Neutron Scattering for Condensed Matter Studies
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Week 7; Lecture 18B
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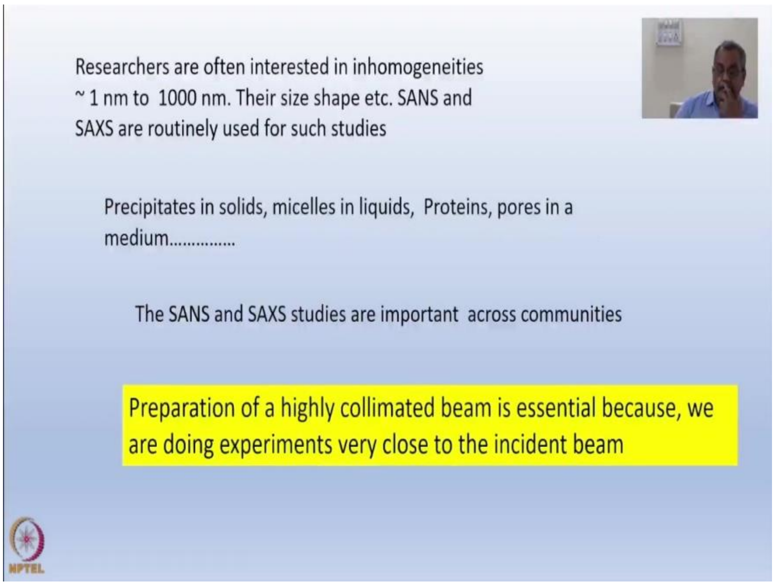

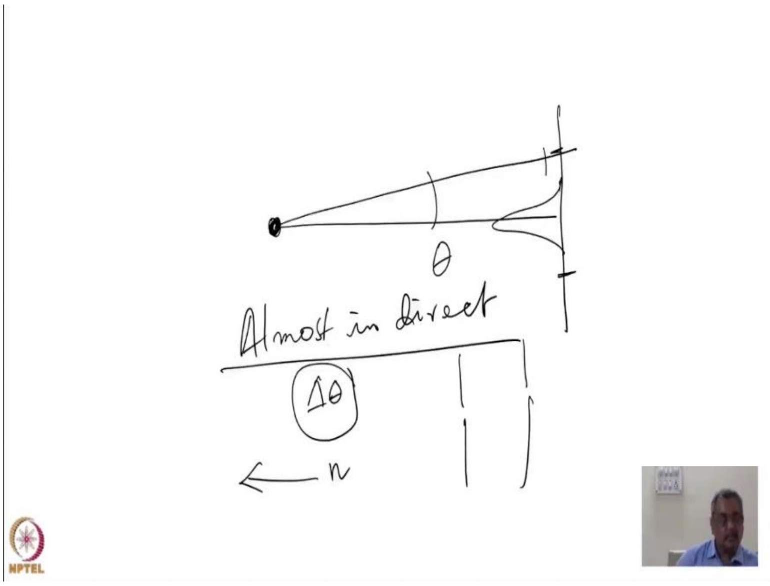

I am just summing it up now. The researchers are often interested in inhomogeneities of size, typically 1 nm to 1000 nm, e.g. precipitates in solids, micelles in liquids, proteins in solutions, pores in a medium etc. And I must mention here, that small angle neutron scattering and small angle x-ray scattering, SANS and SAXS, are important experimental tools across communities for such studies. But here, the thing is that I am doing experiments at a very low scattering angle or at a low *'Q'* .

Please consider the case that I have got a sample and a detector after the sample. I have got a direct beam width and I have got a diffracted beam somewhere here. The fact is that, because I am going to very small angles, I need to be careful that I do not go and intercept the direct beambecause I am almost in direct beam.

For that matter, I have to then collimate the direct beam to a large extent to reduce the $\Delta\theta$ for the direct beam. And this is possible by using collimators in the beam path. But tight collimation comes at a cost. When you put collimators in the beam path, you get a smaller angular spread, but number of neutrons also goes down, because you are cutting down their numbers by putting collimators.

That is why, for the small angle neutron scattering instrument, on a cold neutron source, starts with a larger number of neutrons from the source. That is where the importance of the cold neutron source comes into picture. You use a highly collimated beam in case of a small angle neutron scattering and then you are doing the experiment almost in the direct beam path.

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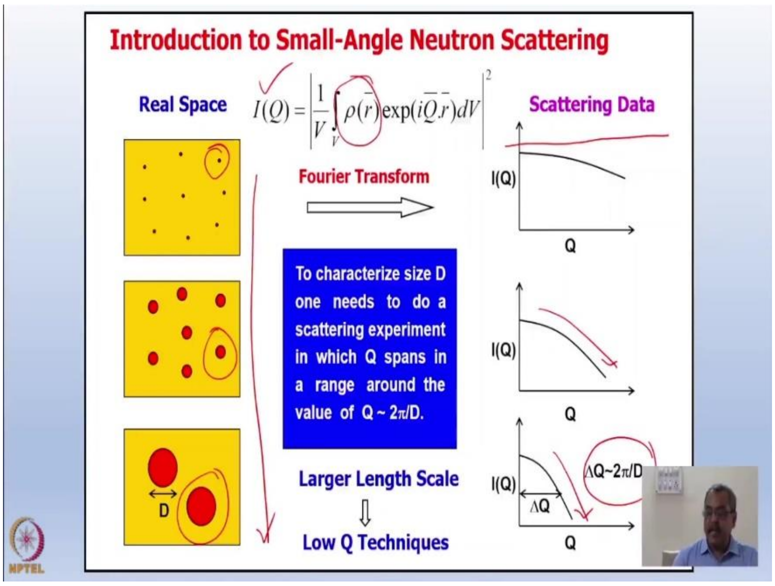

In the pictures there is quick look to the findings in a SANS experiment. Here, I am doing a Fourier transform over a scattering length density. I have done it earlier also for electron density in case of x-rays., If you remember, when I talked about form factor for a spherical electronic charge distribution in an atom, I got exactly the same expression except some constant like 1/V. This is the form factor for a charge distribution.

Now, instead of electronic charge distribution, I take a neutron scattering length density distribution. Please look at this figure where I have these objects that are becoming larger as we go from top to bottom in the page. Now, instead of electronic density, I am talking about neutron scattering length density of these objects. If I want to see that, then I do a scattering experiment and I measure I(Q).

Now, when the objects are smaller, the *'I(Q)'* falls slower. You know if these objects are delta functions, as I showed you earlier, *'I(Q)'* is constant all over Q because a delta function, after Fourier Transform, is a constant in Q space. As the objects becomes larger and larger, I(Q) fall faster and faster with *'Q'* and the typical size is given by ${}^{2\pi}/_{D}$. So, I can look at the size of these particles, looking at the intensity profile in a scattering experiment, but please remember it is not just a qualitative observation. Very shortly, I will come to the expressions that I can use to get size of such particles.

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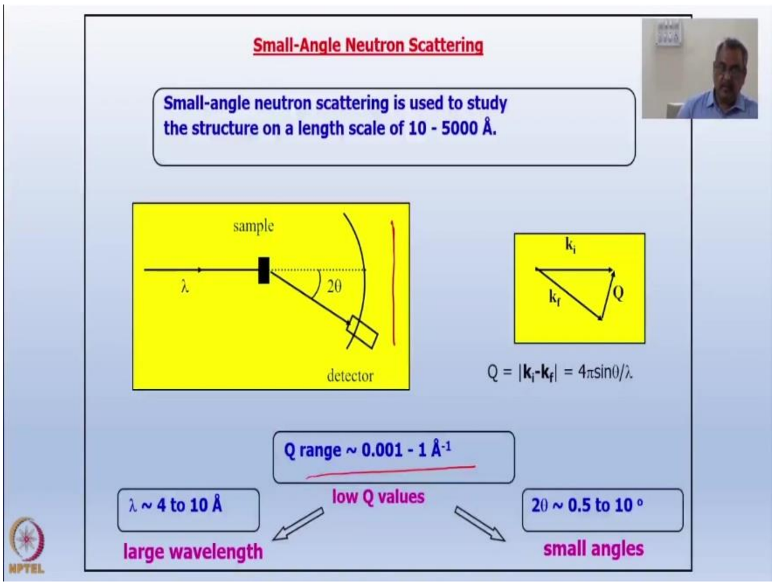

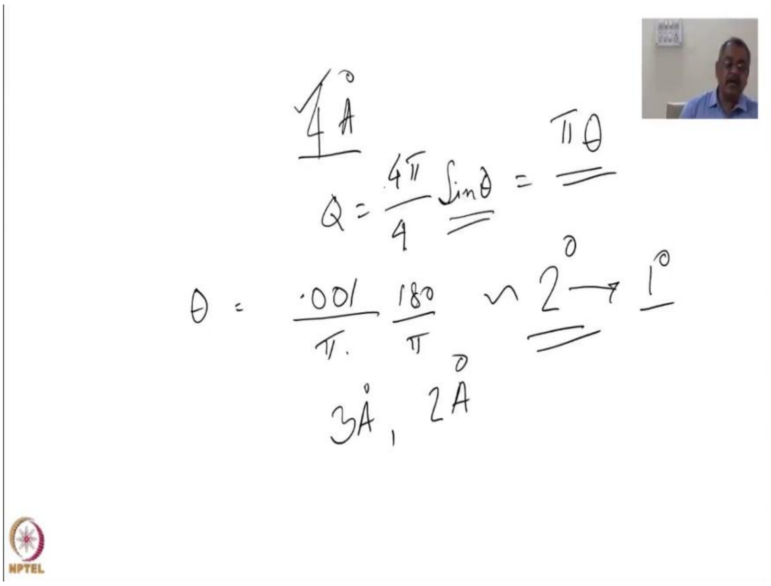

In small angle neutron scattering, you can see that it is close to the direct beam profile on the detector (if 1-dimensional detector). Sometimes we use a position sensitive detector to obtain the intensity of the scattered beam as a function of *'Q'*. , I will show you the instrument in Dhruva which uses a position sensitive detector. The *'Q'* range you can see is typically 0.001 to 1 $Å^{-1}$, λ is in the range of 4 to 10 Å and *'2θ'* the scattering angle, is typically in the range of 0.5 to 10°. So, if I talk about a 4 Å neutron beam then for small angle $Q \approx \pi\theta$. If *'Q'* is 0.001 $Å^{-1}$, then θ will be $0.001/\pi$ in radians or will be ~ 2°. I request you to do the simple calculation and check. So, we have to go to very low angle even with a 4 Å neutron.

If we use a neutron of wavelength 3 Å or 2 Å, because, if I do not have a cold source, then I may not be able to choose 4 Å as the numbers will be less at this wavelength. If I go to smaller wavelength, I need to go to say from instead of 2° (for 4 Å) I need to measure at 1° (for 2 Å) and I have to restrict my direct beam much below 1° in collimation, so that I can do the experiments.

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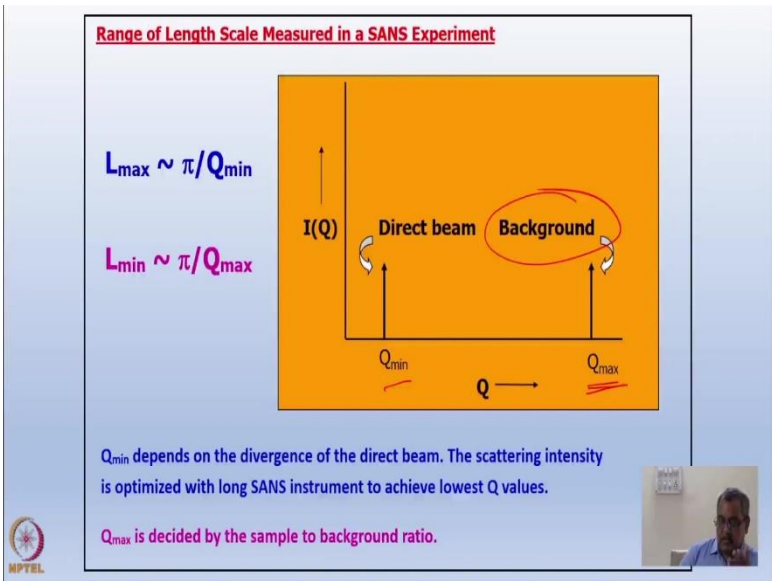

This is the schematic of a small angle neutron scattering set up and now, my experiment is restricted on the lower side in '*Q*' or at smaller angle by direct beam width and as I keep measuring as a function of angle, on the higher angle side, Q_{max} is restricted by the neutron background at the sample area. Background is an important factor because wherever you do the experiment either inside a reactor hall or in a neutron guide hall, you have background neutron and when the scattered intensity, which is falling with Q, matches the background, then I can stop that experiment because now I have gone into the background.

So, Q minimum and Q maximum are dictated by the direct beam and the background on the sample..

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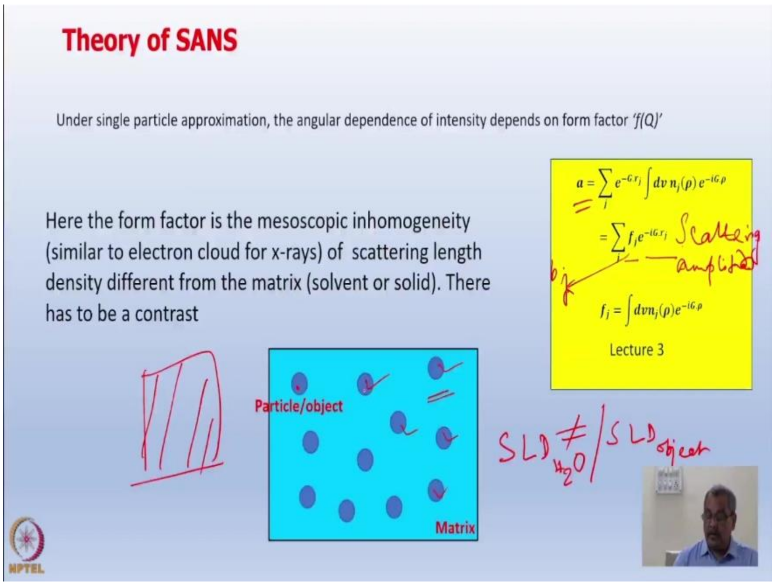

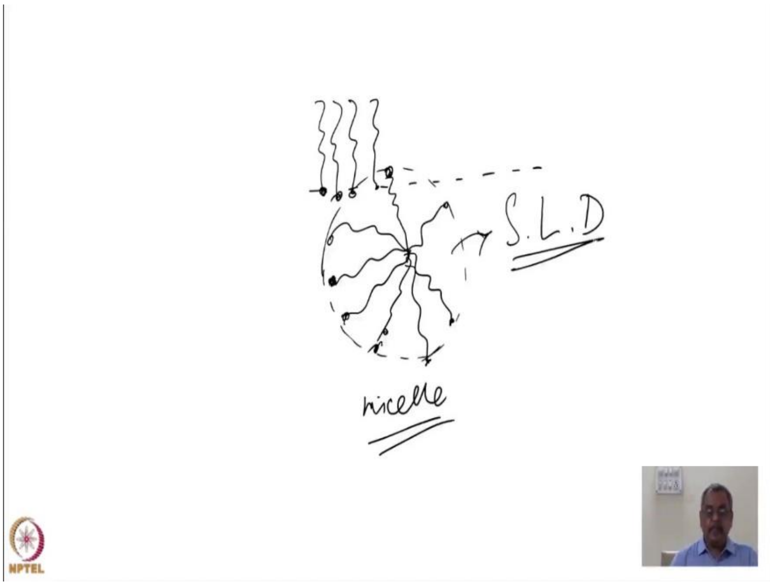

, I will briefly take you through the theory of SANS that you may appreciate. As I told you a few slides earlier that I have a matrix and I have these particles or inhomogeneities, which I want to study. Now, earlier also when I dealt with x-ray or neutron scattering if you remember, this was the expression for the scattering amplitude, and *'Q'* had to be equal to *'G'* because those were crystalline material. t f_j is a Fourier transform of the electronic charge density in case of x-ray.

In case of neutrons, I replaced that with b_j, the coherent scattering length, which gives you a constant function in Q space. But this f_j was a Fourier transform of the electronic charge density in the atom, In lecture 3, I introduced you to this form factor in atoms for the electronic charge density. Here I am introducing the same thing with respect to this kind of inhomogeneities.

What are these objects?

Let us say I have a liquid in which I put these surfactant molecules which have got a hydrophilic head group and a hydrophobic tail group. So, up to a certain density, they will be sitting on the surface, the tail sticking out and the heads on the water. If you keep increasing the density, now to hide the tails from the water this structure will form. it will be near spherical, not always spherical or even cylindrical. But here, the head group looks out to the water because it is hydrophilic and the tail group is inside. This is called a micelle in chemistry. I am looking at the form factor of this object instead of f_j for atomic charge distribution in case of x-rays This is now depending on the scattering length density and the geometry of the object being studied.

Now, I have got a scattering length density contrast between the matrix and the micelle. Here the matrix is water so water has SLD of H_2O and the contrast is with the SLD of the object.

There must be some contrast between thee two. If there is no contrast, this is like putting glass inside water. if I put a piece of glass inside water, the refractive indices match and you cannot see that glass. It is very similar to that. If you have put an object whose neutron scattering length density is same with water you cannot see it in the scattering because it is same as the entire matrix.

But when there is a scattering length contrast of the object, that means, their scattering length density is not equal to the scattering length density of the matrix then you can see them and you can measure, the scattered intensity at small angle to find the form factor for the shape and size of this particle.

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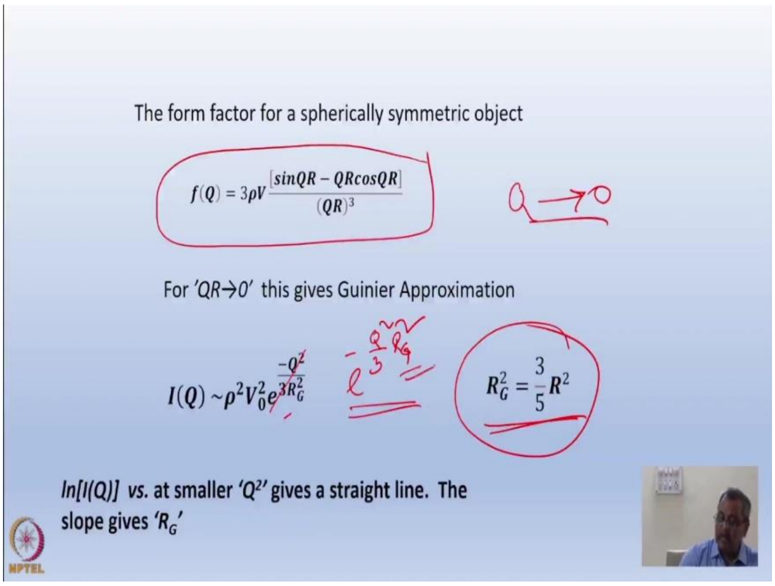

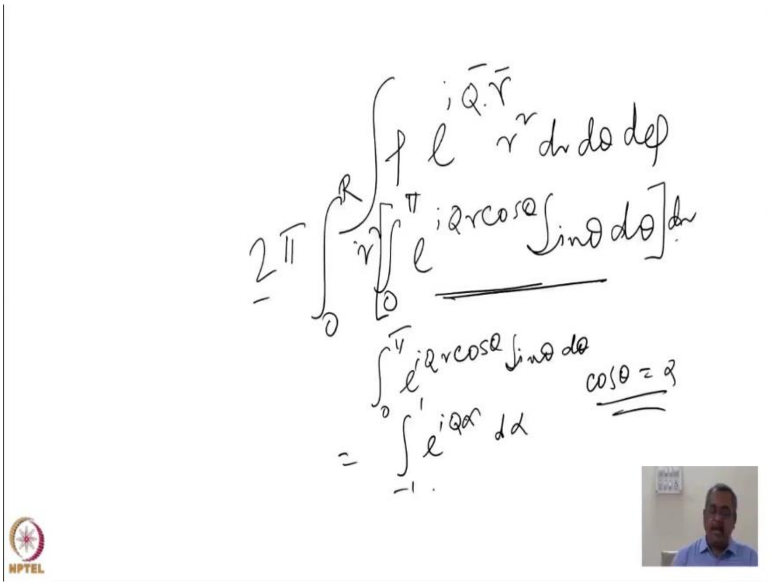

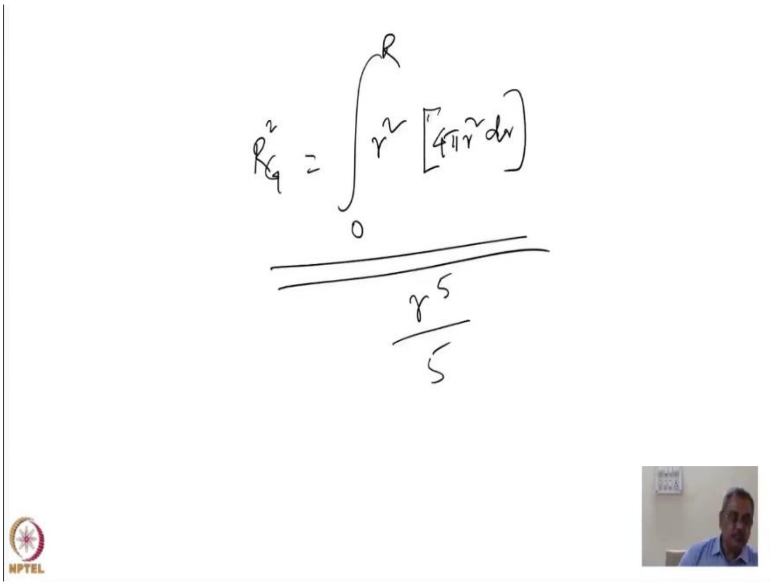

Now, let us take a spherically symmetric object with density ρ. This also I had introduced earlier. It is very simple to evaluate the integral. Then form factor for this spherically symmetric object is,

$$f(Q) = 3\rho V \frac{[\sin QR - QR \cos QR]}{(QR)^3}$$

This expression at low Q when $QR \rightarrow 0$ then

$$I(Q) \sim \rho^2 V_0^2 e^{\frac{-Q^2 R_G^2}{3}}$$

where R_G is the radius of gyration of the sphere, which is given by $R_G^2 = \frac{3}{5} R^2$ for a sphere.

This relationship is known as Guinier relationship where ρ^2 is the (scattering length) density contrast contrast, (not just the density), V_0 is the volume of each particle. Here you can see, if I plot log I(Q) against Q^2, that will be a straight line. And slope of the straight line will give me R_G, the radius of gyration for the sphere.

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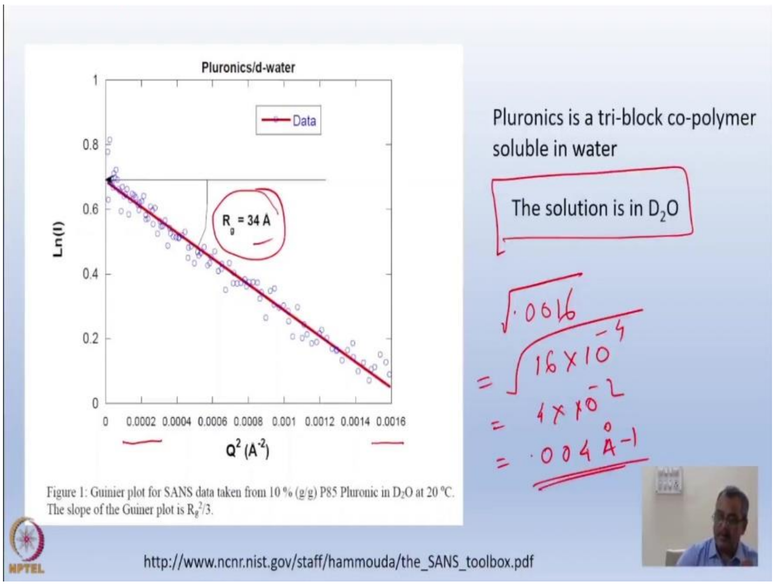

I will use an example from a pluronic sample, which is a tri-block co-polymer soluble in water and in the example it is dissolved in D_2O. This polymer is a hydrogenous sample and if we put it in H_2O, you cannot see because of poor H-H contrast, so it is dissolved in D_2O. I will also talk about something called tailoring contrast factor shortly.

You can see this experimental result. It is called a Guinier plot for small angle or SANS data taken from 10 % (g/g) P85 Pluronic in D_2O at 20 °C. The slope of the plot gives you the R_G sometimes it is also called hydrodynamic radius. You can see this is the average R value for a sphere. So

We can see that this experiment tells me,Pluronics forms a coil in water forming a sphere of this average sizewhen I do a measurement in the low Q region and please note the Q^2 is from 0.0002 Å^{-2} to 0.0016 Å^{-2}. Square root of 0.0016 Å^{-2}is equal to 0.04 Å^{-1}. Hence, we have to go to really, really low Q values for this experiment. I will stop here and go to the next module shortly.