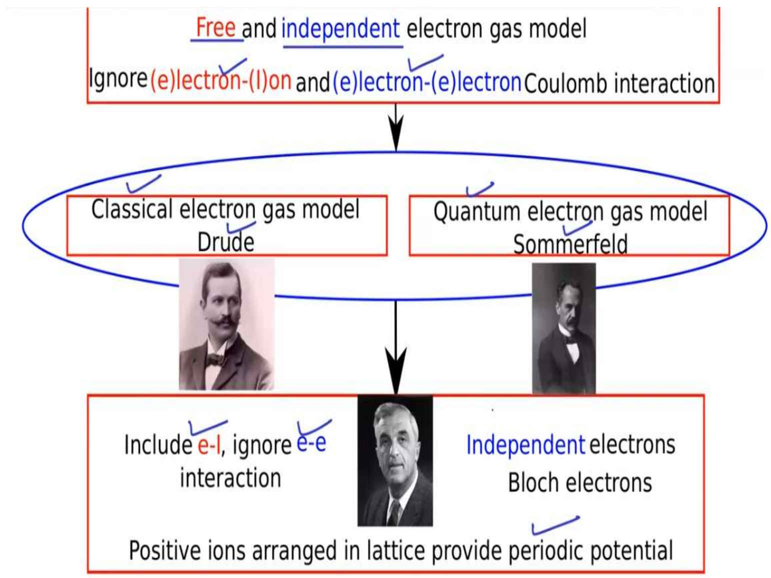
Electronic Properties of the Materials: Computational Approach
Prof. Somnath Bhowmick
Department of Materials Science and Engineering
Indian Institute of Technology, Kanpur

Module No # 06
Lecture No # 26
Fermi Surface: Part 1

(Refer Slide Time: 00:12)

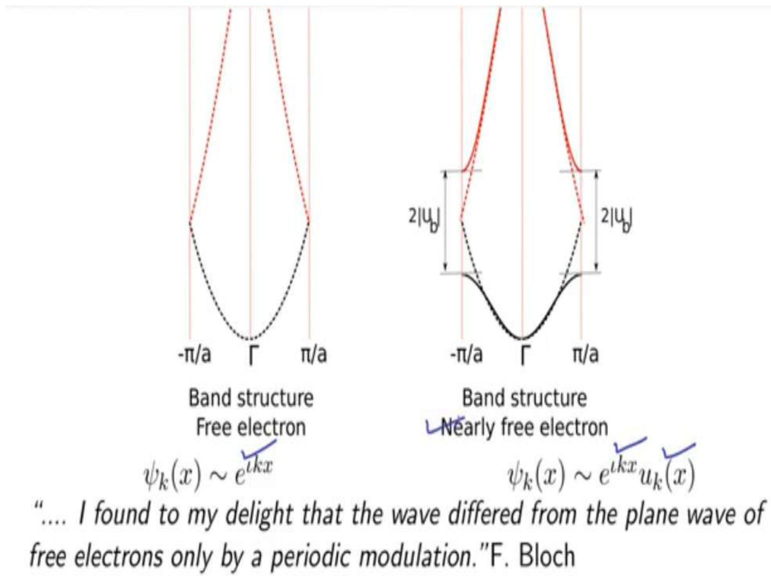


Hello friends let me start with an overall summary of physics of electronic materials at different levels. The simplest Theory ignores electron iron and electron electron interaction ignoring electron ion interaction is known as the free electron gas model and ignoring electron-electron interaction is known as the independent electron gas model. Electron gas model can be solved using a classical as well as quantum theory.

Classical electron gas model was proposed by Drude and quantum electron gas model was proposed by summer wind. Electron gas models provide good explanation for most of the electronic properties of metals other than a few like anomalous all coefficient for certain metals. At the next level we remove the free electron approximation by including the electron wire interaction.

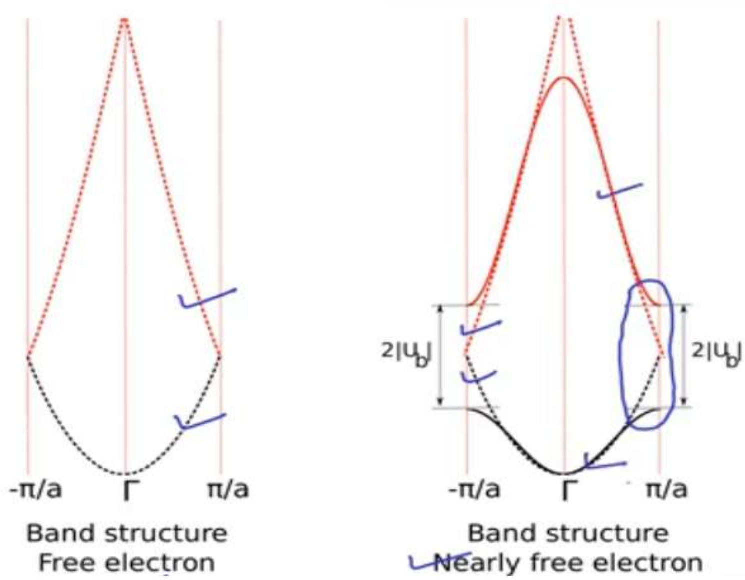
However we continue with independent electron approximation that is we ignore electron- electron interaction valence electrons are assumed to get detached from the atomic course consisting of nucleus and coal electrons thus atomic cores are positively charged ions and the valence electrons find themselves in a potential provided by the positively charged ions in a crystalline solid ions are arranged periodically in a lattice. Thus we solve a problem of electron signal periodic potential such electrons are known as block electrons.

(Refer Slide Time: 02:11)



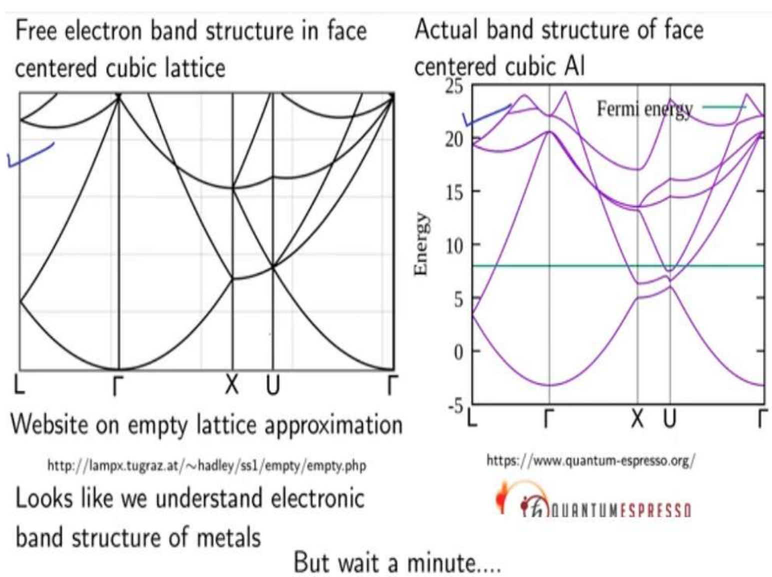
The modification needed to go from free electron to electron in a periodic potential turns out to be very simple. In case of free electrons in function is given by a plane wave in case of block electrons the in function is a plane wave times some function which has the periodicity of the lattice. Let us quote the words of block himself I found to my delight that the wave differs from the plane wave of full electrons only by a periodic modulation. If the potential is weak we call it a nearly free electron model.

(Refer Slide Time: 03:00)



The band structure or E versus K diagram of nearly free electrons differs from the actual free electrons only in a region close to the very low in zone boundary. In this figure the free electron band structure is shown by the dotted line and same here. Note that the free electron and the nearly free electron band structure which is shown by the starting line differ only near the boiling zone boundary. Otherwise away from the reloading zone boundary free and nearly free electrons have identical features.

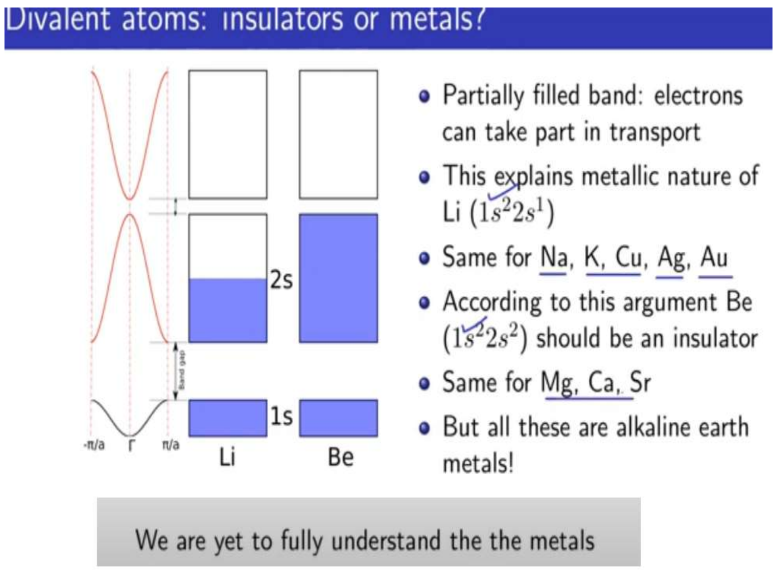
(Refer Slide Time: 03:45)



Nearly free electron model is not just a toy model it indeed works for metals like aluminum. The first diagram from the left shows the free electron band structure in a phase Center cubic lattice. The second diagram shows the actual band structure of aluminum generated by a cabin issue calculations using quantum espresso package. Notice the close match between the free electron and actual band structure.

Indeed the periodic potential has some effect but the effect is not too strong. And the match between the free electron and actual band structure is clearly visible. It looks like that we completely understand the electronic band structure of metals based on what we have done so far but wait a minute.

(Refer Slide Time: 04:47)



We know that if we have a partially field Band then only electrons can take part in transport process a completely full or completely empty band cannot take part in electronic transform. This explains the metallic nature of lithium having electronic configuration of 1s2, 2s1. Since the 2 s band is half field lithium has to be a metal. This also explains the metallic nature of sodium. Which has a half field 3s band copper and potassium which has a half filled 4s band silver which has a half field 5s band and gold which has a half field 6s band.

According to this argument beryllium having electronic configuration of 1s2 2s2 should be an insulator. Similarly all the divalent elements like magnesium calcium strontium should be insulators but these are known as alkaline or metals. How do they show metallic nature despite having no partially filled Banks clearly what we have done so far is not sufficient to explain the metallic nature of divalent metals like beryllium magnesium calcium and strontium.

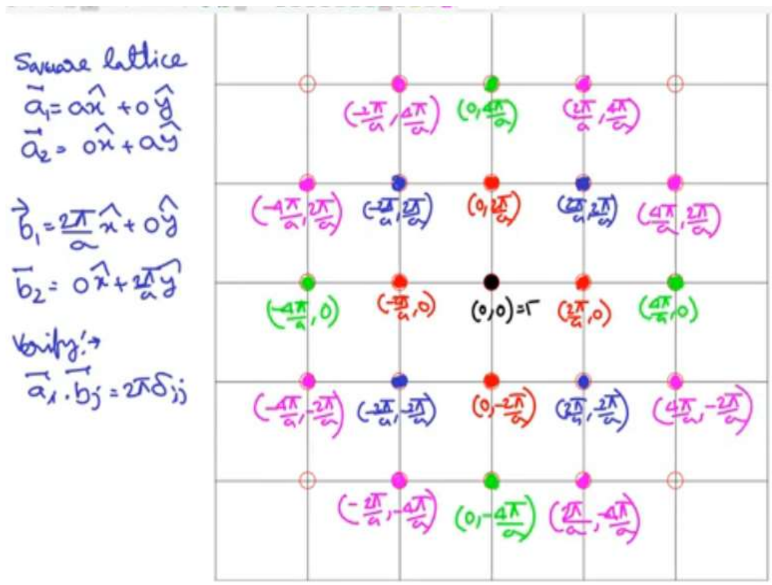
(Refer Slide Time: 06:26)

Fermi surface

A solid with a Fermi surface is a metal

We need to learn one more important concept to explain the existence of divalent metals the Fermi surface later. The same concept will also help us to understand electronic transport properties of metals concept of Fermi surface is so important in a metal that a metal is defined as a solid having a Fermi surface.

(Refer Slide Time: 06:54)



Before discussing about Fermi surface we need to have a very good understanding of reciprocal lattice and doing so. Showing every detail in 3b would be very challenging thus I do it for a 2b square lattice. A square lattice has 2 lattice translation vectors a 1 = a x hat and a 2 = a y hat it is easy to find the corresponding translation vectors in reciprocal lattice. Given by v1 = 2 pi by an x hat and b 2 = 2 pi by a y hat It is left as an exercise for you to verify that a i dot b j = 2 pi delta of i j center of the reciprocal space is the gamma point.

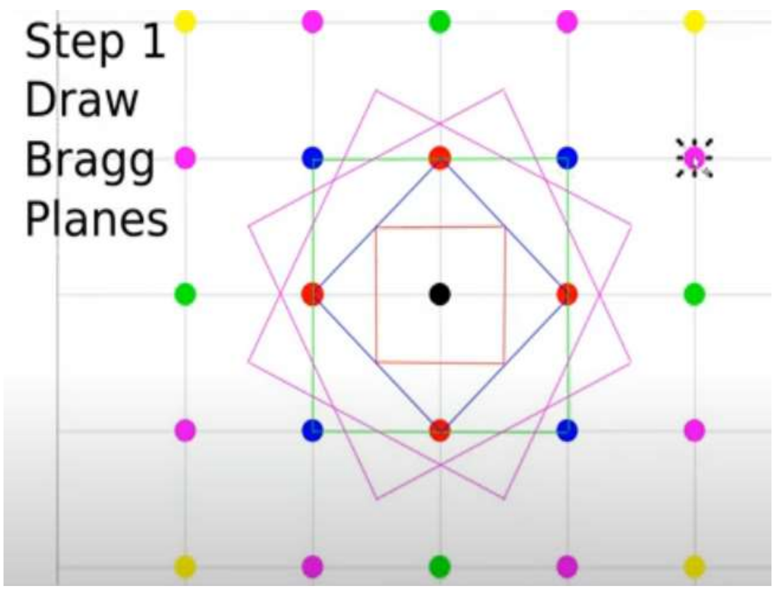
Let us start to mark other lattice points in reciprocal space starting from the origin we will reach the first point at 2 pi by a 0 there are total 4 points located at the distance of 2 pi by a from the origin. And the other points are here at 0 to Pi by a next 1 - 2 pi by a 0 and the fourth one is 0 -

2 pi by a these are the first near neighbors to the gamma point. Now let us find the second near neighbors to the gamma point.

So these Blue Points are the to the gamma point and there coordinates are 2 pi by a 2 pi by a - 2 pi by a 2 pi by a - 2 pi by - 2 pi by a and 2 pi by a - 2 pi by a. Now let us find the third nearest neighbor to the gamma point these green points are third nearest neighbor to the gamma point and they are coordinates are given by 4 Pi by a 0, 0 4 Pi by a - 4 Pi by a 0 and 0 - 4 Pi by K. Finally let us find the fourth nearest neighbor to the gamma point. These magenta points are the fourth nearest neighbors to the gamma point and there are 8 such points.

Coordinates are 4 Pi by a 2 pi by a 2 pi by a 4 Pi by a - 2 pi by a 4 Pi by a - 4 Pi by a 2 pi by a - 4 Pi by a - 2 pi by a - 2 pi by a - 4 Pi by a - 4 Pi by a and 4 Pi by a - 2 pi by a.

(Refer Slide Time: 13:02)



Now let me show you how to draw Brillouin zones for a square lattice. First step is to draw the Bragg plates in order to do that i join the gamma point with its first near table and then draw the perpendicular bisector join the first near neighbour with the gamma point. We get a line and we draw the perpendicular bisector of the line. Join the gamma point with first near neighbour we get a line and we draw the perpendicular bisector of the line.

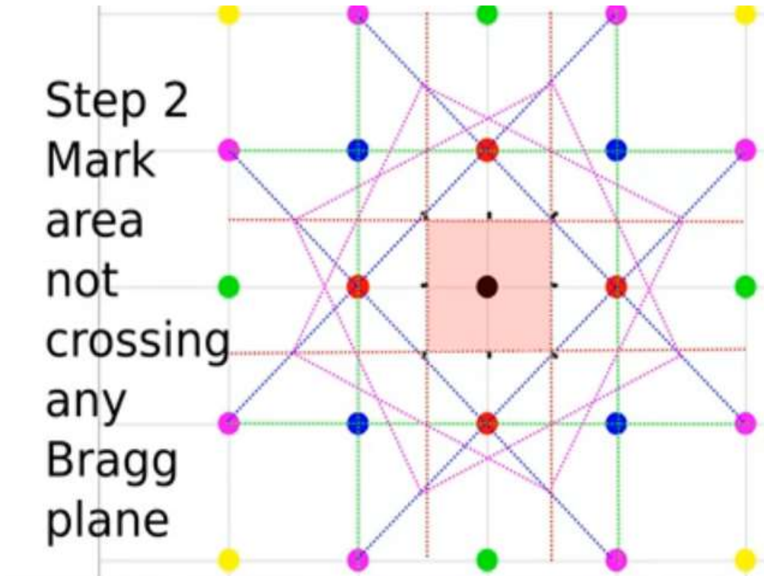
Join gamma point with the first near neighbour we get a line and we draw the perpendicular bisector of this line. Now we have 4 Bragg planes corresponding to the first near neighbor next we join the gamma point with the second near neighbour. We get a line and we draw its perpendicular bisector. We join gamma point and its second near neighbour gets a line and we draw its perpendicular bisector.

We join gamma points with its second near neighbour get a line and draw its perpendicular bisector now we have 4 Bragg planes mart in blue corresponding to the second near neighbour. Then we join gamma point with its third near neighbour we get a line with draw its perpendicular bisector join gamma point with its perpendicular bisector. Join gamma point with its Third near neighbour get a line and draw its perpendicular bisector.

Join gamma point with its Third near neighbour get a line and draw its perpendicular bisector. Now we have 4 Bragg planes mark in green corresponding to the third near neighbour next we joined gamma point with the fourth near neighbour we get a line and we draw its perpendicular bisector. Join gamma point with the fourth near neighbour we get a line and draw its perpendicular bisector.

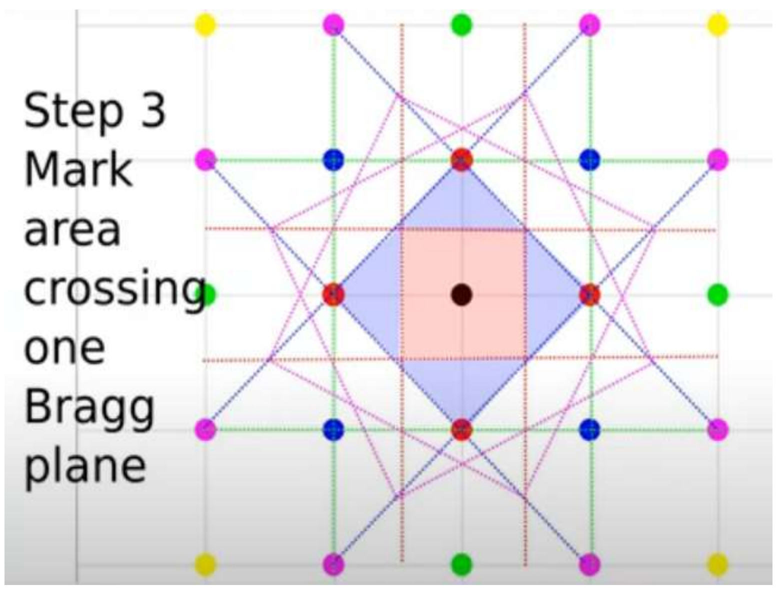
Again we draw a line joining gamma point with the fourth near neighbour and draw its perpendicular bisector join the gamma point with its fourth near neighbour. Get a line draw its perpendicular bisector join gamma point with fourth near neighbour. Join gamma point with fourth near neighbour get a line draw its perpendicular bisector joins gamma point with fourth near neighbour data line and draw its perpendicular bisector. Thus we have 8 Bragg planes corresponding to the fourth near neighbour.

(Refer Slide Time: 18:00)



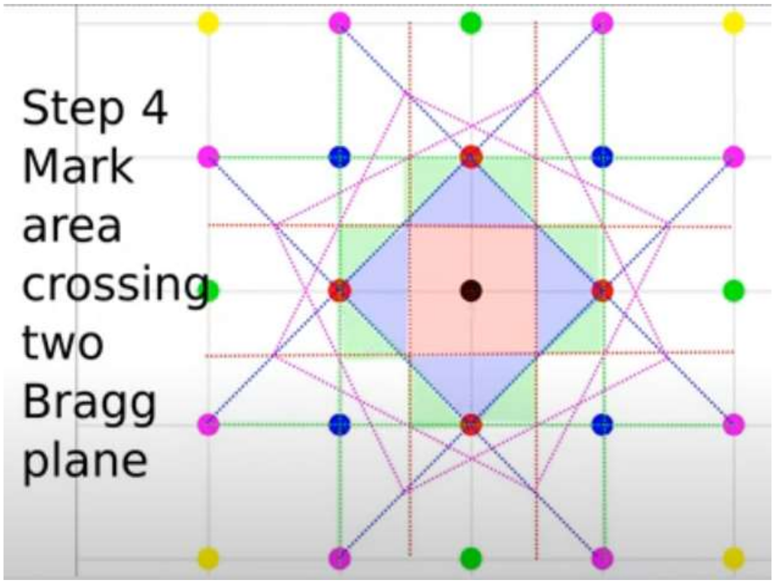
I have shown how to draw the Bragg planes for a square lattice. Now let me last check how to get the Brillouin zones of a square lattice imagine that I start from the gamma point let me find out the regions where I can go without crossing a single Bragg plane clearly. This is the region where I can go without crossing a single Bragg plane this is known as the first Brillouin zone.

(Refer Slide Time: 18:33)



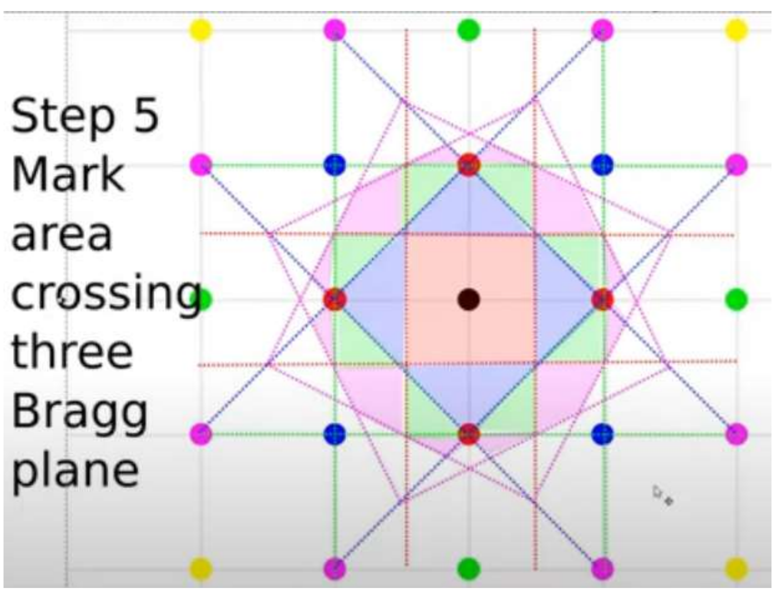
Step 3 let me mark the regions which can be reached from the gamma point by crossing 1 Bragg plane this region can be reached from the gamma point by crossing 1 Bragg plane mark in red similarly this region can be reached from the gamma point by crossing 1 Bragg plane mark in red. In total we have 4 such regions which can be reached from the gamma point by crossing a single Bragg plane mark in red the blue shaded regions constitute the second Brillouin zone.

(Refer Slide Time: 19:31)



Step 4 let me mark the regions which can be reached from the gamma point by crossing 2 Bragg planes. These 2 regions can be reaching from the gamma point by crossing a red Bragg plane and a blue Bragg plane. Similarly these 2 regions can be reached from the gamma point by crossing a red Bragg plane and blue Bragg plane in total there are 8 such regions. This can be reached from the gamma point by crossing a red Bragg plane and a blue Bragg plane. The green shaded regions constitute the third Brillouin zone.

(Refer Slide Time: 20:42)

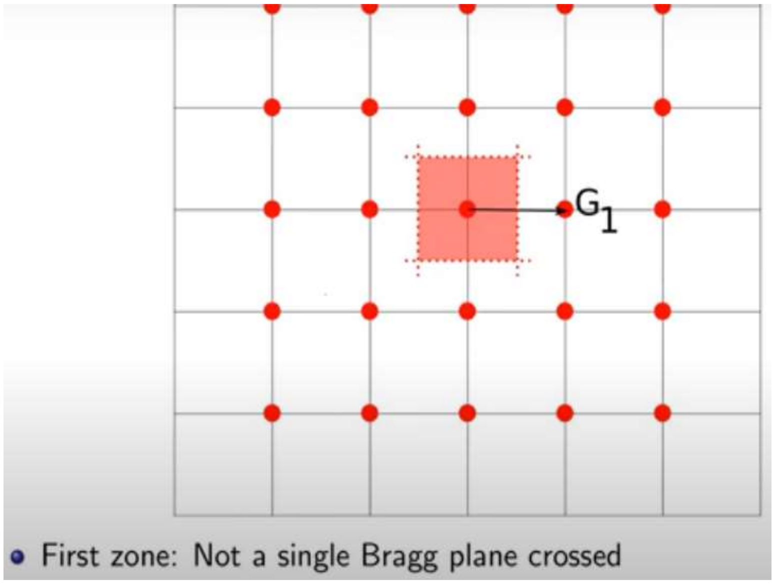


Step 5 I have to mark the regions which can be reached from the gamma point by crossing 3 Bragg planes. Take this region can be reached from the gamma point by crossing 2 red planes and 1 blue

plane now take this small region. This region can be reached from the gamma point by crossing 1 red 1 blue and 1 green plane. Similarly take this small region this also can be reach from the gamma point by crossing a red plane a blue plane and a green plane.

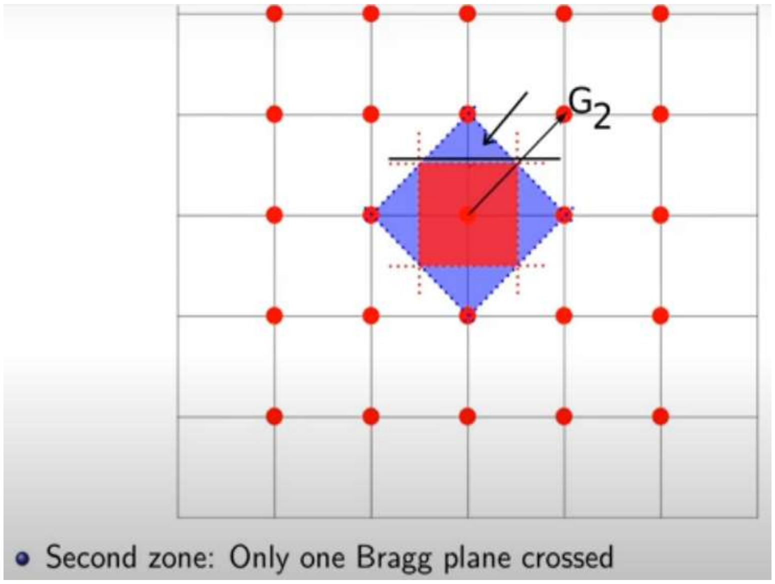
Let us mark all the regions which can be reached from the gamma point by crossing 3 Bragg planes. This regions shaded in magenta can be reached from the gamma point by crossing 3 Bragg planes this regions constitute the fourth Brillouin zone.

(Refer Slide Time: 22:32)



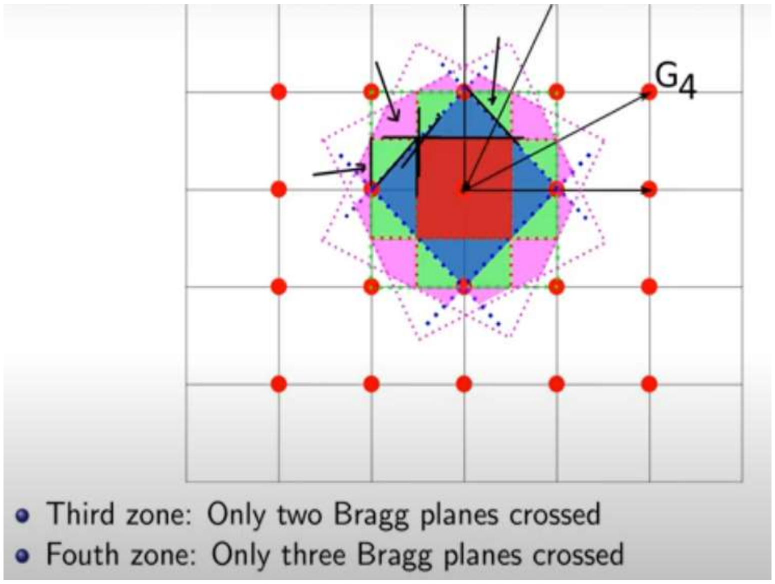
In summary first Brillouin zone is the region which can be reached from the gamma Point without crossing a single Bragg plane.

(Refer Slide Time: 22:43)



The second Brillouin zone is the region which can be reached from the gamma point by crossing only 1 Bragg plane. It is shaded in blue to reach this blue region from the gamma point we just need to cross 1 Bragg plane.

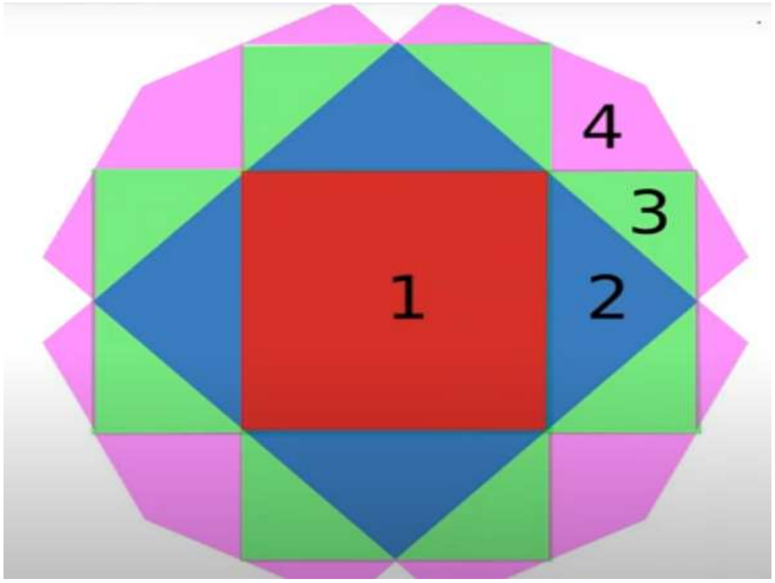
(Refer Slide Time: 23:04)



Third Brillouin zone is the region which can be reached from the gamma point by crossing 2 Bragg plates. It is shaded in green for example if you want to reach this region starting from the gamma point. We have to cross 1 red Bragg plane and 1 blue Bragg plane. Fourth Brillouin zone is the region which can be reached from the gamma point by crossing 3 Bragg planes it is shaded in magenta.

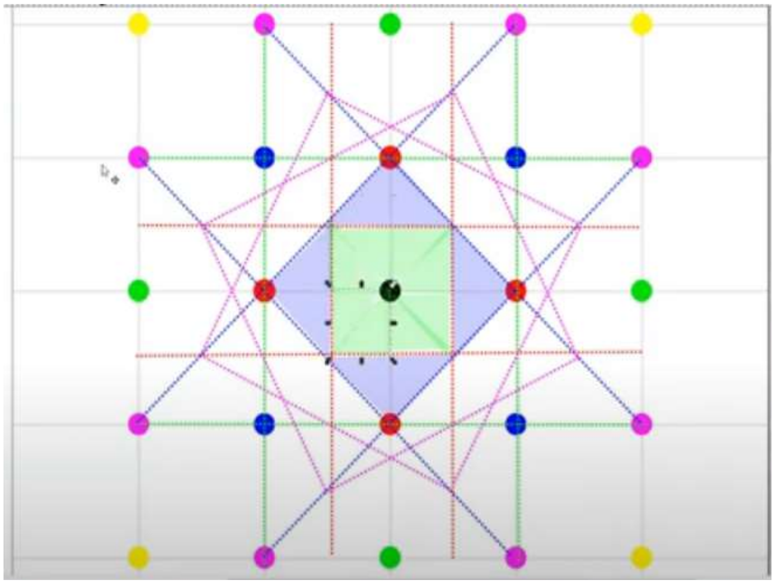
For example if you want to reach this region starting from the gamma point we have to cross 2 red Bragg plates + 1 blue Bragg plane similarly if you want to reach this region starting from the gamma point you have to cross 1 red Bragg plane 1 blue Bragg Plain and 1 green Bragg plain.

(Refer Slide Time: 24:18)



This is an enlarged view showing the first Brillouin zone in red second Brillouin Zone in blue third Brillouin zone in Queen and fourth Brillouin zone in magenta.

(Refer Slide Time: 24:34)

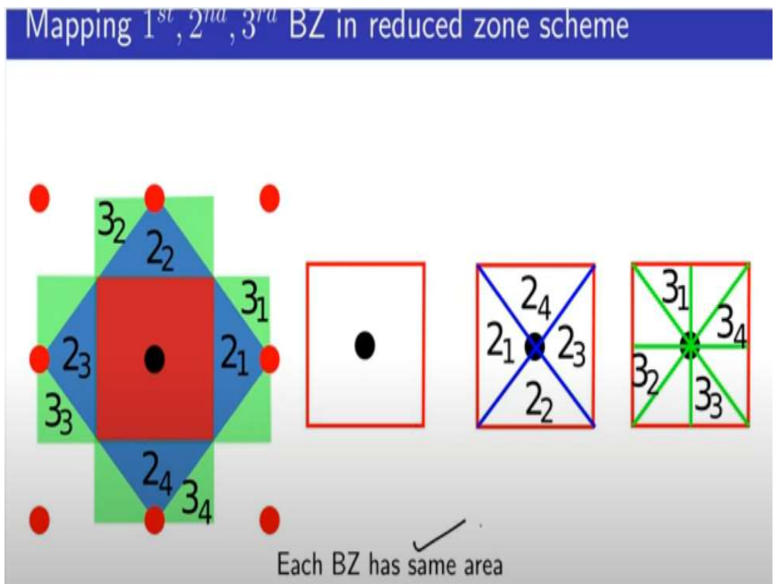


Let me show you that we can map all the Brillouin zones to the first Brillouin zone for example we take this portion of the second Brillouin zone and we bring it back to the first Brillouin zone so similarly we get this portion and bring it back to the first Brillouin zone we take this portion of the second Brillouin zone and bring it back to the first Brillouin zone. We take this portion of the second Brillouin zone and bring it back to the first Brillouin zone.

So similarly we can do it for the third Brillouin zone we take this portion of the third Brillouin zone and bring it back to the first Brillouin we take this portion and bring it back to the first Brillouin zone. We take this portion and bring it back to the first Brillouin zone we take this portion of the third Brillouin zone and bring it back to the first Brillouin zone. We take this portion and bring it back to the first Brillouin zone.

We take this portion of third Brillouin zone and bring it back to the first Brillouin zone and we take this portion of the third Brillouin zone and bring it back to the first Brillouin zone and finally we take this portion of the third Brillouin zone and bring it back to the first Brillouin zone.

(Refer Slide Time: 26:17)



So thus we have map second and third Brillouin zone to the first Brillouin zone in a reduced zone scheme. Since every Brillouin zone perfectly fits in the first Brillouin zone we can conclude that each Brillouin zone has same area. We have finished our discussion on Brillouin zones of a square lattice in the next lecture we are going to discuss about drawing Fermi surface in 2 dimensions thank you.