Indian Institute of Technology
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NP-TEL
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on
Technology Enhance Learning

Course Title
Advanced Characterization Techniques

Lecture-29

by…
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Hello everyone. In today's class on advanced characterization techniques we are going to study low energy, electron diffraction. Now electron diffraction is something that we have encountered in the earlier section of our course wherein we studied diffraction in a transmission electron microscope, as well as in a scanning electron microscope for a technique known as electron backscattered diffraction.

However, in today's class we are going to focus on a completely new technique or rather a completely different technique known as low energy electron diffractions which is used to characterize the surfaces of crystalline materials.

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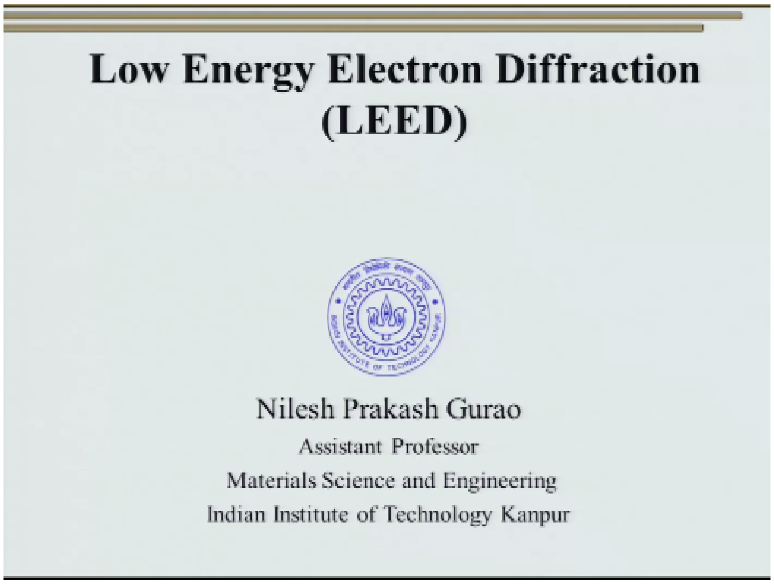

Low Energy Electron Diffraction (LEED)

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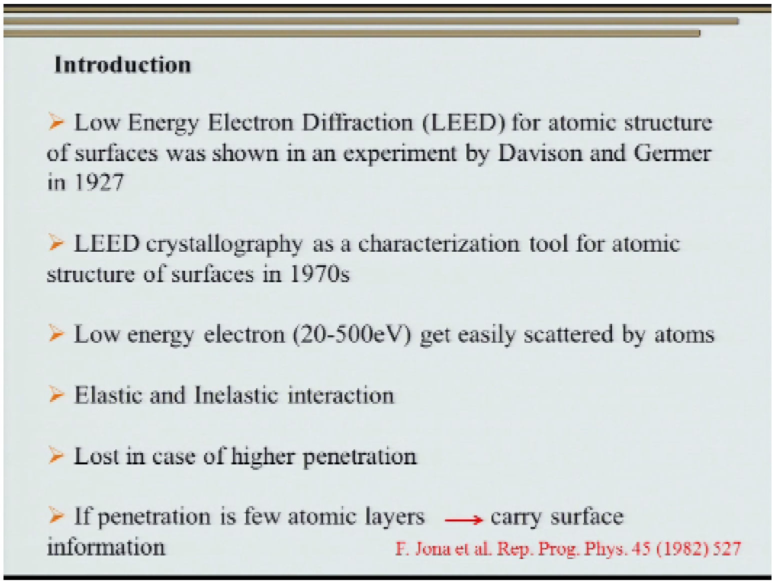

Introduction

- Low Energy Electron Diffraction (LEED) for atomic structure of surfaces was shown in an experiment by Davison and Germer in 1927
- LEED crystallography as a characterization tool for atomic structure of surfaces in 1970s
- Low energy electron (20-500eV) get easily scattered by atoms
- Elastic and Inelastic interaction
- Lost in case of higher penetration
- If penetration is few atomic layers → carry surface information

F. Jona et al. Rep. Prog. Phys. 45 (1982) 527

So talking about Leeds low energy electron diffraction is essentially used for atomic structure of surfaces, and the first experimental observation of low energy electron diffraction was given by an experiment carried out by Davison and Germer way back in 1927. However, the evolution of the field took quiet of you decades and it was not until 1970s that leads was used as a surface characterization tool in laboratories over the world.

So as it we already know as a new in suggest rather this essentially corresponds diffraction from electrons with low energy in the range of 20 to 500 electron volt. We are aware that once electrons interact with matter that needs to elastic as well as in elastic scattering. The in elastically scattered electros get last if the penetration depth is higher within the sample.

However, if the penetration depth is only few surface layers, then we the electron scatter getting diffracted do carry a lot of surface information that can be utilized to get an idea about the structure of the surfaces. We will try to see how essentially it works out in the next few slides.

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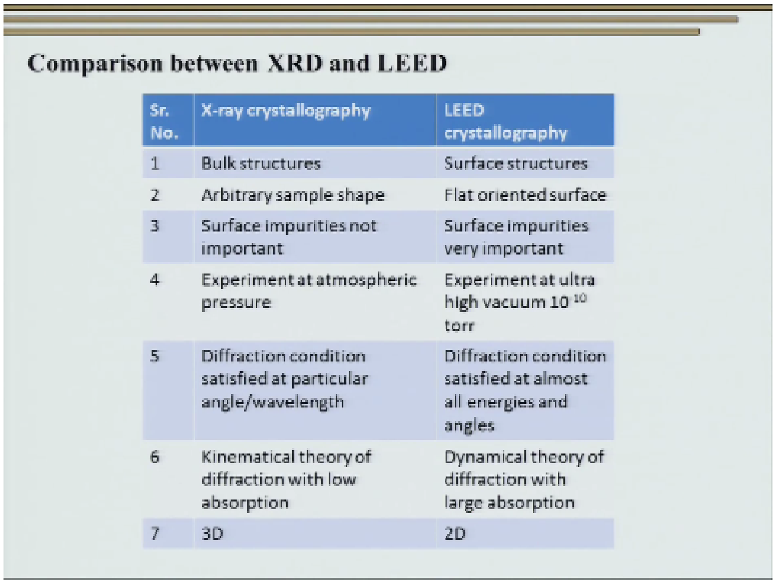

Comparison between XRD and LEED

Sr. No.	X-ray crystallography	LEED crystallography
1	Bulk structures	Surface structures
2	Arbitrary sample shape	Flat oriented surface
3	Surface impurities not important	Surface impurities very important
4	Experiment at atmospheric pressure	Experiment at ultra high vacuum 10^{-10} torr
5	Diffraction condition satisfied at particular angle/wavelength	Diffraction condition satisfied at almost all energies and angles
6	Kinematical theory of diffraction with low absorption	Dynamical theory of diffraction with large absorption
7	3D	2D

But before that let us first compare x-ray crystallography which we had covered in the last three or four classes with leed crystallography. So as the all are aware of x-ray crystallography essentially deals with bulk structures right. While leed crystallography essentially deals with surface structures. I would like to emphasize that x-ray crystallography can be used even to get information about the surfaces.

However the major focus of x-ray crystallography is on bulk structures. Another important thing is that we do not need a particular sample preparation technique or other particular sample preparation condition for carrying out x-ray crystallography. At the same time any arbitrary sample shape can be used in x-ray crystallography while we need extremely flat and oriented surfaces for carrying out leed crystallography.

Surface impurities structurally do not play an important role in x-ray crystallography while and they are very very important in leed crystallography. Generally x-ray diffraction experiments are carried out at ambient temperatures and conditions. However, we need ultra hire vacuum for carrying out lead crystallography. You are also aware that for x-ray crystallography the diffraction condition is satisfied for a particular wave length or particular anger depending on condition of Bragg's diffraction.

However, the diffraction, conditions are pity much relaxed and they get satisfied at almost all energies and angers when it comes to low energy electro diffraction. We had seen that in normal x-ray crystallography kinematic theory of diffraction generally works out, and at the same time we can generally neglect the absorption with the exception of gracing incidents small angle x-rays scattering.

However, when we come to low energy electron diffraction we have to deal with dynamical theory of diffraction and which also accounts for huge amount of absorption in case of low energy electron diffraction. And the basic difference between see something like x-ray crystallography is that it gives us 3D information while a leed crystallography gives us 2 dimensional information of the lattice.

Having talked about it let us go back and try to revise how actually diffraction takes place and this is something that we had covered in the very first class.

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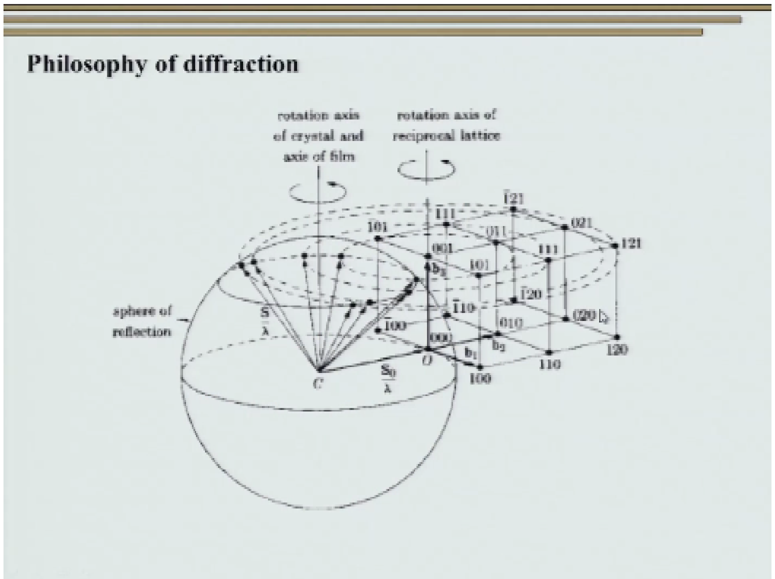

Philosophy of diffraction

Wherein we saw that we have for a every lattice we have a corresponding reciprocal lattice associated with it, during diffraction we use a particular wave length which decides the diameter of the exosphere and all x-ray diffraction are for that matter all diffraction techniques are based on orienting either the crystal or the ewald sphere in such a manner so that the diffraction condition is satisfied. However, as you can easily visualize from this image which were seen earlier diffraction is essentially a 3D phenomenon.

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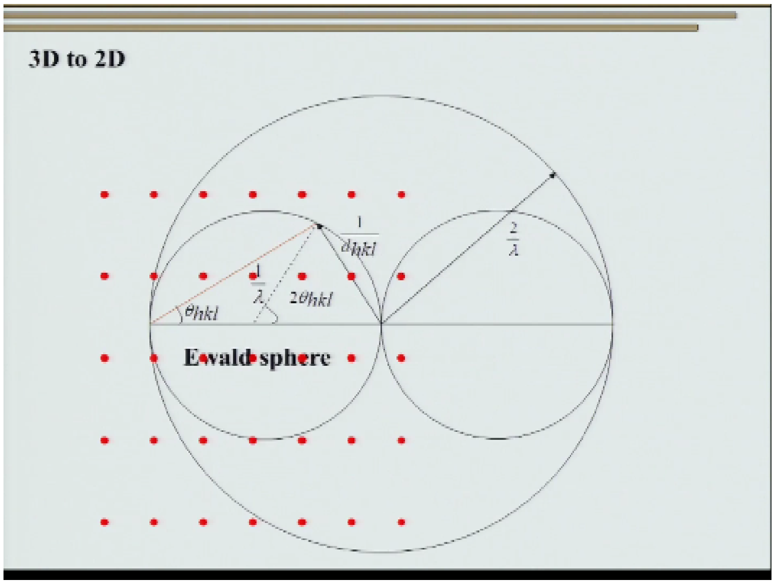

3D to 2D

However, since we are dealing with surface structures if we jump from 3 dimensions to 2D we do see the same construction in 2D, and this figure also we had again seen and here in we see the ewald sphere and the limiting sphere which is a largest sphere and the condition for a diffraction in 2 dimensions.

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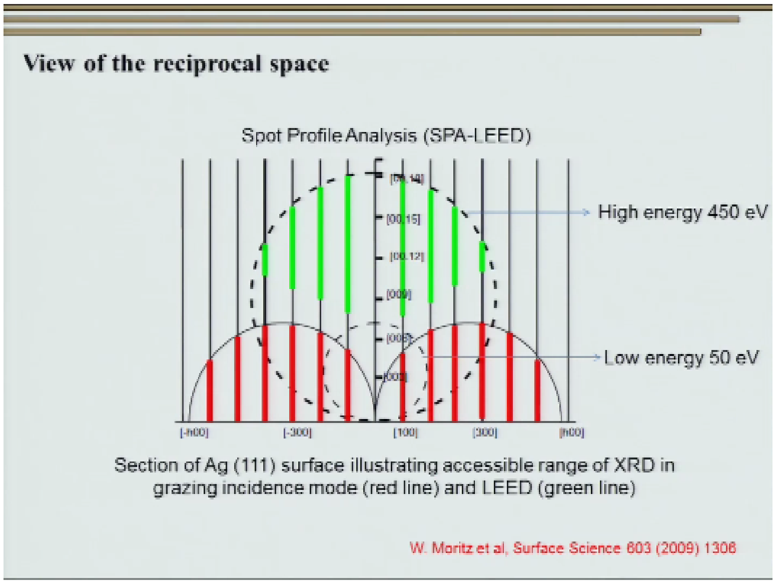

View of the reciprocal space

Spot Profile Analysis (SPA-LEED)

Section of Ag (111) surface illustrating accessible range of XRD in grazing incidence mode (red line) and LEED (green line)

W. Moritz et al, Surface Science 603 (2009) 1306

However, the situation is not as simple and a real picture of this is given through taking a view of the reciprocal space. So in this case we have taken a section of AG111 surface that is the section of the 111 play surface illustrating accessible range of XRD in gracing incidents more which shows the red pot. So herein this is our ewald sphere and you can imagine that with you can always draws as fear comprising of consist with diameter twice that of the diameter of the ewald sphere which comprises of the limiting sphere.

However, what lead essentially offers us is this dotted view or other the dotted circle essentially shows the region which can be viewed, the region of the reciprocal space that can be viewed with low energy electron diffraction. So you can see that part of the region which is not accessible through gracing incidents x-ray diffraction is essentially available through low energy electron diffraction, and this is what the USB of this particular characterization technique.

So as we can see with the changing wavelength with the increase in energy there is a decreasing wavelength and therefore an increase in the diameter of the ewald sphere. So herein this figure we can clearly see that the information given by leed is completely different. It is completely shown here by the green arrows or the green lines over here. So this part or this view of reciprocal space is provided by a leed while the red path the red region shown red lines shown over here is essentially provided by normal gracing incidents x-ray diffraction.

There is another technique which is known as spot profile analysis low energy electron diffraction or what is known as SPA leed which gives us information about exactly perpendicular to the plane, and herein we can get a lot of information about the dimensions of the features on the surface along the Z axis. We will talk more about it in the next few slides, but let us try to understand how exactly 2 dimensional diffraction works.

So you can imagine that once you move from 3D structures to 2D surfaces. The reciprocal space essentially transforms to something like a reciprocal plane.

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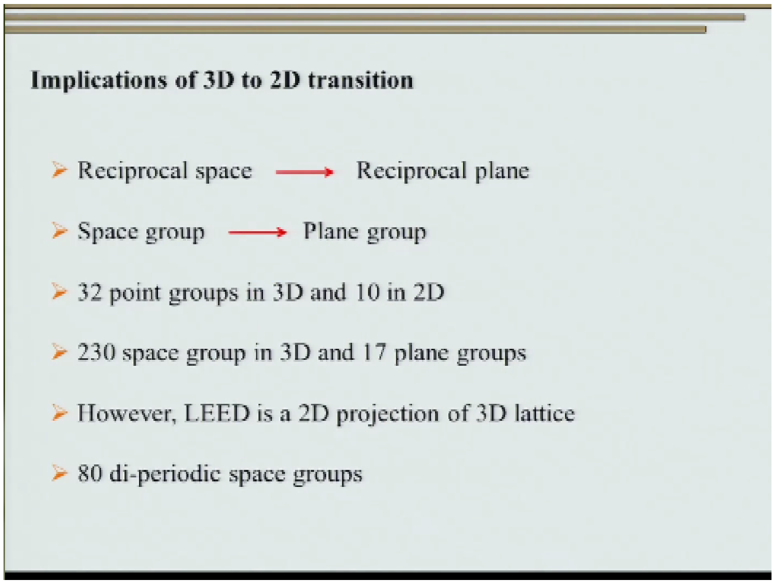

Implications of 3D to 2D transition

- Reciprocal space ⟶ Reciprocal plane
- Space group ⟶ Plane group
- 32 point groups in 3D and 10 in 2D
- 230 space group in 3D and 17 plane groups
- However, LEED is a 2D projection of 3D lattice
- 80 di-periodic space groups

So instead of having the space group we do have a plane group. We are aware that there are 32 point groups in 3D, and there are 10 point groups in 2D. When you talk about space groups we have something like 230 space groups in 3D, and 17 plane groups in 2D right. So the obvious question arises is that when we are looking at 2D patterns of films or eye lanes which are on the surface, are we seeing the 2D structure, well the answer is not really true.

Because we are not seeing the existing 2D planes, instead we have to keep in mind that leed is a 2 dimensional projection of 3D lattice. And therefore, we are not restricted to the 17 plane groups or 10 point groups in 2D. Instead we are left with 80 diperiodic space groups. However, the good news most of them or other all of them have been accounted for, and there are tables like we have tables for all these 32 point groups and 230 space groups.

Even the crystallography community is quite aware of the 80 type periodic space groups which are existing, and this information can be used to characterize or other to index they obtained diffraction pattern. Talking about how exactly the diffraction occurs in 2D this is just the exceptional from the figure which we had shown a couple of slides ago.

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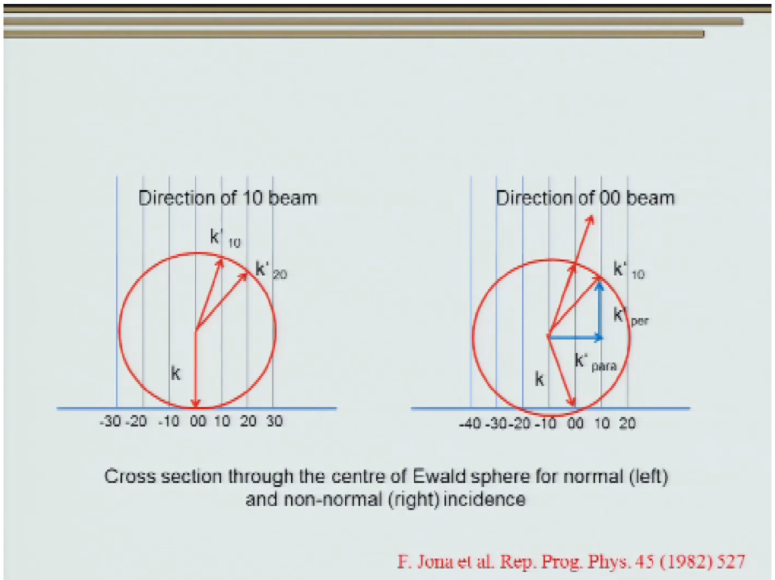

Cross section through the centre of Ewald sphere for normal (left) and non-normal (right) incidence

F. Jona et al. Rep. Prog. Phys. 45 (1982) 527

So here we can have 2 cases or other 2 conditions when it comes to learn as electron diffraction. We can have in normal incidents wherein you can see that your incidents wave is perpendicular to the lattice over here at 000. At the same time in one case we can have incidents which is not normal which can be seen over here in this particular slide. So here we can see that if the incidents are not normal we do get diffraction.

However, this diffraction component can then be classified into a parallel component, the component which is parallel to the surface and component which is perpendicular to the surface right. So this way you can imagine that there are two implications or other 2 conditions were in we can have either normal incidents or we can have non normal incidents in low energy electron diffraction. So this is very similar to what we have in case of x-ray diffraction. So the concept remains the same only thing the implications are slightly different.

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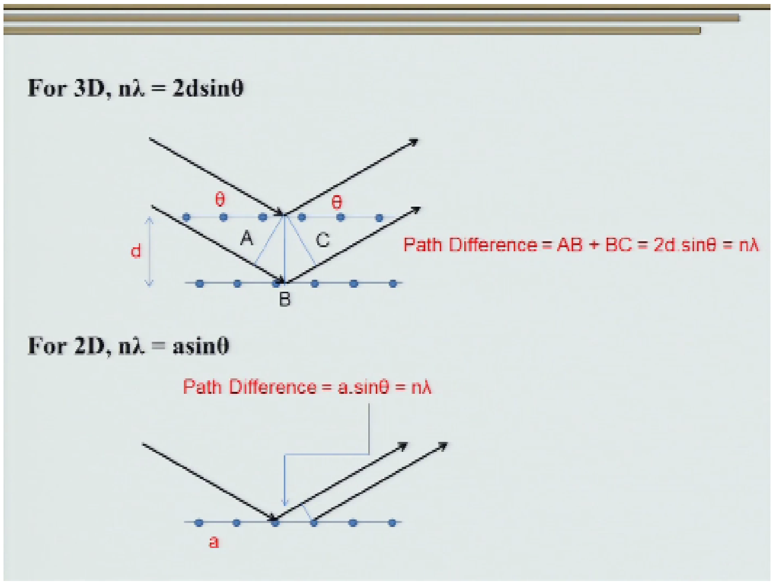

For 3D, $n\lambda = 2d\sin\theta$

Path Difference = AB + BC = 2d sinθ = nλ

For 2D, $n\lambda = a\sin\theta$

Path Difference = a.sinθ = nλ

So talking about how exactly diffraction occurs which is go back and look at the diffraction in 3 dimensions. Now this equation we have come across plenty of times in the last few classes. So the Bragg's law we know that you know $n\lambda=2d\sin\theta$. Having set that we know how to derive to this formula we get and calculate we go and calculate the extra path length that the light X-rays have travel.

In this case it is AB + BC and we know that if the extra path length or the path difference if it is an integral multiple of λ. We do get construct interferers and we essentially the end of getting diffraction. Therefore we have $n\lambda= 2d\sin\theta$. However, when we come to 2D we see that the diffraction occurs in this way having set that we see that this is restricted only to the plane only diffraction occurs only in one plane. There is no diffraction in the third dimension, and therefore the Bragg's law gets modified into the 2D form as $A\sin\theta= n\lambda$.

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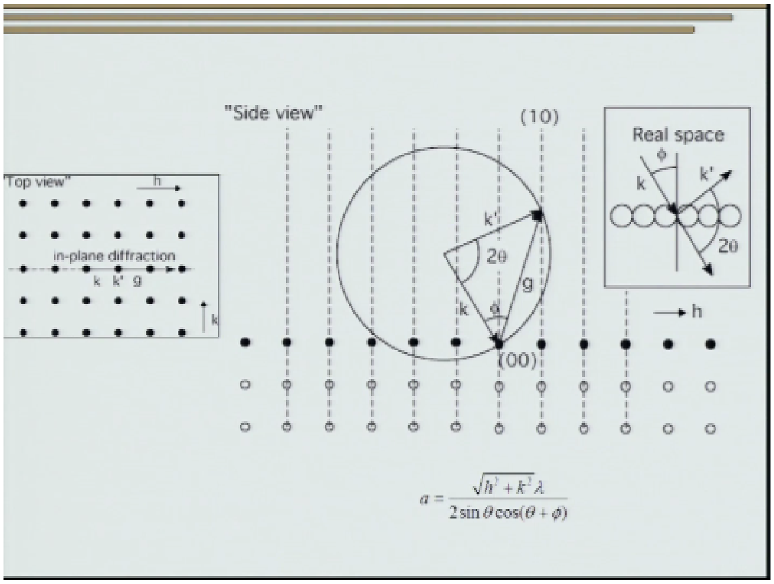

$$a = \frac{\sqrt{h^2 + k^2}\,\lambda}{2\sin\theta\cos(\theta + \phi)}$$

In this particular figure we have given we have shown the actual thing the projection of the ewald sphere. So here again we can see that instead of having a complete space group we are having a plane group, and therefore instead of getting criteria for diffraction all deriving this structural factor in terms of HKL we are just restricted to HNK. Depending on the geometry of the figure we can see that you can derive the Bragg's law for 2D plane condition in with this particular equation.

So this is very similar to our normal $n\lambda = 2d \sin\theta$ stuff. Because you can imagine that this particular term $2 \sin\theta \cos\theta + 5$ essentially accounts for the incident angle, and once taken on this side his particular tell $H^2 + \sqrt{H^2+K^2}$ essentially tells us the distance something which is very similar or analogous to the interregnal distance between the two atoms in case of Bragg's law. So we are all aware.

And I hope we have understood by now that essentially what we are seeing or what we expect to see in low energy electron diffraction is nothing, but the actual reciprocal space corresponding to the 2D lattice under consideration.

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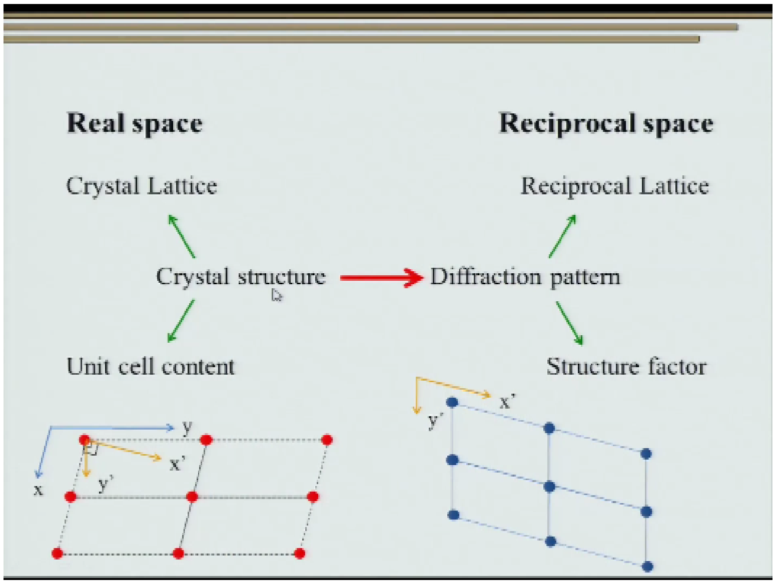

Real space **Reciprocal space**

Crystal Lattice

Reciprocal Lattice

Crystal structure → Diffraction pattern

Unit cell content

Structure factor

So this is again the slide which we had covered that any crystal structure comprises of crystal lattice and unit cell content, and the diffraction pattern associated with it has a reciprocal lattice and a structure factor. So if we have a particular crystal structure with the unit cell and the atom sitting over it, we do get a diffraction pattern which is related in a particular way. So what we are going to actually see in low energy electron diffraction is actually the same thing.

Now the beauty of low energy electron diffraction is that we are essentially looking at 2D structures. So we are really looking at 2D structure in real space and visualize it in 2D reciprocal space.

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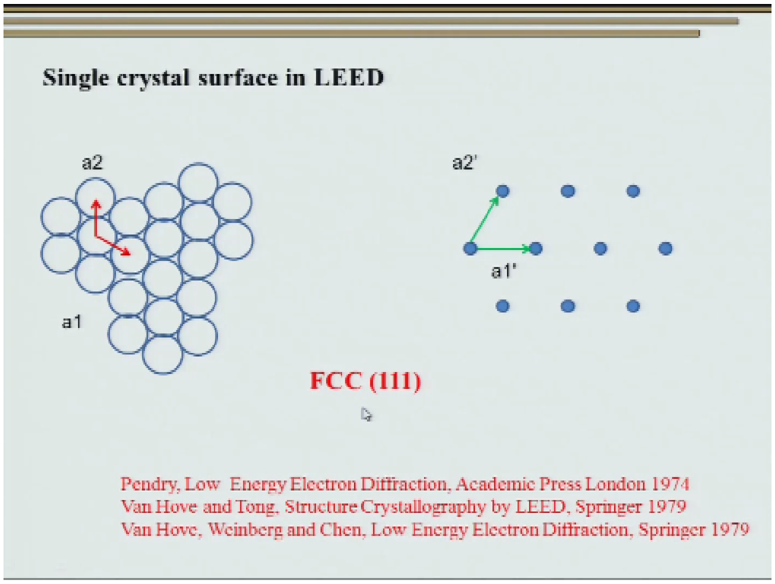

Single crystal surface in LEED

FCC (111)

Pendry, Low Energy Electron Diffraction, Academic Press London 1974
Van Hove and Tong, Structure Crystallography by LEED, Springer 1979
Van Hove, Weinberg and Chen, Low Energy Electron Diffraction, Springer 1979

So just give example so something like 111 plane in FCC which has been shown over here. So you can literally calculate it how we can do that. So I hope you remember the formula for calculating reciprocal factors right, like A* = B x C / A.B x C. so you can extend similar formula and calculate the entire reciprocal space. Now what actually happens in low energy electron diffraction is that you actually see this and this is what I have shown. So this is what we calculated, and this is what you can see over here.

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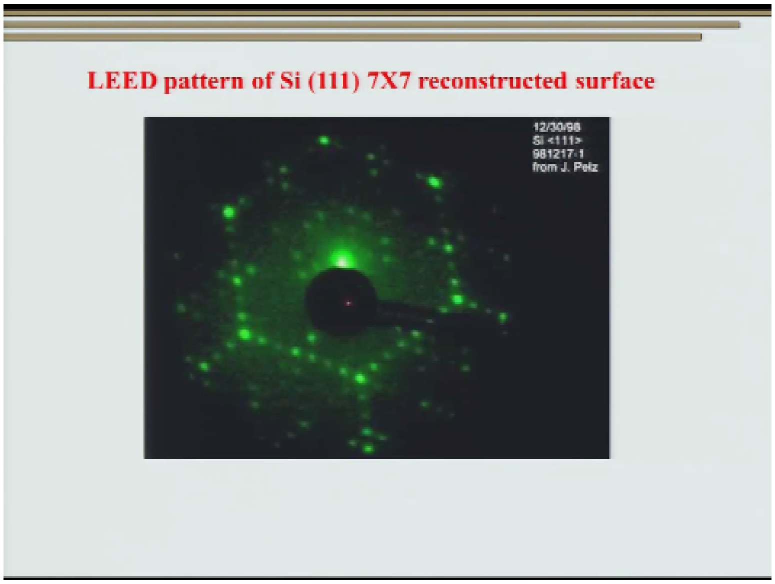

LEED pattern of Si (111) 7X7 reconstructed surface

So in this case we see a low energy electron diffraction pattern of silicon 111 7 x 7 deconstructed surface. So you can see the symmetry get directly reflected in the reciprocal space.

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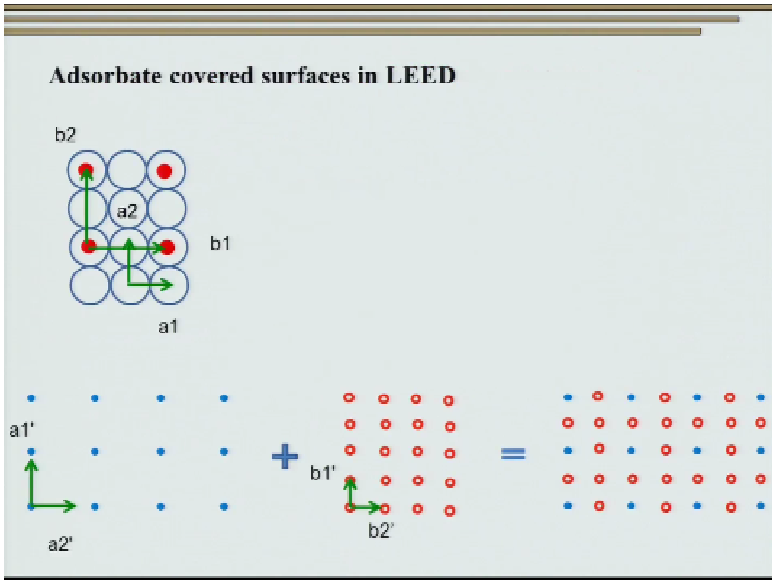

Adsorbate covered surfaces in LEED

Having said that up till now I have just focused and showed you like what all we can do on the surfaces right like looking at the surfaces and all, but there are other important things for the entire branch of surface chemistry that deals with absorption and these options of various chemical entities on the surfaces. So low energy electron diffraction can be used not only to study the structure of the surface, but also to study the structure of the absorbent as well as the sub state.

So here I have shown you a classical example were in we have a sub state which can be characterized by basis vectors of A1and A2 and absorbent. Now the absorbent are sitting at a particular location, and are, if you draw the absorbent lattice you end of getting a basis vector of B1 and B2. So this is what actually exists in the real space. Now how what can you expect in the reciprocal space.

So again we go about and construct the reciprocal lattice of the sub state, and then construct the reciprocal lattice of the absorbent. And then we know that you know what diffraction pattern we are going to get is going to be essentially a super position of these two reciprocal lattices, and this is what we get as a result of existing structure. Having said that what actually happens in an experiment is that we get we do start from something like this the diffraction pattern, and then we kind of go back and essentially derive the structure.

Where the point that I want to emphasize is that we can do a lot of surface chemistry related studies using low energy electron diffraction. However, an important point that needs to be noted that what all we are talking about till now has gives us is only essentially qualitative information that we have often. There are quantitative results that can be obtained through leeds through by leed, but we will talk about it later.

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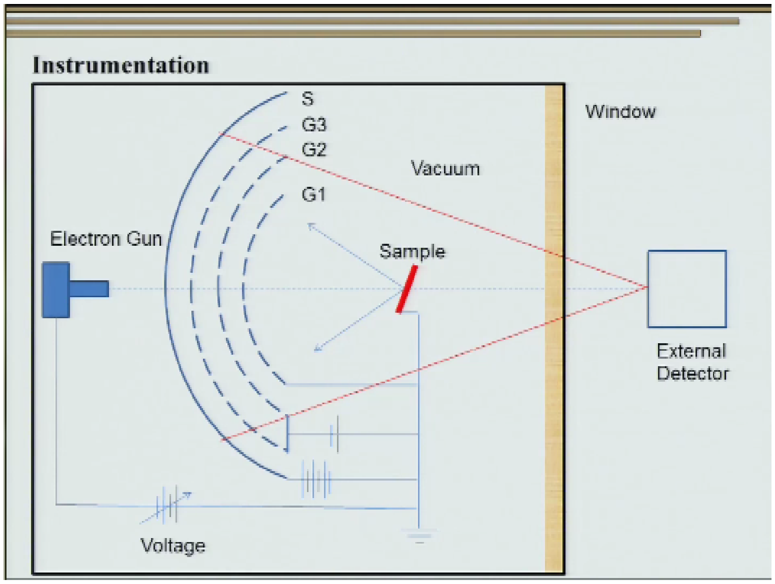

Let us now talk about the instrumentation aspect so talking about leed one of the most striking feature about low energy electron diffraction is this simplicity of the instrument. We talked about small angle axis scattering and greasing incidents small angle extras scattering in the last two classes, and we saw that they involved a lot of instrumentation, right and hardware. However, low energy electron diffraction as such as very, very easy and this can be seen over here.

So all you need is a nice electron gun which gives you electrons with energy in the range of 20 to 500 electron volt. Now this is much lower than what we have in a say a TM or you want to scanning electron microscope. So we need a small electron gun, and entire vacuum chamber were in we keep the sample. The vacuum chamber also comprises of G1, G2, and G3 which are nothing, but the grids at different potentials and the screen to obtain the signal of electrons after diffraction.

So essentially the electron gun axis releases electrons on the samples, the electrons get diffracted partly G1 is the grid which is essentially grounded, while G2 and G3 are kept at in a negative potential to ward of the in elastically scattered electrons and only diffracted electrons go back and hit the screen. This electrons what we are getting we do observed them using external detector.

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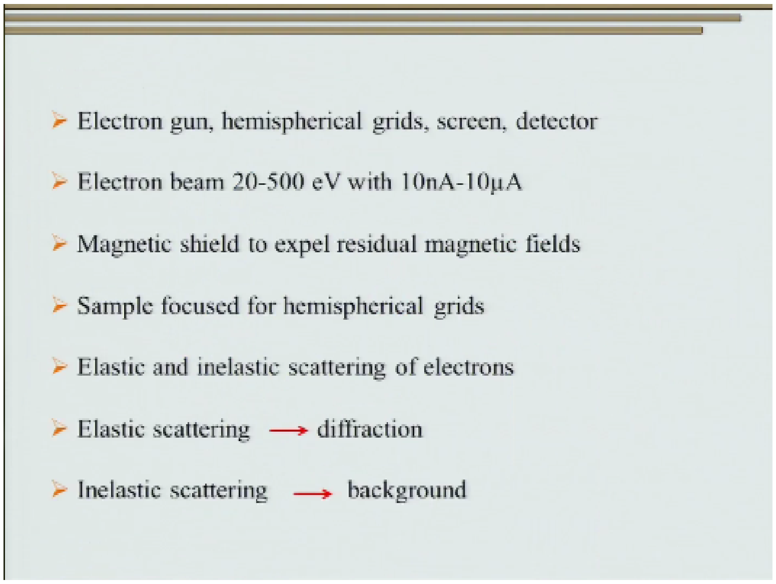

- Electron gun, hemispherical grids, screen, detector
- Electron beam 20-500 eV with 10nA-10μA
- Magnetic shield to expel residual magnetic fields
- Sample focused for hemispherical grids
- Elastic and inelastic scattering of electrons
- Elastic scattering → diffraction
- Inelastic scattering → background

So I had already mentioned we need the instrumentation part is very, very easy and all we need is electron gun hemispherical grid, a screen, and a detector. Now the electron been has to have energy of about 20 to 500 electron volt with current of 10 nanoamperes, 210 micro amps. Another important point is we do need of very strong magnetic shield to expel residual magnetic fields and the sample has to be focused for hemispherical grids.

The elastically scattered electrons which carry all the diffraction information have to reach the screen, while the in elastically scattered electron constitute the back ground and they have to be instead of reflected off.

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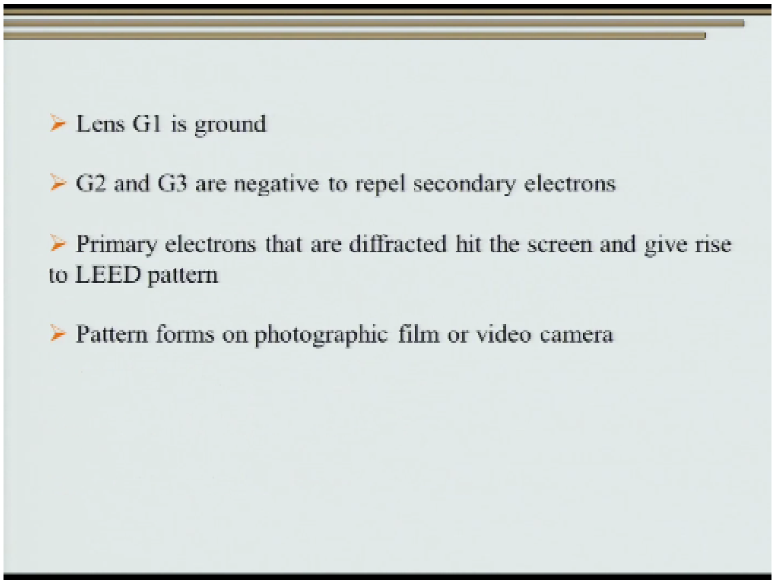

- Lens G1 is ground
- G2 and G3 are negative to repel secondary electrons
- Primary electrons that are diffracted hit the screen and give rise to LEED pattern
- Pattern forms on photographic film or video camera

This is achieved by giving the lens G1 ground, while lens G2 and G3are kept at in the V2 potential. Now what all patterns forming on the screen then we obtained on a photographic film or O video camera.

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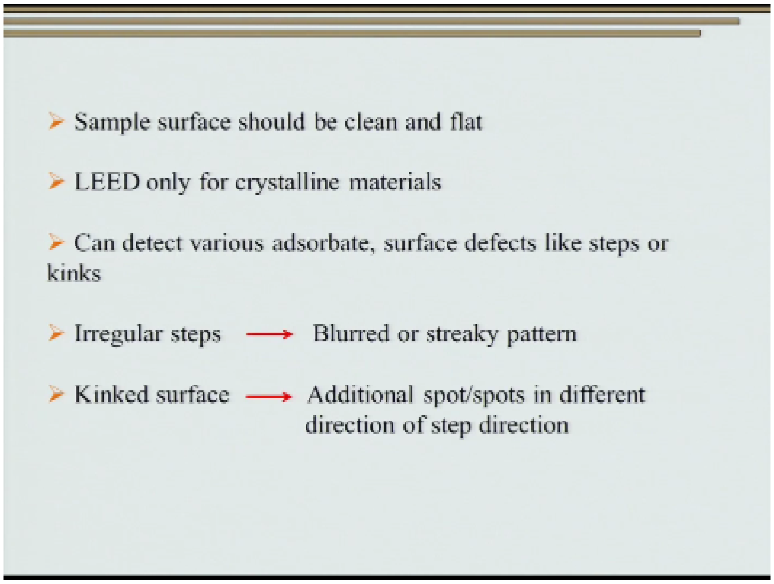

- Sample surface should be clean and flat
- LEED only for crystalline materials
- Can detect various adsorbate, surface defects like steps or kinks
- Irregular steps → Blurred or streaky pattern
- Kinked surface → Additional spot/spots in different direction of step direction

Now one of the important conditions for getting, for carrying out successful low energy electron diffraction is that the sample surface has to extremely clean, at the same time lead gives us information only for crystalline materials which undergo diffraction. We can use lead to detect various absorbent at the same time you can appreciate that if at all there are some defects like steps or kinks on the surface or for that matter.

If there is some kind of relaxation occurring on the surface we do can capture this information using low energy electron diffraction. Therefore, electron diffraction certain features like irregular steps lead to blur or sticky pattern while kink surfaces lead to additional spot or spots in different direction of the step direction. So I would like to emphasize that we need to talk about irregular steps or kinks surfaces.

Essentially we are talking about atomic level of irregularity or kinking. So this kind of ability to really study the structure at atomic level is provided by low energy electron diffraction only. So we have seen the kind of low result we get with low energy electron diffraction were in we see nice spots.

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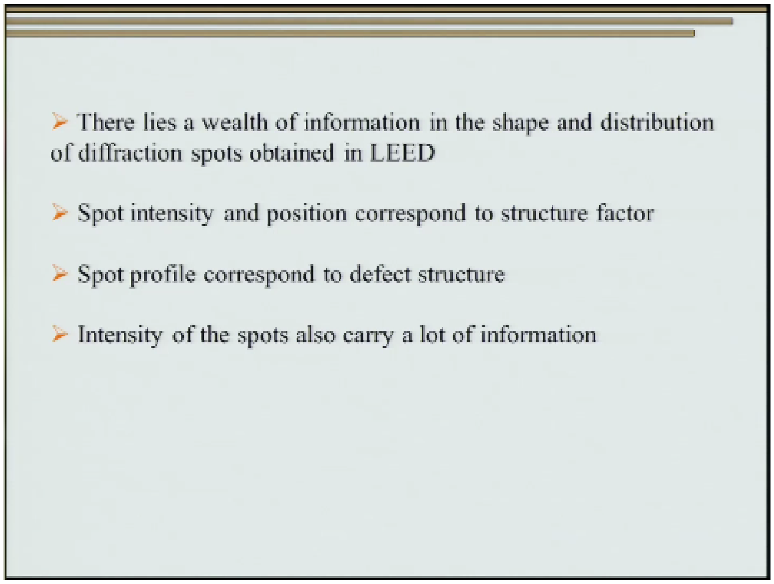

- There lies a wealth of information in the shape and distribution of diffraction spots obtained in LEED
- Spot intensity and position correspond to structure factor
- Spot profile correspond to defect structure
- Intensity of the spots also carry a lot of information

Now there lies a wealth of information in the shape and distribution of diffraction spots of obtained in low energy electron diffraction. The spot intensity and position correspond to the structure factor. Well this is what we agreed actually what we see in low energy electron diffraction is the reciprocal space. At the same time the spot profile can give us a lot of information about the different structure.

This is what we saw that the irregular steps lead to blurring and sticky pattern. Therefore we can see that the spot position as well as the spot intensity and profile carry a lot of information about the surface structure of the material under consideration.

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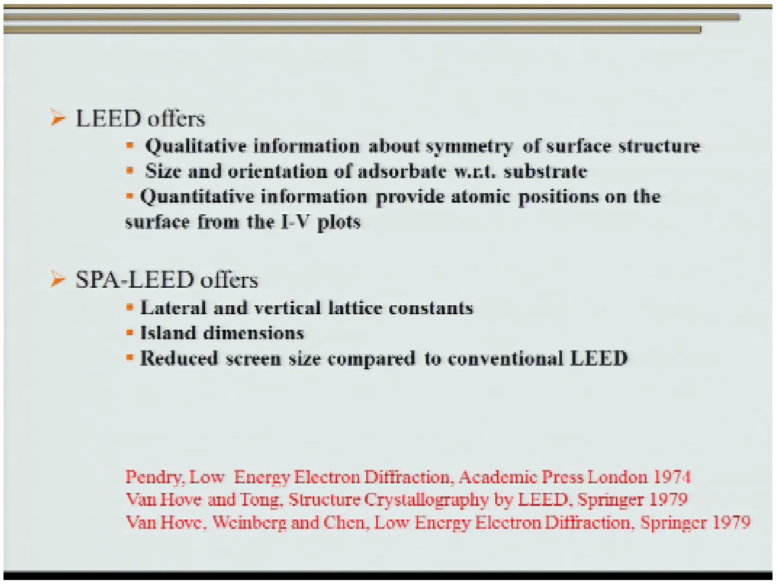

- LEED offers
  - **Qualitative information about symmetry of surface structure**
  - **Size and orientation of adsorbate w.r.t. substrate**
  - **Quantitative information provide atomic positions on the surface from the I-V plots**
- SPA-LEED offers
  - **Lateral and vertical lattice constants**
  - **Island dimensions**
  - **Reduced screen size compared to conventional LEED**

Pendry, Low Energy Electron Diffraction, Academic Press London 1974
Van Hove and Tong, Structure Crystallography by LEED, Springer 1979
Van Hove, Weinberg and Chen, Low Energy Electron Diffraction, Springer 1979

Therefore, we can see that low energy electron diffraction offers us qualitative information about symmetry of surface structures. It also gives us information about size and orientation of absorbent with respect to substrate. It gives us quantitative information of the atomic positions on the surface from IV plans. This aspects we are going to cover in the next few slides, I will like to mention that this is a very involved topic I am going to just touch upon this aspect.

And see that what all we can do with you know IV plots rather than knowing how we can do surface structure analysis using IV plots. Another technique that I had mentioned earlier which was the spot profile analysis low energy electron diffraction. It gives us information about the lateral and vertical lattice constants of serf of islands on the substrate. It also gives us complete island dimensions and reduced.

However, it has a problem that the screen size of offered by SPA leed is much lower compact to conventional lower energy electron diffraction. Therefore, depending on our need we can choose either the lead option or the SPA lead option. I would also like top mention that one thing that we should keep in mind that since we are using electrons for diffraction. We can always use the same electrons for imaging purpose and just use our simple low energy diffraction set up as an electron microscope.

And to get some image to get and electron image and go to the region of our interest and then try to get diffraction from that particular region. Another important point that needs to be discussed is we talked about just single or diffraction even occurring which leads to formation of the reciprocal space.

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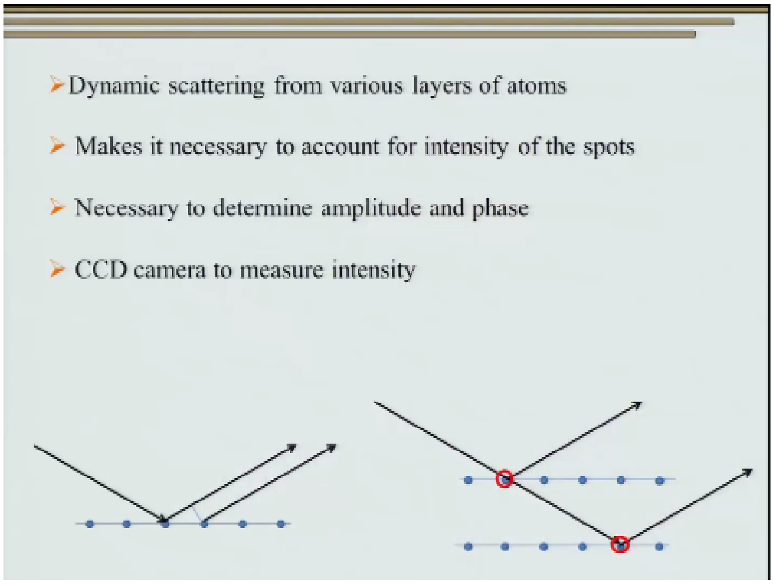

- Dynamic scattering from various layers of atoms
- Makes it necessary to account for intensity of the spots
- Necessary to determine amplitude and phase
- CCD camera to measure intensity

However, as we had mentioned earlier that low energy electron diffraction comprises of dynamic scattering from various the layers of atoms. Now this makes it necessary to account for intensity of the spots. It is therefore necessary to determine the amplitude and phase of the diffracted beam. However, we know that the phase of the beam cannot be determined using a detector. However, the intensity gives us still gives us a lot of information and this is achieved by using a CCD camera in the low energy electron diffraction set up.

So just to illustrate how does dynamic diffraction occurs, this is the classical 2D diffraction that we had seen in the earlier slide. However, when we go and have a dynamic event, right we do see that the diffraction occurs not only from the surface, but also from another from the another level or another plane. Now depending on the kind of things we are having that you have a adsorbent on the sub state, so we can get diffraction not only from the adsorbent atom on the substrate, but also and substrate atom which is below the adsorbent.

So you can imagine that these multiple rather than multiple scattering events are similar to what we talked about in gracing incidents of small angle x-ray scattering. So this essential ensures that this that our bar approximation of single diffraction is no longer valid and we need to modify it extensively.

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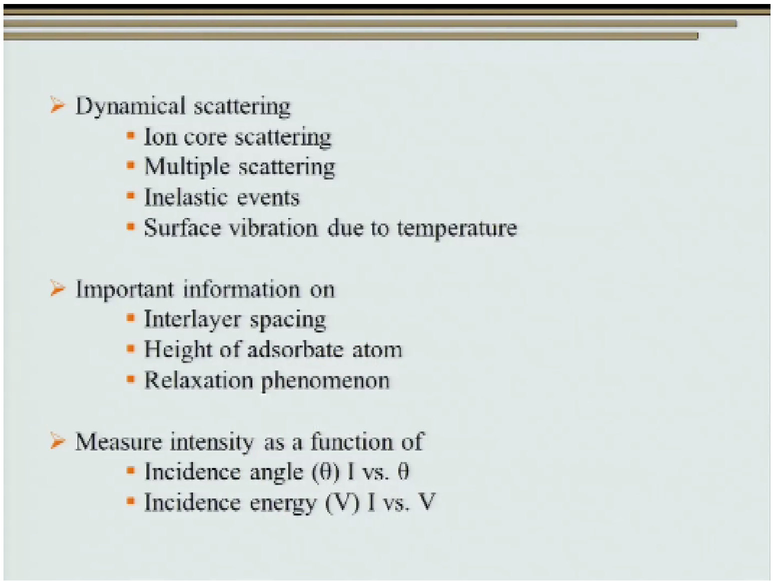

- Dynamical scattering
  - Ion core scattering
  - Multiple scattering
  - Inelastic events
  - Surface vibration due to temperature

- Important information on
  - Interlayer spacing
  - Height of adsorbate atom
  - Relaxation phenomenon

- Measure intensity as a function of
  - Incidence angle (θ) I vs. θ
  - Incidence energy (V) I vs. V

Now this dynamical scattering can be caused because of ion core scattering because of multiple scattering as we had already seen in elastic events like the once that I had mentioned earlier. And at the same time it can occur because of surface vibrations due to temperature. We will come to it and would not go to details and try to find out how exactly this all happens, but all this carries important information on the inter layer spacing in terms of what is the adsorbent and the substrate interlayer spacing.

The height of the adsorbate atoms as well as relaxation phenomena like how relaxation is occurring on of the surface. Now this can be obtained and as at already mentioned by measuring the intensity as a function of incidence angle and incidence energy. We know that if the incidence angle and the incidence energy a changes there is a change in intensity.

So by systematically studying the variation of intensity as a function of incidence angle or incidence energy we do can get different conditions of dynamic diffraction, and then derive back though structure in details.

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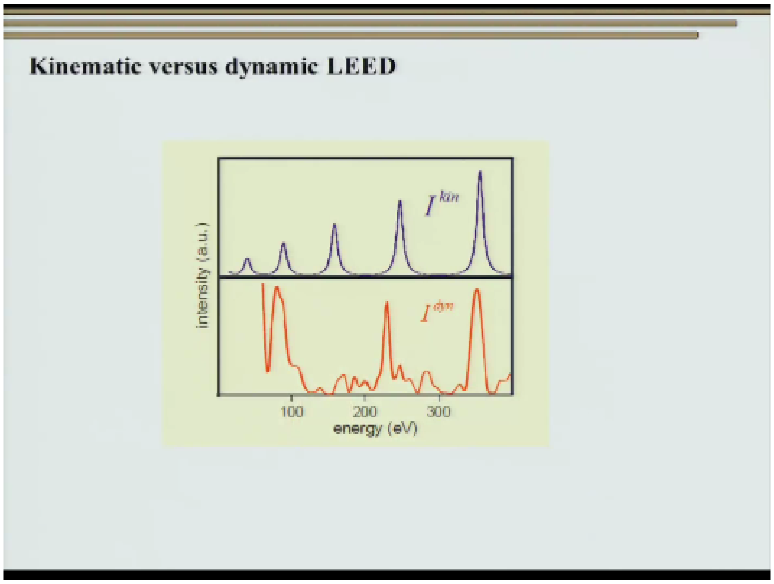

Kinematic versus dynamic LEED

So herein this image how just given you blimps of how actually we can compare kinetics versus. dynamic low energy electron diffraction. So herein we see if at all we are getting kinetic diffraction we see a nice periodic variation of intensity. Though this essentially occurs, I hope you occur because of only single scattering event. Though all this piece that you are seeing is initially corresponds to spot right, all the diffraction spots.

And you should plot the intensity of it and get intensity versus your energy peak versus energy curve, you see that we get a nice periodic pattern. However, if there is dynamic diffraction you see that there is a lot of noise in the diffraction pattern. Now the trouble is it is much easier for us to kind of assume a particular structure and reproduce the diffraction pattern using single scattering event.

However, when you talk about dynamic scattering event I hope you can see that each peak over here corresponds to a different scattering event something what we had noted down over here. And all these events how to be accounted for in order to reproduce this kind of a diffraction curve, and I hope you appreciate that once we are in the dynamic low energy electron diffraction ridging getting information about the structure is very, very difficult.

Having said that one thing that cannot be disputed is that the dynamic leed there is a lot more information than a kinematic leed or leed occurring due to kinematic diffraction. Therefore, it is very important to see what is the effect of θ as well as that of energy on the intensity.

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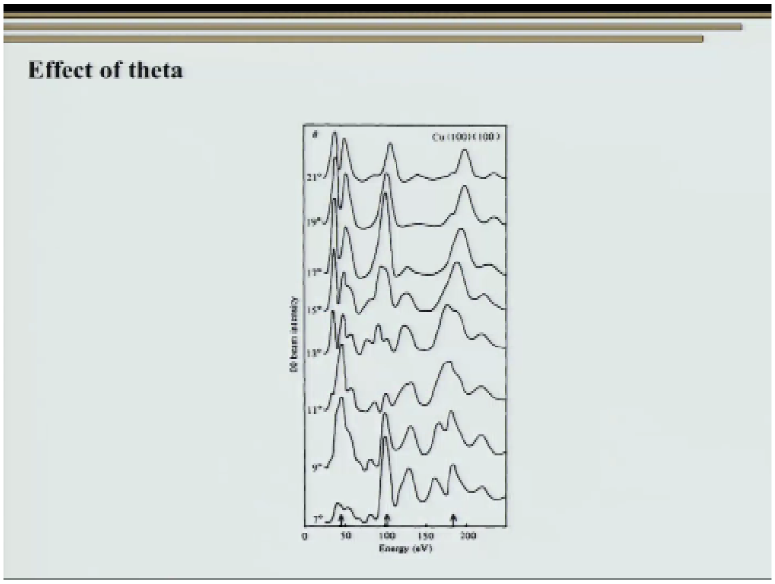

Effect of theta

So herein I have just shown the effect of energy on the beam intensity. So this is for copper 100 surface, and herein we can see that all the peaks that we are having over here. They not only change their position, but also they provide so look at this peak which is at around 100 we see that with the change in our incidence angle which is shown over here you see that not only the peak position is shifting consider the peak position is shifting in fact even the peak profile is changing.

Now this essentially indicates that as we change our incidence angle we are not only getting a change in the kind of the intensity of diffraction or the structure factor. In fact we are getting additional scattering events. Now all this scattering events are to be accounted for when we try to back calculate the structure from the low energy electron diffraction data. So again to go back all these kind of electron or other scattering events.

The multiple scattering events that are likely to occur they have being terminated and are well known. So actually once we get this kind of a pattern our job is to essentially assume a structure and then consider all these diffraction events and try to reproduce this diffraction pattern.

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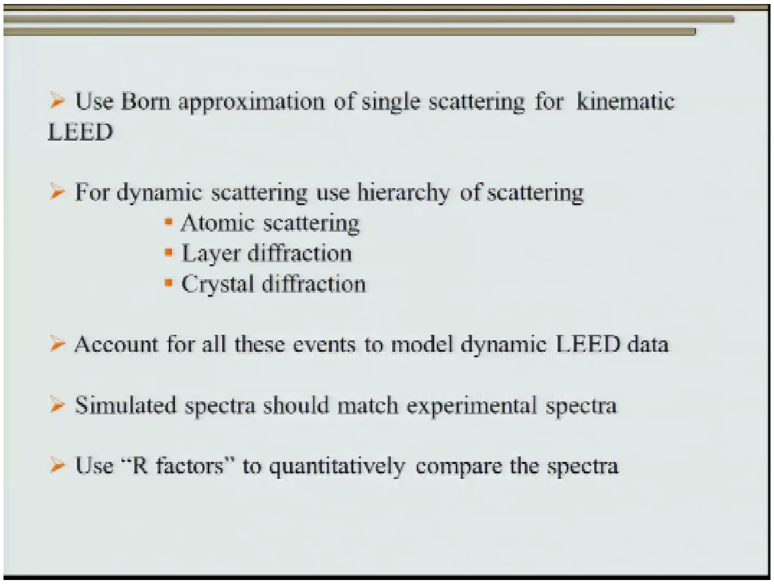

- Use Born approximation of single scattering for kinematic LEED
- For dynamic scattering use hierarchy of scattering
  - Atomic scattering
  - Layer diffraction
  - Crystal diffraction
- Account for all these events to model dynamic LEED data
- Simulated spectra should match experimental spectra
- Use "R factors" to quantitatively compare the spectra

However, this is much easier certain done and as we had already seen that we use bar approximation of single scattering for kinematic leed. However, for dynamic scattering if we start looking at all the events that are occurring it becomes very difficult, and therefore we follow a particular strategy wherein we consider the hierarchy of diffraction. So at the lowest level we have the atomic scattering were in we get scattering from the substrate from the adsorbate atoms right, so that is the atomic scattering or for that matter diffraction from the first atomic layer.

So that corresponds to atomic scattering. The second level of hierarchy is the layer scattering right, so if you have an adsorbate on a sub state the diffraction occurring from the entire adsorbate that corresponds to your layer diffraction. However, depending on your energy or your anger of incidents you can also get diffraction from the crystal itself or the sub state itself. So again going back you can see here that is what seems to be happening that as your incidence angle is increasing which see that you know there is merging of this peaks.

You have a peak which essentially first disappears and then again it reappears. So what exactly is happening? So you can understand we can try to understand it in terms of hierarchy of diffraction and get some idea on it. Now when we actually get the low energy electron diffraction data we account for all this events to model that data. Now our entire job once you get this your spectra is to obtain or rather simulated get a stimulated spectra which shows a good match with the experimental spectra.

However, having said that it is very difficult to compare to spectra and therefore we use what are known as R factors to quantitatively compare the spectra, and there are going two strategies which have been used till date.

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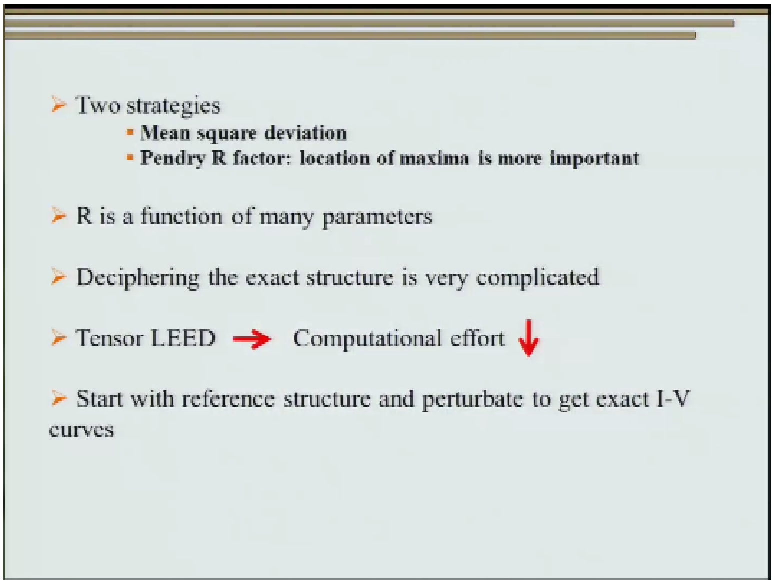

- Two strategies
  - **Mean square deviation**
  - **Pendry R factor: location of maxima is more important**
- R is a function of many parameters
- Deciphering the exact structure is very complicated
- Tensor LEED → Computational effort ↓
- Start with reference structure and perturbate to get exact I-V curves

They includes means to here deviation and pendry R factor. So I need not emphasize much on mean square deviation were we see that you know that the mean square deviation is minimum in the simulated and the experimental pattern, while in pendry R factor approach we see that the location of maximum maxima is more important. I would not go in details, but I would like to just emphasize that what we are trying to do is we assume different diffraction events at corresponding to different hierarchies.

And try to simulate the diffraction pattern on the diffraction spectra. However, we do see that there are lots of parameters that are used to fit the spectra and to know how good our fit is we do use these two strategies. Now our R is a function, the R factor which I showed is a function of many parameters and desafering the exact structure though is possible is very very complicated. However, there are some advances made in data analysis, and one of the latest advantage or one of the latest advancement is what is known as tenser a leed.

Wherein the computational effort required is reduced a drastically. Now in case of tenser lead what essentially we end of doing is that we start with a reference structure and pertubate it to get exact IV course. The intensity was versus voltage course. So this is essentially ensures that we start with a structure and pertubate it to get some idea about the IV curve, and once we get a exact match according to the R factor we get sufficient information about the structure of the surface.

I am not touching upon and going in details of data analysis in this part, because it is to involved and is beyond the scope of for this particular lecture. However, I want to emphasize that essentially we can get lot of information regarding not only key condition of the surface, but also a lot of information about the adsorbate on it not only the kind of adsorbate, but also the orientation of adsorbate using low energy electron diffraction.

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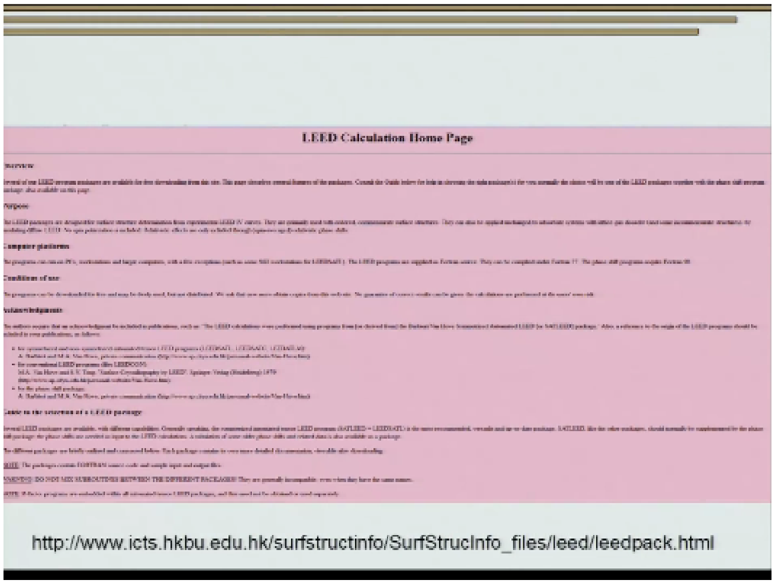

LEED Calculation Home Page

http://www.icts.hkbu.edu.hk/surfstructinfo/SurfStrucInfo_files/leed/leedpack.html

So there is to do all this data analysis there are dedicated software's which are availables I have listed down one of the lead calculated homepage wherein you can go and take your data and do the calculation. But calculation of your structure from low energy electron diffraction is a field in itself and it requires a lot of analysis and understanding of the diffraction processes occurring in 2 dimensions in various materials.

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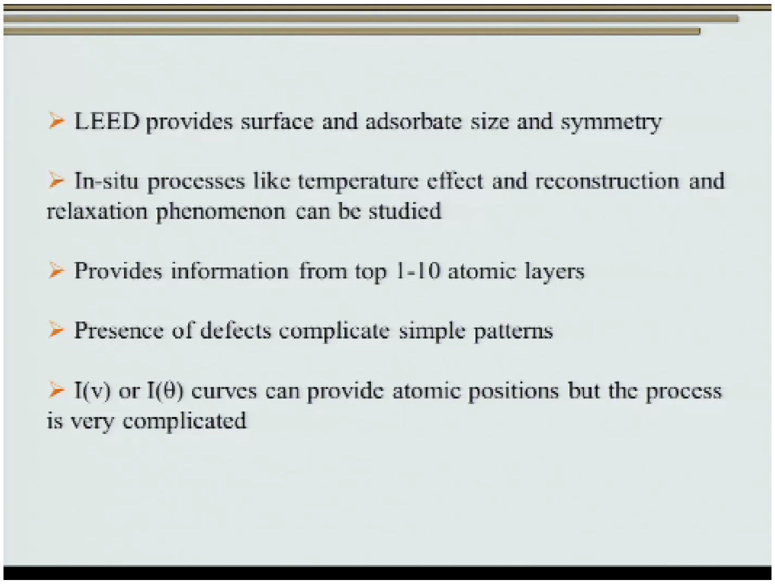

- LEED provides surface and adsorbate size and symmetry
- In-situ processes like temperature effect and reconstruction and relaxation phenomenon can be studied
- Provides information from top 1-10 atomic layers
- Presence of defects complicate simple patterns
- I(v) or I(θ) curves can provide atomic positions but the process is very complicated

So just to summarize I would like to emphasize that low energy electron diffraction provides surface and adsorbate size and symmetry. It is very good or a very sophisticated tool to study in-situ processes like temperature effect and reconstruction and relaxation phenomena in crystalline materials. It provides information from the top 1 to 10 atomic layers and can account for all the surface reactions which are occurring in different materials.

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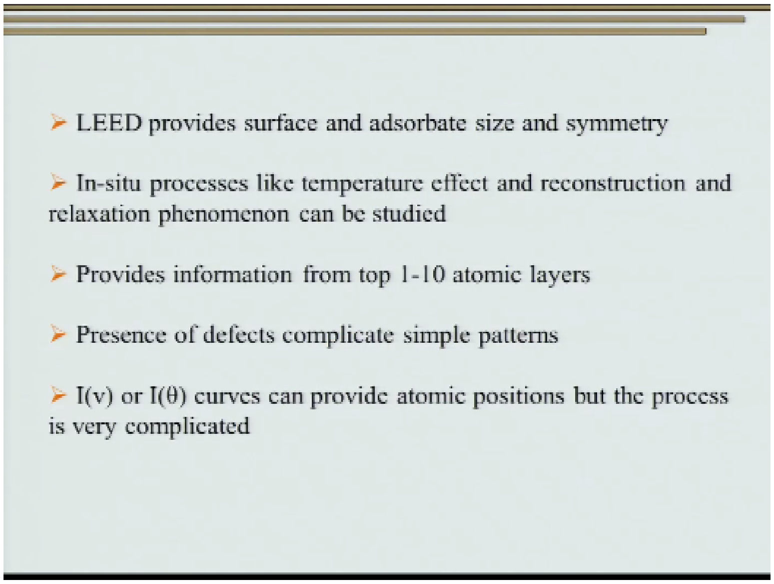

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However, the presence of defects like kinks and ledges can complicate the simple diffraction pattern that we had elevation from the derivation of the reciprocal space. The IV on Iθ curves which gives us the variation of intensity with the voltage or the incidents angle have a lot of information about the, not only the structure and orient, but also the orientation of the adsorbate and the surface. But they are very complicated and need a much careful analysis to get to derive any important information.

(Refer Slide Time: 36:13)


Thank you

Thank you.

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