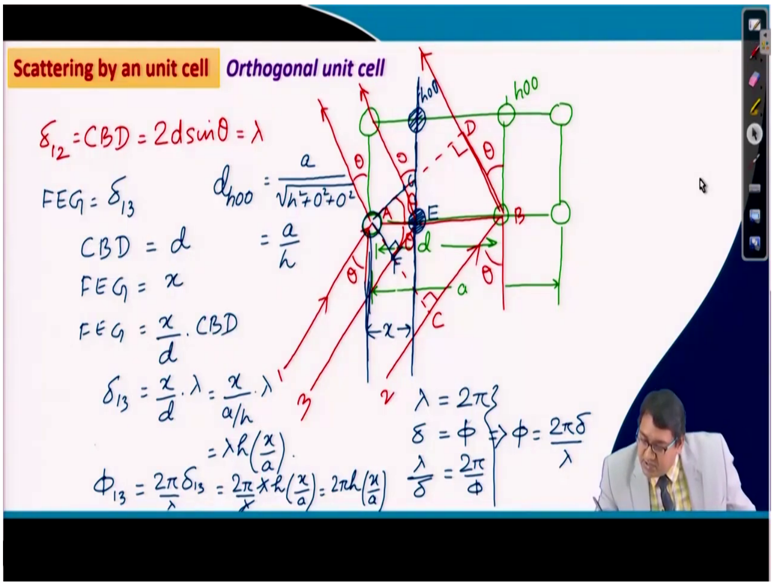

So, in order to understand the scattering of a unit cell let us consider a two-dimension orthogonal unit cell. The orthogonal unit cell let me draw it.

Let us say that an orthogonal unit cell of two-dimension has a unit cell size of a and there are atoms present somewhere in between at a distance and corresponding to a plane h00 and having a distance d from the atom which is present at this position. If an incident X-ray beam is falling at say for this is atom A, and is diffracting by an angle theta. So the incident beam is falling at an angle theta and is diffracted at an angle theta, and that similar incident beam is falling the same incident beam. So, 1 is falling on atom A and 2 is falling on atom say atom B, and is diffracting at the same angle theta, right. The extra path length traveled by the incident X-ray beam 2 will be greater than the incident beam 1, right.

And in order to find that we can draw perpendicular to this incident and the diffracted beam, and then if we say that it is C and it is D position, then the path difference delta 12 which is equal to CBD is equal to. , how much it is equal to? It is equal to D times, this D times the sin of theta that means, B, D and then D times sin of theta that is C B. So, 2 d sin of theta. Now, if we consider that the combination of the diffracted beam from 1 and 2 to atom A and B is giving a constructive interference, then this must be at least equal to lambda, right. Now, if we consider that there is another atom, another atom somewhere here, right and say this atom is at position E. Now, an incident the same incident beam say now it is the incident beam 3 is falling over the atom and this atom basically represents the same h00 plane, right. And this is present at a distance x from the atom A, right. So, now that when the incident beam 3 is falling over atom E and it is diffracted in the same angle theta, then one can find out the angle, if we consider that this is F, this position is F, and if this position is G, then one can find out that this F, E, G is basically the path difference for this particular plane to diffract, right with respect to the beam 1, right.

So, if we say that the atom E is x distance away from the atom A, which is the distance of this h00 plane from the h00 plane present at the origin of the orthogonal unit cell, then one can relate it is something like that, right. So, I am going to relate it to say, for example, if CBD is a path difference corresponding to the distance d of the h00 plane, then FEG is a path difference corresponding to the distance x, right.

So, FEG is basically x by d times CBD, right. And what is CBD? CBD is basically lambda, so x by d times lambda. Now, if we consider that what is this d, so d is basically the distance between the h00 planes which is equal to the unit cells distance a divided by h square plus 0 square plus 0 square and that becomes equal to a by h.

So, FEG which is basically equal to delta 13 is equal to x by a by h times lambda, right. So, this is basically equal to lambda times h x by a. Now, we know that if the path difference is lambda this is equivalent to the phase difference 2 pi, right. Now, if the path difference is delta then this equivalent phase difference should be phi, right.

And phi should be equal to, how to find out this one? That means, that lambda by delta is equal to 2 pi by phi and this implies that phi is equal to 2 pi times delta by lambda. So, instead of the phase difference delta 13 if we write in terms of phase difference phi 13, then phi 13 is equal to 2 pi, delta 13 path difference by lambda is equal to 2 pi times let us write delta 13 is equal to 2 pi by lambda times lambda h x by a. Lambda and lambda is canceled, and therefore, it is 2 pi h x by a.

So, that the phase difference in terms of for an orthogonal unit cell in two-dimension is given by 2 pi h x by a which is basically the distance of the h00 plane which is present because of this atom E and the other which is present in between the orthonormal unit cell.

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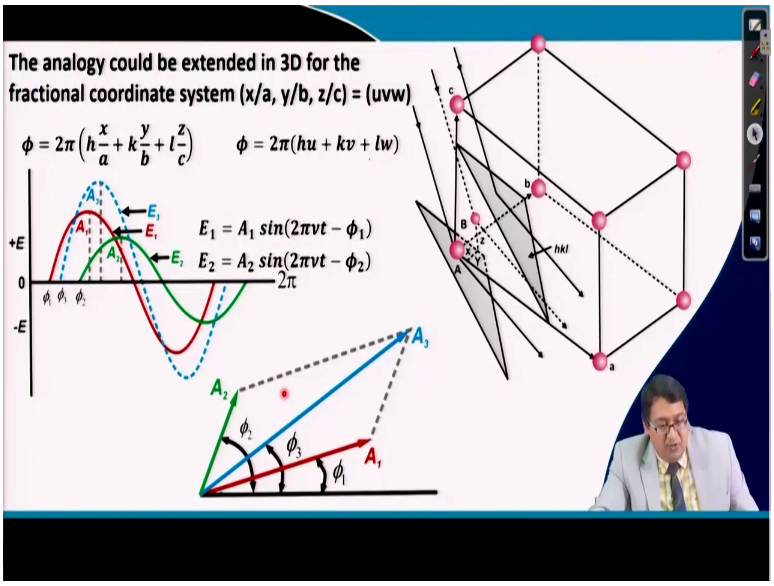

Now, that we can take this analogy to the; let me delete it first. We can extend this analogy of this two-dimension unit cell into the three-dimensional orthogonal unit cell and the figure of the three-dimensional orthogonal unit cell is shown here. Let me take the pointer.

And that if an atom, if an atom is present at a certain position and say, for example, we were talking about one plane, the atom position is at the origin; another plane, the atom position is at a certain distance to the inside the unit cell, but both the atoms represent planes which are basically initially it was two-dimensions. So we took h00, but if it is three-dimension then it represents hkl.

And if there is another atom present in between these two planes and it also represents the hkl plane, and if this the if this atom is present in between and the position of the atom can be given by x by a in the x-direction y by b in the z-direction and z by c in the z-direction that is u, v, and w.

And then, the phase difference phi which was 2 pi times h x by an in the two-dimension can be extended to 2 pi times h x by a plus k y by b plus l z by c for the three-dimensional case. So, phi is equal to 2 pi times hu plus kv plus lw. So, this is the phase difference that is created because of the presence of an atom in inside the unit cell.

Now, that this analogy of phase difference can be used to find out the amplitude of the diffracted wave related to the structure factor. Now, let us say that the amplitude of the wave generated by the first atom at the origin A is given by this red A 1, right.

And the amplitude of the wave generated by the other atom for the hkl plane is given by A 2, right. Now, if that if we add A 1 and A 2 we get this amplitude. So, there is always a phase difference present when a number of waves are coming from different positions.

So, E 1 is equal to A 1 sin of 2 pi mu t, mu is the frequency and t is the time, minus of phi 1 which is the phase difference because of this A 1 wave, electromagnetic radiation. The E 2 radiation has A 2 equal to sin mu 2 pi mu t minus phi 2 and phi 2 is the phase difference of the A 2 radiation. And if we add like that, and we can get the cumulative addition of the wave, and therefore, the resultant wave A 3 can be obtained.

This addition is basically the vector addition, right, where if you say A 1 is having an amplitude A 1 at a phase difference phi 1, whereas, A 2 is having this amplitude at a phase difference phi 2. So, if we add these two like this, means if we draw a line parallel to this A 1, and another line parallel to A 2, and we get if we draw this body diagonal then we get the final amplitude total amplitude at a phase difference phi 3.

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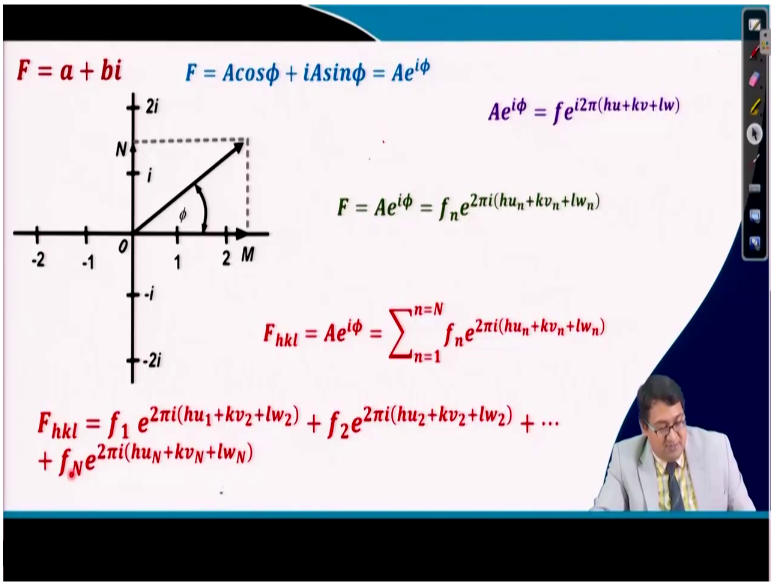

Now, doing this like this becomes quite complex. So, what it is done is that usually instead of doing it like that a complex number system is used, so that one can find out the amplitude in terms of x-axis a, which is the real axis, and y which is the imaginary axis. So, if we consider if the factor F, that is the structure factor F in terms of a plus bi, which is a is the real axis, and b which is multiplied by i because i is the imaginary number i which is equal to root of minus 1. Then, the structure factor F can be said to be equal to A times cos of phi because the value small a is equal to the amplitude a resultant amplitude of the wave a times cos of phi, right and B is equal to the resultant amplitude of the electromagnetic wave times sin of phi. So, F which is the structure factor is equal to A cos of phi plus i times A sin of phi and this can be written as an exponential to the power i phi, right, where phi is the resultant phase difference that we just calculated. So, if we say that a to the power i phi is, where phi is the resultant wave resultant phase difference that we calculated then this can be written as equal to the atomic scattering factor f for that certain atom times exponential to the power i 2 pi times hu plus kv plus lw, right.

So, that F is equal to amplitude A times exponential to the power i phi is equal to the struck atomic scattering factor f for the nth atom to the power exponential 2 pi i times hu plus kv plus lw for the nth atom, right. Now, this can be written in terms of summations of all the atom which is present in a unit cell. So, n can be equal to 1 to n equal to N.

So, now that if we can write then we can find out the structure factor for a particular hkl plane in terms of the atomic scattering factor and the exponential of 2 pi o times h times u plus k times v plus l times w. And this, by this way we can find out the atomic scattering factor for a certain hkl plane for different atoms 1, 2, 3, 4 up to n which are present in a unit cell, right.

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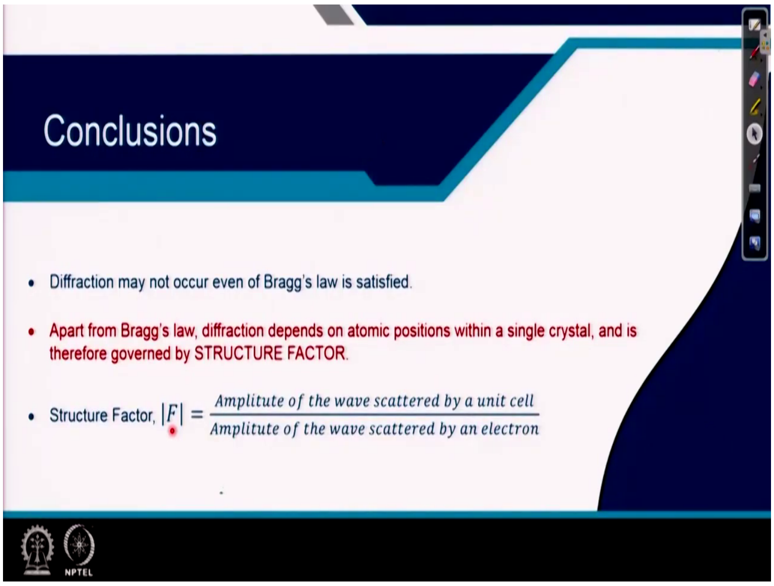

So, this is what in this class and therefore, we can conclude that diffraction may not occur even if the Bragg's law is satisfied. Apart from Bragg's law, diffraction depends on atomic position within the single crystals and is, therefore, governed by the factor which is known as the structure factor. Structure factor given by this symbol is equal to amplitude of the wave scattered by a unit cell by the amplitude of the wave scattered by an electron.

Thank you.