***Transcript of the audio narration for the presentation on reflectometry (June 2021)***

SLIDE 1 (an1.m4a)

Hello everyone. My name is Chuck Majkrzak and I am a research scientist and have been involved in neutron reflection studies of the micro-structure of both hard and soft condensed matter systems for many years.

I would be pleased to share with all of you today some of what I have learned about this technique -- much of which has come through association with gifted mentors and colleagues I've had the privilege to work with.

SLIDE 2 (an2.m4a)

In general, the primary goal of most elastic neutron and x-ray scattering studies of both "hard" and "soft" condensed matter is to obtain information about the micro-structure of a given material object through the analysis of its corresponding scattering pattern. Typically, for such studies, the length scale at which structural features can be resolved is of the order of 1 to 100 Angstroms or 0.1 to 10 nm.

In particular, for a specular neutron reflectivity measurement -- which yields the composition depth profile perpendicular to the surface of a layered thin film structure, a spatial resolution approaching a fraction of a nanometer is possible for certain properly prepared systems.

SLIDE 3 (an3.m4a)

At the relevant free neutron velocities in a beam emanating from a thermal or sub-thermal source, the interaction of a neutron with condensed matter must be described according to quantum theory -- which accounts for the wavelike nature of the neutron. The wavelength range corresponding to such velocities is of the order of 1 to 10 Angstroms.

An individual neutron can be associated with a wave packet function which is partially localized in space. The interaction of the neutron with the arrangement of atoms making up the scattering material produces a characteristic diffraction pattern. From a mathematical analysis of that pattern the real-space structure of the scattering object can be deduced. The reflected neutron wave amplitude r as a function of its wavevector **k** can be related to the incident neutron wave function and the distribution of scattering power of the constituent nuclei of the atoms composing the material (in the continuum limit the strength of the interaction for a given material is characterized by a scattering length density). The neutron wavevector **k** points along the direction of propagation and its magnitude is proportional to the inverse of neutron wavelength.

In this slide are shown several wave forms or representations thereof. In the upper left of the slide is shown an electromagnetic wave with electric and magnetic field vectors perpendicular to the direction of propagation. On the upper right half of the slide is shown a two-dimensional circular wave diffracting through a slit. On the lower right is a two dimensional representation of an incident plane wave that has diffracted through a single slit -- note that perpendicular to the horizontal axis of propagation (from left to right) the wave amplitude diminishes significantly beyond a well-defined finite width -- characteristic of wave packet spatial localization. On the lower left is a schematic representation of a beam of quasi-monochromatic neutron wave packets (each of which is associated with a material neutron) defined by a crystal monochromator and pair of slits in series.

SLIDE 4 (an4.m4a)

The top half of this slide shows the electron diffraction pattern for a polycrystalline piece of aluminum which has a relatively simple face-centered cubic unit cell. In the lower half is shown the x-ray diffraction pattern produced by the relatively complicated structure of the biomolecule pea lectin. In both of these examples, the diffraction data were collected out to sufficiently high wavevector transfers, $\mathbf{Q} = \mathbf{k}_F - \mathbf{k}_I$ , that the real-space resolution attainable was of the order of an Angstrom or less.

On the other hand, in typical specular reflectivity measurements, the wavevector or momentum transfer is typically an order of magnitude lower so that the spatial resolution is often no better than a nanometer. In this case the positions of individual atoms are not discernible and the scattering material appears more as a continuum than a collection of distinct atoms. An important phenomenon in scattering is the fact that spatial resolution in real object space is inversely proportional to the maximum wavevector transfer attainable in a scattering pattern. This point which will be discussed further in subsequent slides.

SLIDE 5 (an5.m4a)

This slide gives a partial outline of what will be presented in this lecture along with several references to the history of the development of neutron reflectometry to become an important method for studying the microscopic structure of layered materials.

Although the theory underlying the means by which structures are mathematically deduced from the reflectivity or scattering data will be discussed, it will be a relatively elementary description of the essential concepts. Scientists from a broad range of backgrounds and disciplines who possess widely varying degrees of mathematical knowledge currently engage in neutron reflectivity measurements. Scientific studies involving neutron reflectometry are typically a team effort requiring people with expertise in many different areas such as biochemistry, polymer and other materials sciences, condensed matter physics, etc.. For example, for a biochemist to study how proteins interact with a lipid membrane by employing reflectivity measurements as a structural probe does not require that they be an expert in scattering theory -- provided another member of their research team is. But it is certainly useful for everyone to know something about the fundamental physical principles upon which the analysis of the scattering data is based to help appreciate both the sensitivity and inherent limitations of the method.

SLIDE 6 (an6.m4a)

In this figure is given the definition of and geometry for specular reflectivity. The incident beam of neutrons (or x-rays) is incident at glancing angles relative to a flat surface where the direction of the incident beam is defined as that of the mean value of the wavevectors of the individual neutrons composing the beam. To satisfy the specular condition, the angles of incidence and reflection are maintained to be equal (e.g., by proper orientation of the defining slits for the incident beam and the position of the detector for the reflected neutrons). Note that in this configuration the wavevector transfer **Q** is parallel to the mean surface normal. As will be discussed further in what follows, information about the composition depth profile along that normal is obtained if the specular condition is maintained. To obtain information about in-plane scattering density distributions, off-specular measurements are required. In this talk, the primary subject of interest will be specular reflection. And although the presentation is focused on specular neutron reflectometry, much of the discussion pertains

to x-ray reflectometry as well with the appropriate accounting for the different scattering potentials.

SLIDE 7 (an7.m4a)

See slide.

SLIDE 8 (an10.m4a)

This slide illustrates, by both numerical and color schematic, how specular reflection of a neutron wave packet in effect provides information about the average in-plane (i.e., a plane perpendicular to **Q**) scattering density -- as a function of depth along the surface normal. For example, in the top row of blocks, averaging the blue blocks (2 scattering strength units) with red blocks (10 units) -- where the blue and red blocks are of equal size -- results in an average in-plane scattering strength of 6 units -- represented in the separate column to the left as an equivalent purple block.

This averaging effect can be rigorously proven mathematically, but such a proof is beyond the scope of this presentation.

SLIDE 9 (an11.m4a)

Here is another schematic illustration of the relationship between the specular reflection measured as a function of wavevector transfer Q -- or glancing angle of incidence theta -- and the scattering length density depth profile along the surface normal. How this relationship arises mathematically is considered in slides to follow. But in general terms, an incident wave interacts with a material structure to produce a reflected wave that is created from the superposition of wave amplitudes originating from scattering centers (individual nuclei for neutrons) at different locations in the material sample object. For the particular case of specular scattering, the relative positions of the scattering centers along the surface normal are what determine the shape of the interference pattern observed as a function of Q. In other words, it is the variation of the in-plane averaged scattering length density along the surface normal that determines the shape of the specualr reflectivity observed as a function of Q.

Although it is difficult to see on the inset at the top of the figure -- which shows the reflectivity as a function of Q -- that at values of Q below a certain critical value, which depends on the overall scattering length density of the film and/or substrate, the reflectivity approaches unity. That is, below the corresponding critical angle all incident neutrons undergo total external mirror reflection -- a reflectivity of unity (although this might not be evident in raw reflectivity data since a geometrical footprint correction must first be made). As we will see in forthcoming slides, the specular reflectivity rapidly diminishes with increasing Q, decreasing by as much as eight orders of magnitude before the signal-to-noise ratio makes further measurement impractical.

SLIDE 10 (an12.m4a)

This slide illustrates the fundamental relationship between real space and scattering or reciprocal space -- the smaller the feature to be resolved in real space, the higher the magnitude of wavevector transfer **Q** to which scattering data must be obtained. Note also that for material structures with periodic variations in scattering density along a real space direction that is parallel to **Q** , peaks in the specular reflectivity appear with a periodicity in Q that is inversely proportional to the real space period.

SLIDE 11 (an13.m4a)

In the upper section of this slide is summarized the description of the scattering potential in terms of material density and neutron scattering power (specifically scattering length density) that is appropriate for use in the quantum mechanical wave equation (otherwise known as the Schroedinger equation) that predicts the specular reflection of the neutron wave packet in the continuum limit.

The central section of the slide shows how that wave equation derives from imposing the condition that energy be conserved.

In the bottom part of the slide the scattering potential is characterized in the form of a refractive index analogous to that typically employed in wave optics descriptions of ordinary light.

SLIDE 12 (an14.m4a)

This slide illustrates how the wave equation for the specular reflection process can be solved in a so-called piece-wise continuous manner by imposing the conditions of conservation of momentum and neutron particle number.

Any scattering length density profile (i.e., the potential) can be represented -- to an arbitrary degree of accuracy -- by slicing the profile into rectangular segments or "bins" where within each individual segment the SLD is a constant value appropriate for that particular segment. The solution of a corresponding set of linear algebraic equations relates the reflection amplitude r as a function of Q to the scattering length density value in each bin.

It is important to keep in mind in what follows, that the SLD profile does not directly correspond to the actual material composition profile -- some modeling is typically required to relate the two distributions.

Moreover, as to be discussed subsequently, a single set of specular reflectivity data does not necessarily correspond to a unique scattering length density depth profile. This is because only the reflected intensity -- the absolute square of the wave function -- and not the reflection amplitude r (a complex quantity with real and imaginary parts) can be measured directly.

We will return to this important point later in the presentation.

SLIDE 13 (an15.m4a)

The left-hand side of this figure shows a specular neutron reflectivity pattern on top and and a number of corresponding scattering length density profiles below -- as would be obtained for reflectivity data sets cut off at various maximum Q values. This illustrates, by example, one of the key relationships between diffraction or reflection patterns and the corresponding real space material objects which produce them -- namely, that the smallest length scale to which features of the object can be resolved in real space is inversely proportional to the largest value of Q out to which the reflected intensity pattern can be measured.

On the right is shown a picture of a trans-membrane protein embedded across a lipid cell membrane with corresponding scattering length density depth profiles as obtained for various scattering length densities of the surrounding aqueous reservoir in which the system is immersed. Advantage can be

taken of the fact that the scattering length densities of protonated and deuterated materials, such as ordinary water and $D_2O$, can differ greatly -- thereby making it possible to engineer a relatively high contrast between different parts of a structure.

SLIDE 14 (an16.m4a)

See slide.

SLIDE 15 (an17.m4a)

Employing polarized incident and reflected beams, the scattering of a neutron from a nucleus and an atomic magnetic moment can be distinguished -- thereby making it possible to measure not only material composition depth profiles but the magnitude and orientation of magnetization density as well.

In general, scattering in which a neutron spin "flips" from plus to minus state or vice versa is indicative of purely magnetic scattering and arises from components of the sample magnetization lying in the scattering plane defined by the incident and reflected neutron wavevectors. On the other hand, components of the sample magnetization perpendicular to the scattering plane can produce magnetic scattering without change of neutron spin state -- non-spin-flip -- that can also interfere with the nuclear scattering potential of the material. By measuring four distinct neutron spin-dependent reflectivities -- namely, corresponding to ++, --, +-, and -+ incident and reflected neutron spin states respectively -- the orientation of the sample magnetization as a function of depth can be deduced.

This important application of polarized neutrons will be discussed further in following slides and other talks in the school.

SLIDE 16 (an18.m4a)

On the right are shown characteristic reflectivity patterns for the simple ferromagnetic and antiferromagnetic sample atomic layer magnetization configurations adjacent to the left. Note that the effective "doubling" of the magnetic repeat period of the antiferromagnetic structure is associated with a peak in the corresponding spin-flip reflectivity at half the Q value.

SLIDE 17 (an19.m4a)

These canted and helical configurations of the sample atomic plane magnetization are associated with more complicated spin-dependent neutron reflectivity patterns. Polarized neutron reflectometry is an extraordinarily sensitive probe of the magnetic structure of layered film materials.

SLIDE 18 (an20.m4a)

On the top of this figure is shown a schematic of the spin polarizing and rotating or flipping devices used to produce and control the polarization states -- in this case either neutron spin + or spin - -- of the neutron beams incident upon and reflected by the sample under study. With the devices pictured, it is possible to measure the four possible spin-dependent reflectivities, namely correspnding to ++, --, +-, and -+ neutron incident and reflected spin states, respectively.

The lower part of the figure is a photograph of an earlier version of the NIST polarized beam reflectometer, PBR. Near the center of the photo is a blue cryostat inserted in a pair of copper wire

Helmholtz coils for controlling the temperature of and a magnetic field applied to the sample, respectively.

SLIDE 19 (an21.m4a)

Now we will talk about specific applications of neutron reflectometry in the study of the micro-structure of layered film systems composed of both hard and soft condensed matter. A broad range of examples will be covered to show the remarkable diversity of research areas in which neutron reflectivity measurements can make a contribution -- but because of the limited time available, we will concentrate principally on the key aspects common to all. Some of the examples will not be discussed at all and are included only for your future reference to read about should you be interested in that particular subject.

The examples of neutron reflectivity studies presented here are from work involving facilities at NIST -- primarily because of my greater familiarity with them either via participation or observation of the work of colleagues. Similar research has been and continues to be performed all over the world.

SLIDE 20 (an22.m4a)

Some of my colleagues at NIST who are principally engaged in the study of magnetic thin films, multilayers, and superlattices.

SLIDE 21 (an23.m4a)

See slide.

SLIDE 22 (an24.m4a)

See slide.

SLIDE 23 (an25.m4a)

This slide illustrates how interlayer correlations between magnetic layers separated by non-magnetic segments in a periodic sequence can be studied by polarized neutron reflectometry. In this case the degree of correlation between the magnetic structure in one layer segment to that in an adjacent magnetic segment depends upon the thickness of the intervening non-magnetic material.

SLIDE 24 (an30.m4a)

An example of a more recent polarized neutron reflectometry study of a skyrmion magnetic system -- of current interest for its relevance to potential spin-dependent electronics ("spintronics") applications.

SLIDE 25 (an31.m4a)

And one more example of an application of polarized neutron reflectometry to study a magnetic system currently of interest for both its fundamental physical behavior and potential technological applications -- in this case the possible control of oxidation by applied electric fields.

SLIDE 26 (an32.m4a)

Here is a slide showing some of the NIST researchers studying soft condensed matter systems -- such as the transmembrane protein embedded in a lipid bilayer shown in the inset.

SLIDE 27 (an33.m4a)

Heterogeneous polymer film systems constitute one class of soft condensed matter that has benefited significantly from neutron reflectometry studies.

SLIDE 28 (an34.m4a)

For instance, consider the morphological transitions which can occur in di-block copolymer systems -- as a function of molecular weight or chain length -- when constrained to a surface. The morphology changes from homogeneous to lamellar with increasing molecular weight. One specific case in which such structural changes occur is the di-block copolymer poly(ethylene-propylene) - poly(ethylethylene) (PEP-PEE).

SLIDE 29 (an35.m4a)

The morphological changes in these di-block copolymer systems were discovered by neutron reflectometry. On the left of the figure are shown specular neutron reflectivity data sets obtained as a function of the di-block chain length. On the right are shown the corresponding concentration depth profiles -- directly related to the scattering length density profiles obtained from fitting the neutron reflectivity data. The morphology progresses from that of a single film of homogeneous density (on the relevant length scale of the order of a fraction of a nanometer) at lower molecular weight to a stratified lamellar multilayer structure -- with aligned alternating layers of PEP and PEE segments -- at the higher weight. This latter structure is evident in the periodic variation of the density which results from protonating one of the di-block constituents -- producing a relatively low scattering length density for neutrons -- and deuterating the other to increase its scattering density.

SLIDE 30 (an36.m4a)

Here is a more recent example in which key aspects of solvent vapor annealing -- a technique for directing nanostructure ordering and morphology in block copolymer films -- has been studied by neutron reflection.

SLIDE 31 (an37.m4a)

The biosciences is another area in which neutron reflectometry can contribute in unique ways to understanding the micro-structure and function of important systems such as membrane proteins. It is not difficult to imagine the implications for understanding how pathogens, like the virus causing the current pandemic, interact with the receptors on the cell membranes of the host organism. Given several key properties of neutrons -- including their ability to penetrate through macroscopic distances in single crystal materials such as silicon and the significant difference in scattering power of hydrogen and deuterium -- the interactions of biomolecules and lipid membranes can be investigated in vivo, approaching a more natural state of the system.

SLIDE 32 (an38.m4a)

In this example of a neutron reflectivity study of a biomimetic membrane, the goal was to determine the microstructure of an engineered, organic multilayer for application as a biocompatible coating in artificial organs -- e.g., synthetic replacements for blood vessels. The project was a collaboration between a vascular surgeon and medical researchers at Emory University School of Medicine (E.L. Chaikof and K.M. Faucher) and Ursula Perez-Salas at the NIST Center for neutron Research.

SLIDE 33 (an39.m4a)

On the left hand side of the figure is an overall schematic of the layered structure constituting the deposited coating. On the right is a more detailed version with chemical compounds identified. The goal of performing neutron reflectivity measurements on this system is ultimately to identify areas into which water diffuses when the film is placed adjacent to an in contact with an aqueous reservoir.

SLIDE 34 (an40.m4a)

Neutron reflection data for the phospholipid terpolymer and polyelectrolyte multilayer structure are shown on the left. On the right is shown the scattering length density profile which results from analysis of that neutron reflectivity data. In particular, by collecting multiple neutron reflectivity data sets corresponding to different aqueous reservoir scattering length densities (various $H_2O$ and $D_2O$ combinations) it is possible to uniquely determine where the water fraction resides. In this case, the water diffuses primarily into the polyelectrolyte layer. Neutron reflectivity measurements are the only way to obtain information such as this at nanometer scale resolution.

SLIDE 35 (an42.m4a)

On the left is a typical design schematic for a fluids cell in which a film structure deposited on a single crystal support substrate such as silicon or sapphire can be placed adjacent to and in contact with an aqueous (or other) fluid medium. The use of single crystalline silicon, along with a minimum fluid reservoir thickness of the order of 10 to 100 microns thick, helps minimize the amount of background scattering. On the upper right is an expanded view of the cell components. At the bottom right is a photograph of an actual fluids cell used in neutron reflectivity measurements. Fluids can be exchanged into and out of the reservoir volume through inlet and outlet orifices, respectively.

SLIDE 36 (an46.m4a)

This slide illustrates the significant advancement and evolution of neutron reflectivity studies of biological membrane systems. Neutron reflectivity studies have now been performed that investigate the interaction of pathogens with membrane structures in a more natural aqueous environment.

SLIDE 37 (an52.m4a)

A study of how the structural protein tubulin is attached -- as well as oriented with respect to -- a lipid membrane. In this study, the specular neutron reflectivity data was analyzed in combination with information obtained by x-ray protein crystallography and molecular dynamics simulations. Combining the information obtained from several complementary techniques is a powerful means for obtaining a more complete and accurate picture of relatively complicated systems.

SLIDE 38 (an53.m4a)

A final example of a neutron reflection study of a cell membrane system in which information is obtained about the structure and function of voltage-sensing proteins that reside within the cell membrane and play a role in the operation of ion conduction pores.

SLIDE 39 (an54.m4a)

Electrochemistry and photovoltaics are other areas in which neutron reflectivity studies can provide important structural information on a nanometer scale -- and in operating systems employing sample environments similar to those described earlier for biological systems.

SLIDE 40 (an58.m4a)

Now that we have taken a look at some examples of the applications of specular neutron reflectometry over a broad range of scientific research fields, let's conclude with a discussion about its accuracy. After all is said and done, a method is worthless for scientific investigation unless it is objective and accurate in both principle and practice.

SLIDE 41 (an59.m4a)

The upper left-hand side of this figure shows a plot of a family of very similar scattering length density depth profiles obtained by repeated fitting -- through variation of fitting parameters describing a model structure via least squares methods -- the single neutron reflectivity data set directly below it. The reflectivity data were obtained from a partially oxidized titanium film in contact with an aqueous reservoir across which an electrical potential could be applied. The relatively modest amount of variation among this family of fitted profiles is indicative of a high level of confidence in the result -- the variations are as would be expected for a measurement given the statistical uncertainty in counting statistics, truncation of the reflectivity pattern at a finite maximum value of Q, and other typical systematic instrumental uncertainties.

However, consider now the right hand side of the figure. It was found that if the same fitting process described previously were continued (on the identical set of reflectivity data) for a sufficient number of iterations, eventually another family of solutions emerged wherein each member was similar to one another within the new family -- but all in stark contrast to the original family of fits obtained. (Note that in the upper right plot, only one representative fit from each of the two families of solutions is plotted for the sake of clarity.) The second family of solutions possesses chi-squared goodness-of-fit values comparable to those of the first family. Based on the single neutron reflectivity data set alone, it is not possible to distinguish between the two possible solutions for the scattering length density profile. (Of course if other information about the film system were known, it might be possible to identify which of the solutions obtained from the reflectivity data corresponds to physical reality.)

Nonetheless, these results from the analysis of the neutron reflectivity alone is disconcerting. As we will now discuss, the ambiguity is a consequence of the loss of phase information (alluded to earlier) inherent to the measurement of the reflectivity -- which is proportional to the reflected intensity. The intensity does not explicitly yield the phase information intrinsic in the reflection amplitude (the reflected neutron wave function) which is a complex number composed of both real and imaginary parts.

SLIDE 42 (an60.m4a)

Another illustration of the phase problem in reflectivity measurements. On the left are two apparently significantly different model scattering length density profiles. On the upper right plot are the two specular reflectivity patterns corresponding to the two dissimilar density profiles. The two different reflectivity data sets, although not exactly identical, are nearly so with discrepancies appearing only at a relatively few Q values where the magnitude of the reflectivity is exceedingly small and problematic to measure accurately. So, cases can arise where reflectivity data is not very sensitive to different material density profiles.

On the other hand, the lower right graph showing the real part of the reflection amplitude corresponding to each of the two density profiles -- presuming that it was possible to obtain the amplitude in some way -- reveals relatively large differences between the two amplitudes that would clearly distinguish the two different density profiles from one another.

As it happens, this so-called phase problem is common to all diffraction phenomena. Hauptmann and Karle were awarded a Nobel prize for finding one solution to this problem applicable to the diffraction of x-rays from crystal structures. But there is another solution possible, applicable to specular neutron reflectivity, which involves the use of known reference structures located either within or adjacent to the "unknown" part of interest in the sample being studied.

SLIDE 43 (an61.m4a)

The left half of this figure schematically summarizes the phase problem for specular reflectivity measurements. Following the loop from the top of the schematic counter-clockwise, we go from a conventional measurement of the reflectivity through what amounts to a trial-and-error fitting of the data to a model scattering length density profile -- according to the underlying quantum wave equation which connects the profile and reflectivity data -- to aresultant density profile. As we have seen, accurate results can be obtained, but they may be ambiguous because of the loss of the important phase information in measuring an intensity rather than the reflected wave function itself -- which is not directly accessible.

On the other hand, taking the loop on the right in a clockwise sense outlines what would have to be done to perform a direct inversion of the reflection amplitude -- presuming it was obtainable -- yielding a unique solution for the scattering length density profile. The solution is in principle exact, to within the limitations imposed by truncation of reflectivity data at a finite maximum value of Q and statistical counting uncertainties -- and assumes that bound states and absorption processes are negligible (which are typically the case).

The right side of the figure shows the essential relations underlying the mathematical justification, the detailed derivation of which is beyond our scope here, for this one-to-one correspondence between specular neutron reflection amplitude and scattering length density depth profile.

So how might it be possible to obtain the reflection amplitude in practice when only reflected intensities can be measured?

SLIDE 44 (an62.m4a)

The answer to the preceding question is to employ reference structures, either underlying known layers

or variable media surrounding the film system region of interest. The linear algebraic formulation of the solution of the one-dimensional neutron wave equation is well-suited to a mathematical analysis that extracts the reflection amplitude corresponding to the segment of the density profile of interest -- the part we are trying to obtain -- from the segments of the composite film system structure which serve as the *a priori* known references. It is necessary, however, to use at least two, and in certain cases, three composite systems -- each with a different reference part but all with the same, common section of interest. That is, composite system j = reference j + common segment of interest.

Once the reflection amplitude for the "unknown" part of the system of interest is extracted from the composite system reflectivity data sets, a direct inversion can be performed as outlined on a previous slide.

Alternatively, the composite system reflectivity data sets can be simultaneously fit to a model scattering length density profile. Although this latter approach still requires fitting algorithms, it will ultimately converge, in principle, to the same unique scattering length density profile that would be found by the direct inversion process. In practice, the latter fitting approach is the one typically preferred for a number of practical reasons. As you might recall, the neutron reflectivity study of solar cells that was presented as an example of an application earlier, employed both approaches to analyzing the reflectivity data and consistent results for the density profile were obtained.

SLIDE 45 (an63.m4a)

This figure shows the application of the reference method of phase determination for neutron reflectivity to the membrane system used to investigate the interaction of melittin with bilyer lipids. The phase-sensitive experiment confirms that the solution obtained previously for the the scattering length density profile by conventional means (i.e., without phase information) was indeed correct. The exaggerated oscillation of the scattering length density across the gold film region is primarily a result of the lower truncation of the Q range in the phase-sensitive data compared to that for the conventional data (0.3 as opposed to 0.72 inverse Angstroms, respectively).

To summarize, properly conducted specular neutron reflectometry measurements on appropriately prepared sample film systems, can, in principle and practice, yield reliable structural information about layered film systems with quantifiable accuracy.

SLIDE 46 (an64.m4a)

It is also important to point out that the in-plane averaging process that occurs in the specular reflection of a neutron wave packet depends upon the transverse spatial extent of the packet. The packet can only average over the area of the reflecting surface of the sample on to which its wavefronts are projected.

SLIDE 47 (an65.m4a)

Fortunately, the projected length of a neutron packet wavefront on a surface -- at the relatively small glancing angles common in specular reflectivity measurements -- is typically tens of microns in practice.

Moreover, when necessary, the transverse dimension of the wavepacket can be measured through the use of standard reference diffraction gratings -- either through observation of the specular reflection pattern in the vicinity of the critical angle (as illustrated in this slide) -- or via a transmission diffraction

pattern.

SLIDE 48 (an66.m4a)

Example of specular neutron reflectivity data from thin film diffraction gratings that are indicative of the transverse extent of the neutron packet wavefronts.

SLIDE 49 (an73.m4a)

Finally, I would like to let you know about the NIST reflectometry website where you can find and make use of online neutron reflectivity calculators.

SLIDE 50 (an74.m4a)

On this website you can create models of layered thin film structures related to actual material systems that you are interested in and might consider probing by neutron reflection. It is possible to use these calculational tools to help optimize the sensitivity of the neutron reflectivity pattern to particular structural features of potential interest -- for example, by exploring the effects of film thicknesses or various substrates.

You can also contact any of the reflectometry team staff at the NCNR for help in evaluating the feasibility of a particular measurement on a system of interest to you -- and in writing proposals for beam time.

SLIDE 51 (an75.m4a)

An example of what the online neutron reflectivity calculator tools look like.

SLIDE 52 (an76.m4a)

In conclusion, I want to thank you all for listening to this introduction to reflectometry. I hope that it will be of some use to some of you at some point in your future careers -- even if only to know that the technique exists and what its applications are.

Please do not be reluctant to ask questions -- either during this school or anytime afterwards by e-mail. I'll try to answer as best I can or at least refer you to someone who is more qualified to do so.