Neutron Scattering for Condensed Matter Studies
Center for Distance Engineering Education Programme
Indian Institute of Technology, Bombay
Lecture 8B

Keywords: monochromators, Maxwellian, Vertical focusing, Mosaic spread, Position Sensitive Detector

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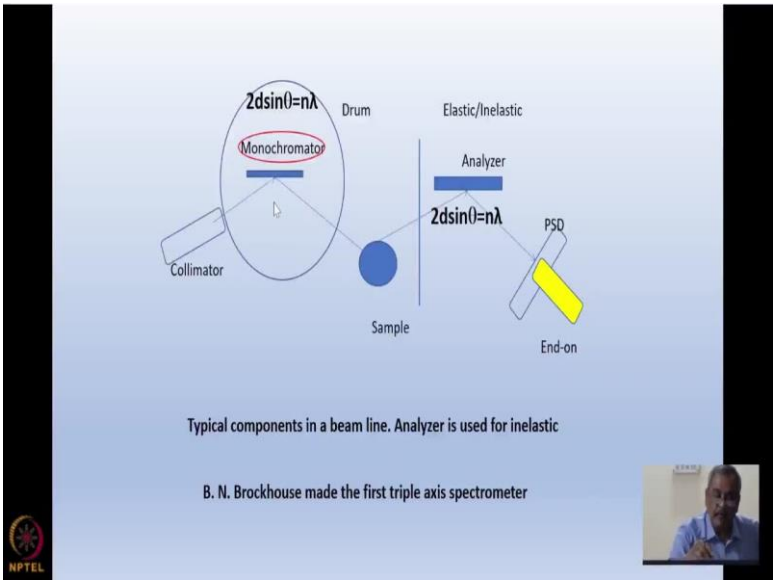

Now, I have come to a very important part of a neutron spectrometer known as monochromators. As you can see the diagram, there is a collimator in the beam path known as in-pile collimator and then it is followed by a monochromator. This is a monochromator actually. Polychromatic beam is falling on the monochromator and what goes out is a monochromatic beam. The circle you see in diagram represents the monochromator drum and at the center of this drum is the monochromator. The first triple axis spectrometer was designed by BN Brockhouse: you can rotate the monochromator and the whole spectrometer rotates around it, including the sample, the analyzer and the detector.

By rotating the monochromator, you can choose different wavelengths (λ) of neutrons then there is sample which scatters the beam and afterwards there may be an analyzer. If you have an analyzer in the beam path, then while keeping the rest of the things fixed, you can rotate the analyzer and do an analysis of the scattered beam's energy before it goes to a detector.

I must mention that neutron detectors cannot distinguish energy of neutron because neutron has to be converted to some other radiation before it is detected. And I just showed that you

have choices of having a position sensitive detector or an end-on detector which we will discuss later. In earlier days, we used to have a single detector which moves from one position to another to cover the angular range for monitoring the scattered beam and it takes longer time.

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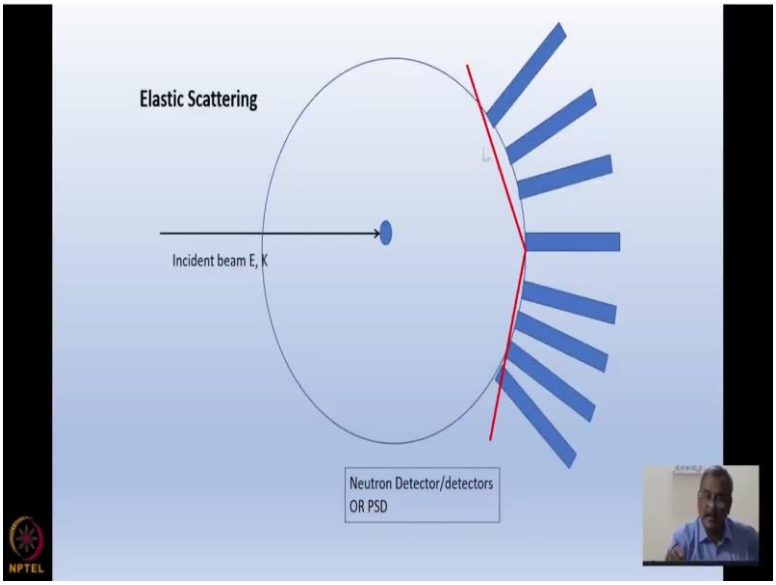

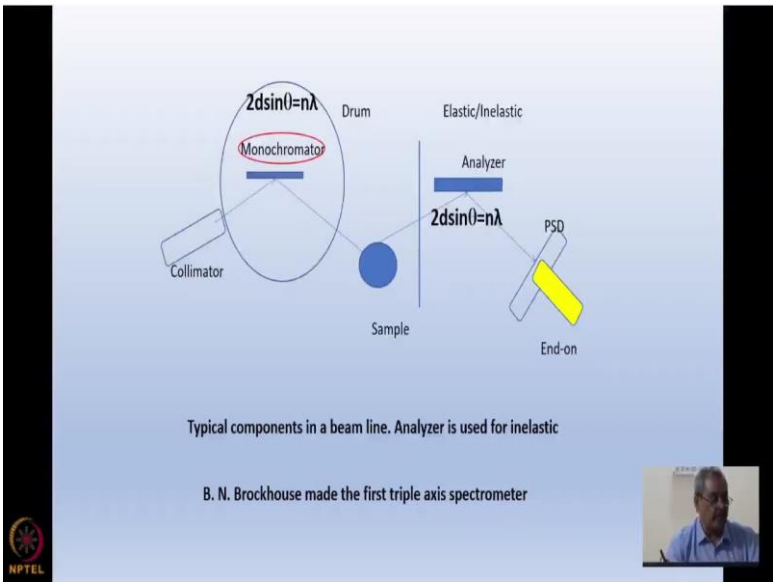

Nowadays, we have got something called position sensitive detectors. The beauty with these detectors is that you know at which point the neutron has hit the detector and once you know the point, knowing the distance from the sample, you can find out the angle of scattering. So, in one shot, you can collect the data unlike the previous case where you go on collecting the data over time serially. This is sort of a parallel processing all the data at the same time. Three axes of triple-axis spectrometer are the monochromator, the sample, and the analyzer.

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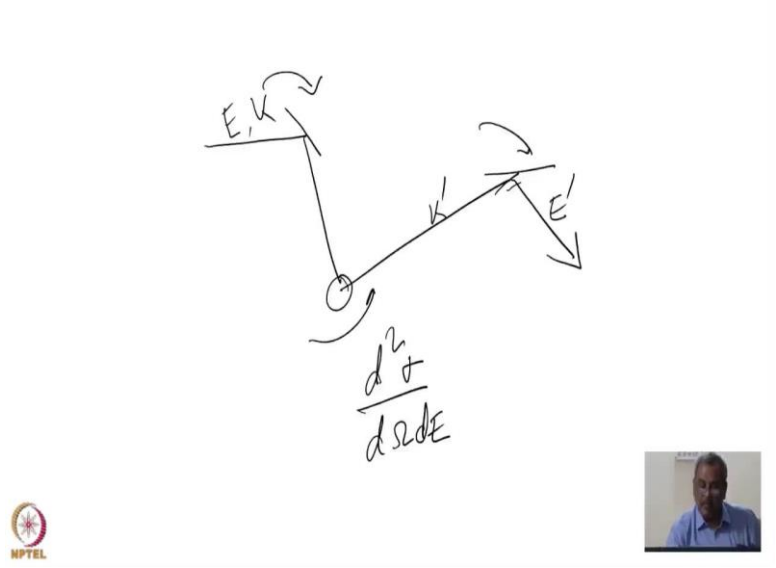

The monochromator axis is followed by the sample axis which is followed by the analyzer axis. This is what was done by BN Brockhouse and he got a Nobel Prize for his studies. This is for inelastic scattering experiment; here we know the energy of the incoming beam and after analyzing the we can tell about the energy of the outgoing neutron. So, in such experiments we do have knowledge of both E' and K'. This is the measurement, which I discussed with you earlier. Inelastic differential scattering cross section is given by $\frac{d^2\sigma}{d\Omega dE'}$, which is measured for getting the dynamical processes in the system at various timescales.

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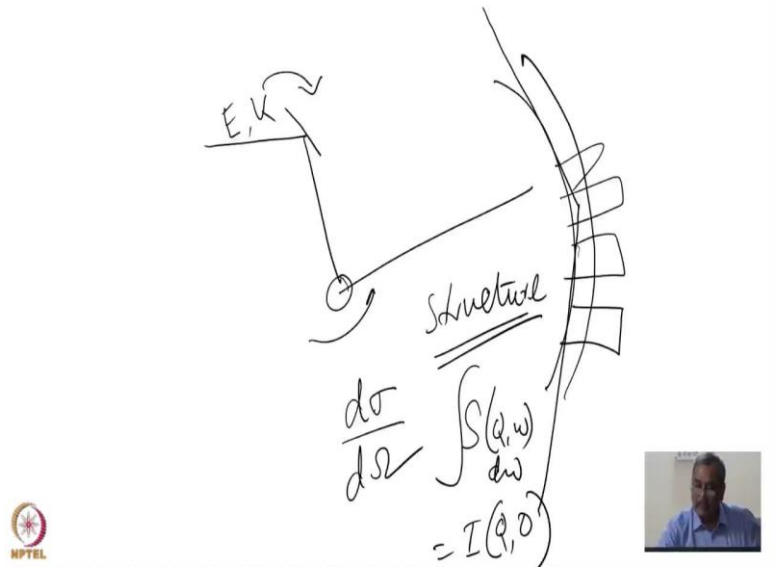

However, if I take out the analyzer part then there is just a sample followed by a detector. This arrangement is used to determine the structure at various length scales with scattering cross section, here shown as $\frac{d\sigma}{d\Omega}$. these are also integration of $S(Q,\omega)$ over ω which gives $I(Q,0)$. I hope you remember when I discussed the kind of correlations in case of neutron scattering.

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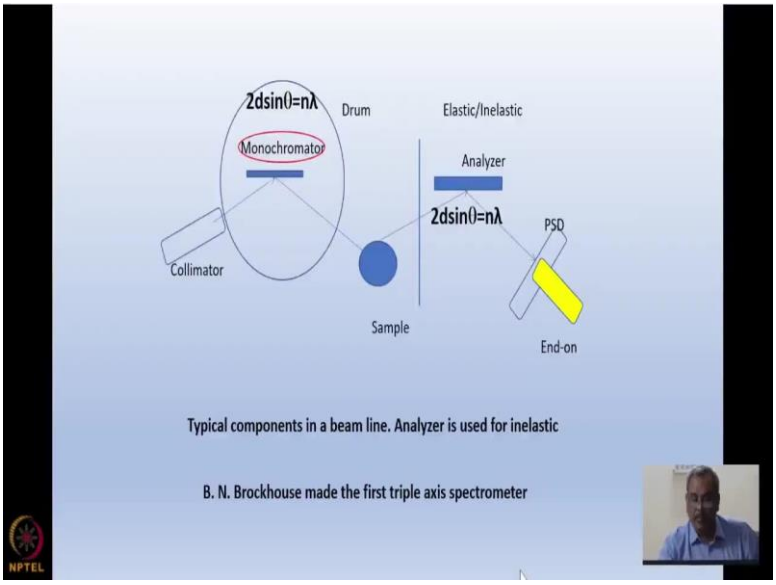
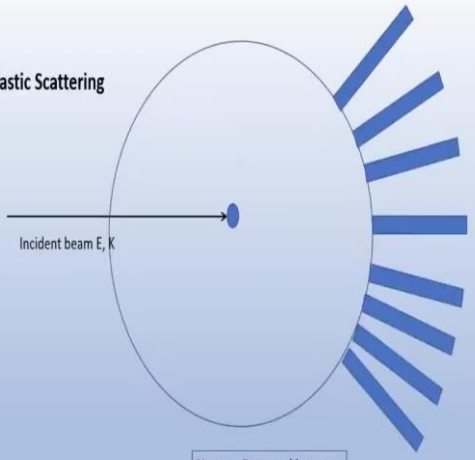


Monochromator selects a single wavelength from the Maxwellian spectrum using Bragg's law.

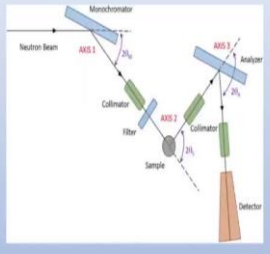
$$2d \sin\theta = n\lambda$$

This is usual. Sometimes one uses filters to allow a larger band of neutrons

Elastic Scattering



A typical neutron scattering set up



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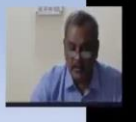

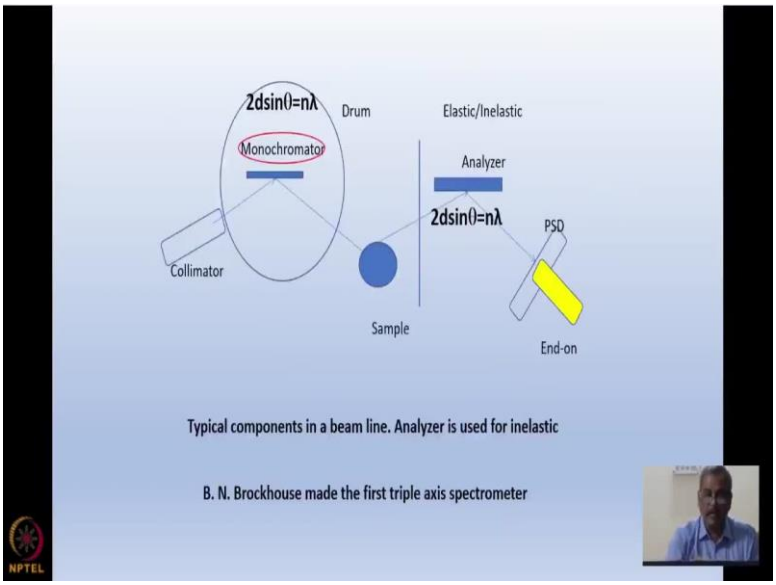

Now, we have reached an important point that is the monochromators and we will discuss how to monochromatize the beam. The monochromatization is not a difficult task. You know that we use Bragg's relation, $2d \sin\theta = n\lambda$ on the Maxwellian spectrum to choose a particular wavelength for experiment. One can also use a filter instead of monochromator where filtered beam is used for a low-resolution experiment and then you can look at the analyzer and at the detector. The configuration shown is also one possible configuration.

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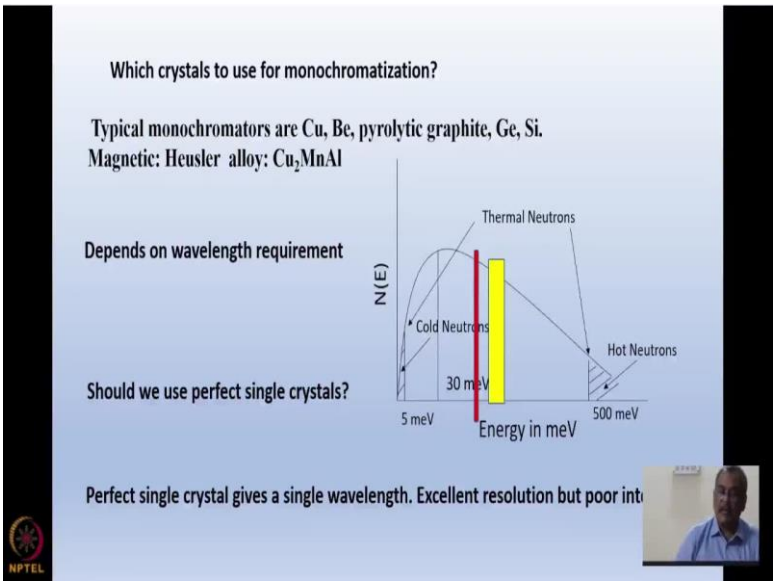

Typical monochromators that are used, are Cu, Be, paralytic graphite (PG), Ge, Si crystals. We also have magnetic polarizing monochromators. Heusler alloy, Cu_2MnAl, is a monochromator cum polarizer which not only monochromatizes the neutron beam but also chooses one particular polarization of the neutron beam. I will come to it later.

The angle and the plane that we choose depends on the wavelength as we need to satisfy the Bragg's relation and for that correct interplanar spacing (d) must be chosen for a particular wavelength. Now, should you use perfect single crystals? In the figure, I have drawn here two vertical blocks. If I use a perfect single crystal then you have one very specific plane which satisfies Bragg's relation and it gives out only a narrow slice of the neutron beam. It certainly gives a monochromatic beam, but you also have the added requirement that you need more neutrons because already the neutron flux is reduced largely when it comes out from the reactor beam line. Now, you are monochromatizing it but then you have competing interests, that is you need a monochromatic beam, but you also need large number of neutrons to do your experiments. How to have those dual purposes serve? What we do need actually is a larger slice of this beam.

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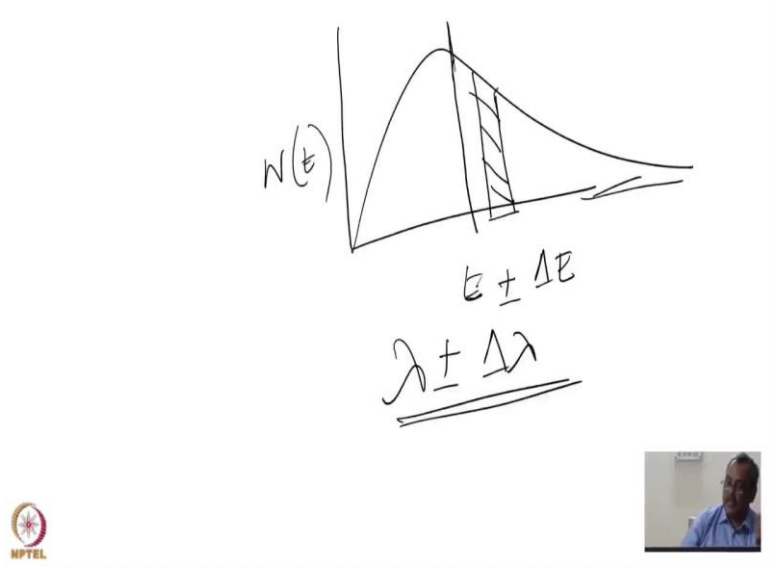

In summary, if I put a perfect single crystal then out of the Maxwellian distributed neutron beam, which has come out from the reactor, we will have a delta function in energy and we will be left with very few neutrons. But what I need actually is, more number of neutrons. That means, I need $E \pm \Delta E$. But of course, immediately the question arises that the lambda becomes undefined and there will be uncertainty in the wavelength. I am ready to accept uncertainty at the cost of resolution where we also need more number of neutrons.

Every experiment is a design where you have a compromise between resolution and intensity. I want intensity and I also want to have resolution reasonably good. So, I have to make a compromise between these two by taking a larger slice of the beam from the Maxwellian. It is usually done by the mosaic crystal.

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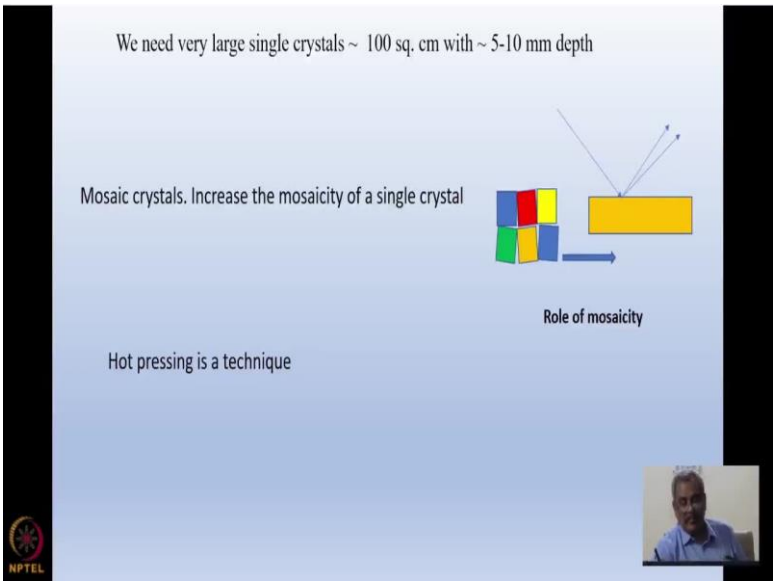

Mosaic crystal is one which has got crystallites which are perfect in themselves. These are the crystallites shown in various colors, but now they are slightly oriented with respect to each other. The way it can be done actually is: you take a perfect crystal, (and then) you can hot press it. That means you take it to a higher temperature and then press it and then it will introduce grain in the system. and you can have slightly misoriented, note my words slightly misoriented crystallites.

In that case, when the beam falls, if I take a polychromatic beam with a single direction, for the outgoing beam some will scatter at a lower angle, some of them will scatter at a higher angle and you have a range of angles and a range of wavelengths in the outgoing beam, which is desirable. Similarly, we can also use bent single crystals, I will come to that.

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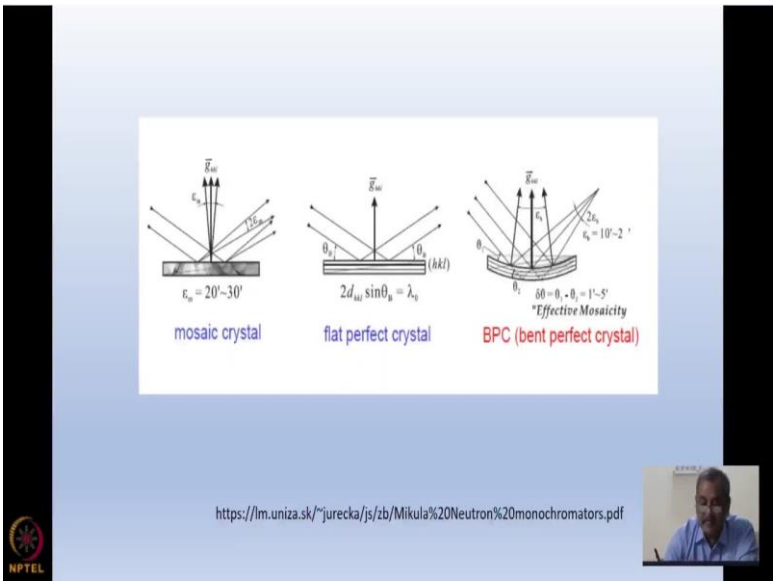

In the figure, I just show you that if you have a flat perfect crystal, in that you have only a parallel outgoing beam of single wavelength. In a mosaic crystal, you have a parallel beam coming. But there is some angular variation in the planes that are offered to the incoming polychromatic beam. So, the angle becomes slightly different for another wavelength from the incoming beam. So, you have got is around 20 - 30 arc minutes of angular variation and hence you have got a resolution compromise, but you gain in the intensity using a mosaic crystal.

Another way of increasing this angular width is to use a perfect crystal but to bend it. Look at it from left to right. You can see that when the parallel beam falls at the left side then the angle of incidence is smaller while towards (another end) it is larger. This (geometry) focuses the beam. It is like an elliptic mirror, which focuses the beam but it also gives you larger spread in wavelength. That means it makes some compromise on the resolution to give me intensity. So, instead of flat perfect crystal, I will try to use either mosaic crystals or bent perfect crystals. Both of these help me to gain the intensity at the cost of resolution.

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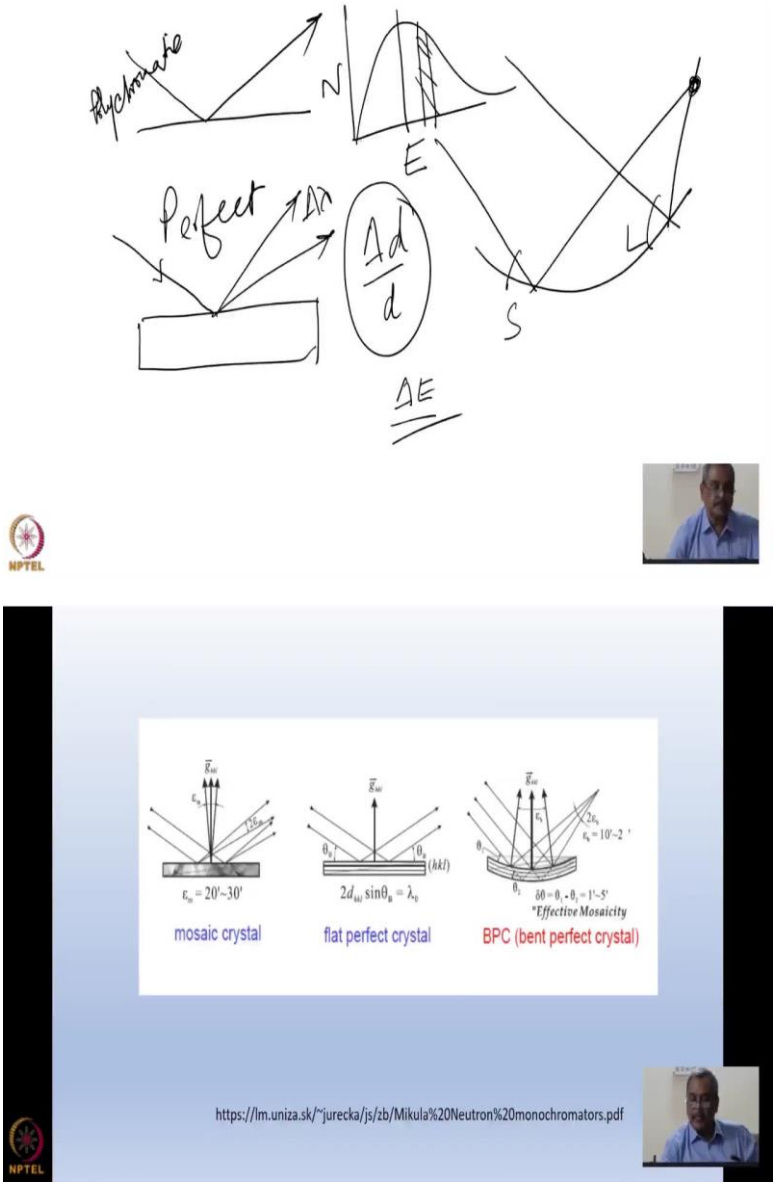

Hence, if it is a perfect single crystal, you have only one angle going out for the incident polychromatic beam. The incident direction has been fixed by the soller collimator but with many energies. The single crystal chooses one of the many energies but it will highly reduce the intensity. Hence, I don't want this.

Now, I have a mosaic crystal. As I showed you in case of Mosaic crystal, there are lots of small crystallite inside. So, for the polychromatic beam, the (Bragg) direction becomes slightly uncertain. It gives me a broadening in wavelength, that is a larger slice from the Maxwellian. So, the neutron flux gets enhanced and I had to make some compromises on the wavelength resolution, and also on the *d* resolution, because when I am doing Bragg diffraction, $\frac{\Delta d}{\mathrm{d}}$ is the

parameter of interest for us. How good we can resolve our *d* spacing, and that depends not only on ΔE but also on $\Delta\theta$.

Also, I can use a bent crystal when I put a parallel beam on a bent crystal, you can see the angle here is small and the angle here is large. So, you have got a focusing effect. And again, it gives you a ΔE. These are the tricks for that one uses to improve the intensity in the beam at the cost of resolution.

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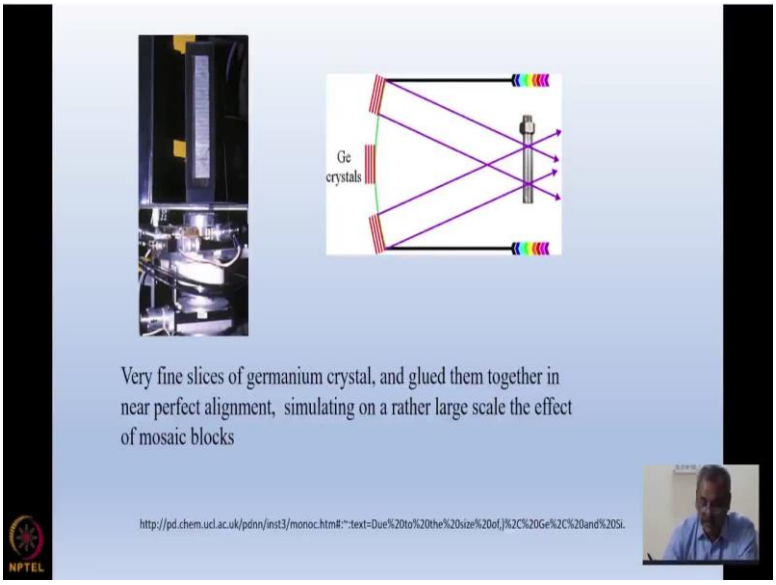

Now I am just showing you a photo where very fine (thin) Ge crystal slices are used. This photograph will give you some idea about a specific assembly of monochromator. Here, height is almost 20 – 25 cm, and at each point there is stuck a single crystal which is bent and the curvature is in the vertical plane. Due to this geometry, the reflected beam is focused onto the sample. So, it makes the beam size smaller, it makes a compromise on the angle and as I told you here the resolution is not compromised, because you are doing the focusing in the vertical plane, but you are doing the experiment in the horizontal plane so you gain in intensity using the Ge crystals, but you get high resolution data in the horizontal plane. Usually if the neutron beam is large and you want to use a smaller sample size then this (arrangement) is required. It is very difficult to grow large quantity of samples especially if the samples are novel and you need to get data from them, then this is one way it can be done. This arrangement is in RAL, UK.

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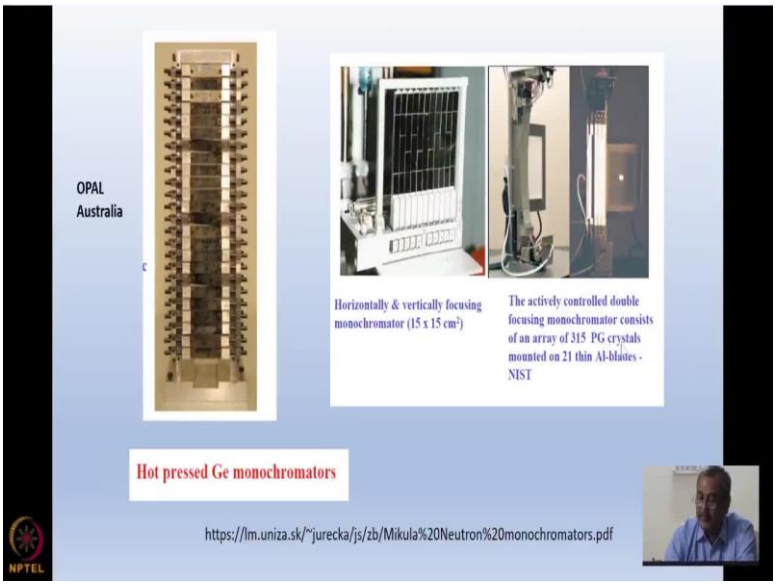

Also, I will show you the OPAL reactor in Australia. These are hot pressed Germaniums. They have made a vertical stack of these germanium (crystals). Each one has been hot pressed. That means they have a lot of mosaic spread in them. First you make the vertical focusing so you reduce the size of the beam and then there is mosaic spread so that there is wavelength spread and you get more intensity. This is in OPAL Australia, (where) they have these hot press germanium monochromators. And as I showed you that there is a horizontally and vertically focused monochromators and all these sizes are typically 15 - 20 cm. Hence, these are the large assemblies and ultimately the beam size can be as low as 1 cm^2. You can see that these are actively controlled double focusing monochromators consisting of an area 315 paralytic graphite crystals. This is in NIST USA. Possibly, monochromator is a single most very important component in our beam path. Now, let me come to the fact that I talked to you about (regarding) beam tailoring inside the reactor and the target and after the beam tailoring, how they are transported out. I talked about beam holes, beam lines and the guides. And after have brought them to the beam, I talked to you about various collimators and filters that you put in the beam path and at the end, I have talked to you about how to get a monochromatic slice from a polychromatic beam using these techniques. In the next lecture. I will discuss with you the role of detector and monitor counters in neutron experiments and then we will get into real experiments with samples.