Introduction to Neutron Scattering

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Neutron scattering is a traditional probe for many magnetic and spectroscopic studies. It is now firmly established as an invaluable complement to x-ray scattering for structural and dynamic studies with many other areas of the materials sciences, chemistry, and biology[1]. This paper presents a brief introduction to neutron scattering. At last, two examples will demonstrate the applications of neutron scattering on structural biology and superconductivity which represent structural and dynamic properties respectively.

Keywords: neutron scattering, probe, structural and dynamic, neutron source

I. PROPERTIES OF NEUTRONS

Generally, the nuclei of nearly all atoms consist of protons and neutrons. As one of the fundamental particles in nature, neutron consists of an up quark and two down quarks. [2]This combination leaves it no net charge, a half spin and magnetic moment that plays an important role in scattering. To explain this, we usually take advantage of the neutrons wave-like nature using the de Broglie relationship of

$$\lambda = \frac{h}{p} = \frac{h}{mv} \tag{1}$$

Where the λ is the wavelength of neutron, h is the Plancks constant, p is the momentum, m is the mass of neutron that is $1.67495 \times 10^{-27} Kilogram$ and v is the velocity. With this relationship, a neutron with 81.8 meV of energy will be traveling 4000 m/s and have a wavelength of 1 Å. By cooling down the neutrons, the wavelength can be increased to about 9 Å. This range has reached to atomic scale that makes neutron possibility to probe more micro-structures.

People may ask, Why use neutrons? You already have X-ray scattering, electron scattering and STM, AFM, SPM. Some of these techniques seems also can reach that scale. Or how can you get neutron beam? It seems not common in universities and research affiliate, and what is more, not cheap.To answer these questions, we need to know the basic properties of a neutron. From aspect of scattering interaction, it is neutrality makes neutrons uniquely useful in probing. Neutron also has magnetic moment which can helps to investigate the magnetic interaction in materials. It is the only techniques to directly observe magnetic excitation. In summary, the properties of the neutron bring about some very important consequences that make the neutron a valuable tool in the science community. In this paper, the advantages and disadvantages of the neutron scattering comparing to X-ray Scattering will be first introduced, followed by a detailed theoretical scattering principle, then two kinds of neutron resource will be demonstrated. At last, the research areas related to neutron scattering and two applications on structural biology and investigating materials are presented.

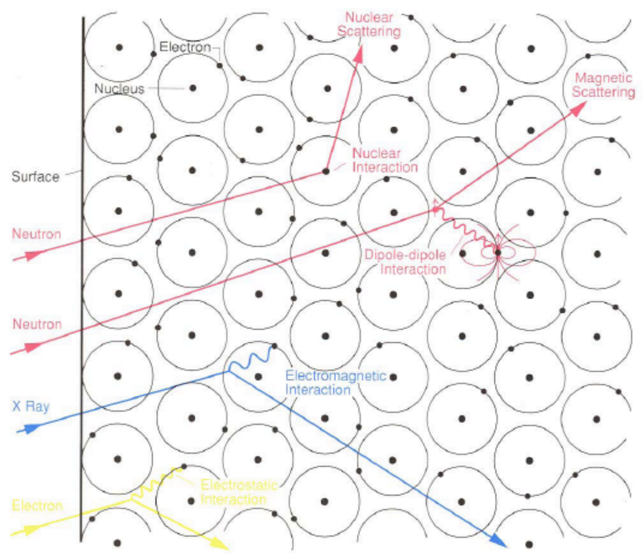

FIG. 1: Scattering interaction

II. NEUTRON SCATTERING

A. Advantages and Disadvantages: Comparing to X-rays Scattering

When a particle beam shooting into a sample, first we need to know what kind of interaction it is going to meet. Figure 1 shows beams of neutrons, x-rays and electrons interact with materials with different mechanism[3]. X-rays(blue) and electron beams(yellow) both interact with electrons in the material. With X-rays the interaction is electronmagnetic, whereas with an electron beam it is electrostatic. Both of these interactions are strong, and neither type of beam penetrates matter very deeply. Neutrons(red) interact with atomic nuclei via the very short-range strong nuclear force and thus penetrate mat-

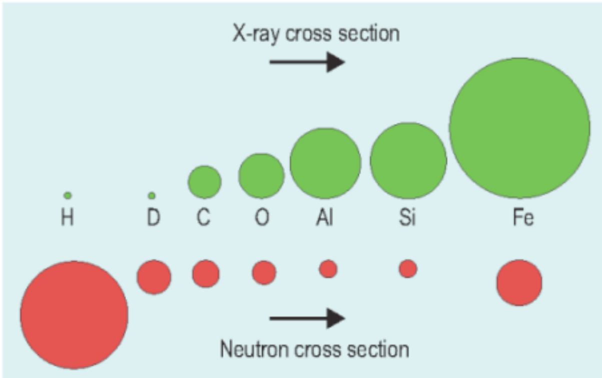

FIG. 2: Neutron and X-ray sattering cross-section compared

ter much more deeply than that x rays or electrons. If there are unpaired electrons in the material, neutrons may also interact by a second mechanism: a dipole-dipole interaction between the magnetic moment of the neutron and the magnetic moment of the unpaired electron.

As we know, X-rays are scattered by electrons; neutrons by atomic nuclei, or magnetic interaction. So with X rays it is easiest to see atoms that have many electrons. However, Hydrogen, for example, which has only one electron, is not easy to see. With neutrons, nearly all kinds of atoms are visible.

In a scattering, we define cross section to identify the effective area presented by a nucleus to an incident neutron. If neutron hits this area, it is scattered isotropically. Figure 2 shows the cross section comparing between neutrons and X-rays. X-rays are easier to probe the structures of many-electrons systems while neutrons scattering are easier to cover the light atoms like hydrogen.

Neutron scattering is a point scattering, that is, scattered with equal probability in any direction. This is different with X-rays because the range of the nuclear potential is tiny compared to the wavelength of the neutron, while X-rays are not. This is the same reason that neutron are usually penetrate in the body of the sample. Neutrons interact with atoms via nuclear rather than electrical force, and nuclear forces are very short range, at the order of a few fermis. Thus, as far as the neutron is concerned, solid matter is not very dense because the size of a scattering center(nuclear) is typically 100,000 times small than the distance between such centers. As a consequence, neutrons can travel large distance through most materials without being scattered or absorbed. Figure 3 illustrates this point with considering the penetration depth of neutrons and X-rays[3].

However, sometimes, we usually combined the two methods to cover different aspects of materials structures. This situation can be showed from Figure 4. A neutron diffraction map[4] can show the positions of the nuclei while X-ray diffraction map can give the distribution of the electrons. The two maps are folded up together that clear that the electron density is shifted in relation to the positions of the positions of atomic nuclei. Since a chemical bond involves a shift in eletron position, a direct picture of the chemical bond is obtained in this way.

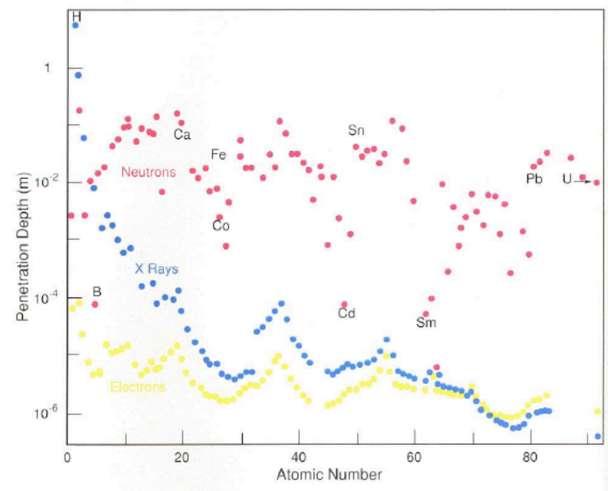

FIG. 3: The plot shows how deeply a beam of eletrons, X rays or thermal neutrons penetrate a particular element in its solid or liquid form before the beam's intensity has been reduced by a fact of $\frac{1}{e}$, that is to about 37 percent of its original intensity. The neutron date are for neutrons having a wavelength of 1.4 $Angstroms(1.4 \times 10^{-10})$

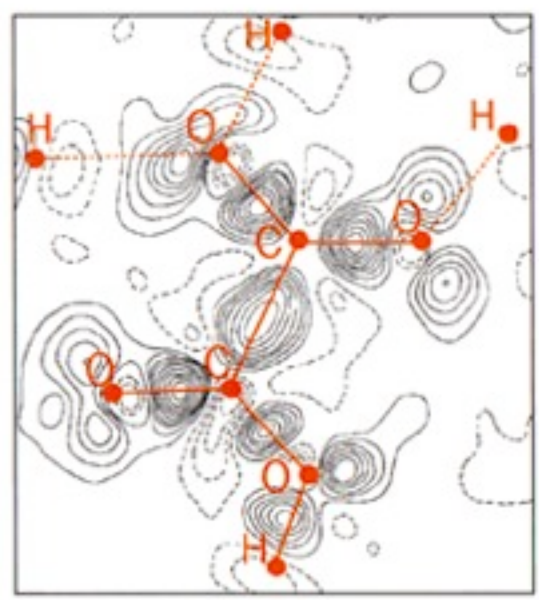

FIG. 4: Neutron and X-ray diffraction mix map[4]

Above all, a summary to the advantages and disadvantages of neutrons scattering are as follows[1].

Advantages:

1. Wavelength comparable with interatomic spacings
2. Kinetic energy comparable with that of atoms in a solid
3. Penetrating. Bulk properties are measured and sample can be contained
4. Weak (point-like) interaction with matter aids interpretation of scattering date
5. Isotopic sensitivity allows contrast variation (especially important in bio-applications)
6. Neutron magnetic moment couples to B. so neutrons can see unpaired eletron spins
7. Possible to use a wide range of solvent conditions (in bio-studies)

Disadvantages:

1. Neutron sources are week, low signals, need for large samples
2. Neutrons are only available at centralized facilities and are expensive
3. Some elements, like Cd, B, Gd absorb strongly
4. Kinematic restrictions(Cant access all energy and momentum transfers)
5. Measured date needs to be corrected for Instrumental effects
6. The measured signal may correspond to a combination of physical phenomena

B. The Principles of Neutron Scattering

The 1994 Nobel Prize in Physics[4] was honored for pioneering contributions to the development of neutron scattering techniques for studies of condensed matter with one half to Professor Bertram N. Brockhouse, for the development of neutron spectroscopy and one half to Professor Clifford G. Shull, for the development of the neutron diffraction technique. In some terms, Shull made use of elastic scattering i.e. of neutrons, which change direction without losing energy when they collide with atoms. Brockhouse made use of inelastic scattering i.e. of neutrons, which change both direction and energy when they collide with atoms.

Figure 5 represents the two kinds scattering where **k**, **k'** are incident wave vector and scatter wave vector respectively and **Q** is an important vector proportional to momentum transfer vector. In all neutron-scattering experiments, scientists measure the intensity of neutrons scattered by matter(per incident neutron). It is a function of the momentum and energy transferred to the sample during the scattering. This $neutron-scatteringlaw$ is written as $\mathbf{I}(\mathbf{Q},\epsilon)$, where $\hbar\mathbf{Q}$ is the momentum transfer, and ϵ is the energy transfer which characterized by

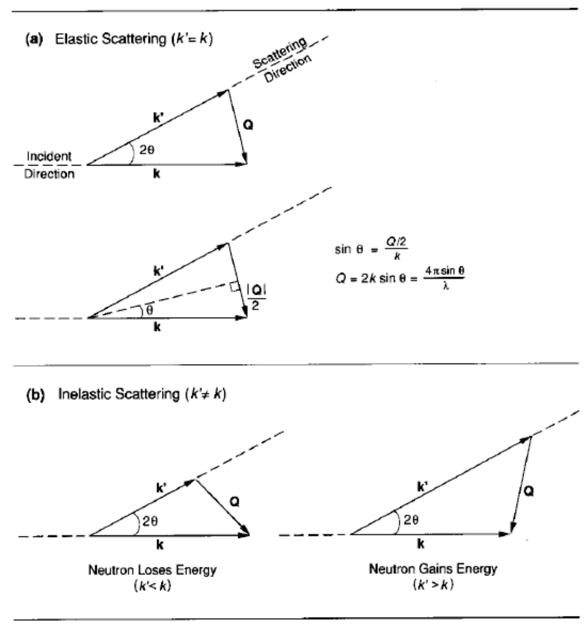

FIG. 5: Scattering Triangle

$$\frac{\hbar^2(k'^2-k^2)}{2m} \tag{2}$$

In a complete and elegant analysis, Van Hove, in 1954, showed that this scattering law can be written exactly in terms of time-dependent correlations between positions of pairs of atoms in the sample. See $\mathbf{I}(\mathbf{Q},\epsilon)$ expression follows(see appendix of [3]:

$$\mathbf{I}(\mathbf{Q},\epsilon)=\frac{1}{h}\frac{k'}{k}\sum_{j,k}b_jb_k\int_{-\infty}^{\infty}<e^{-iQ\cdot r_k(0)}e^{iQ\cdot r_j(t)}>e^{-i\epsilon t}dt \tag{3}$$

where the sum is over pairs of nuclei j and k and that the neclues labeled j is at position $r_j(t)$ at time t, whereas the nucleus labeled k is at position $r_k(0)$ at time $t=0$. The angular brackets $<\dots>$ denote an average over all possible starting times for observations of the system, which is equivalent to an average over all the possible thermodynamic states of the sample.

Van Hoves result implies that $\mathbf{I}(\mathbf{Q},\epsilon)$ is simply proportional to the Fourier transform of a function that gives the probability of find two atoms a certain distance apart. It is the simplicity of this result that is responsible for the power of neutron scattering. Van Hove also provide a way of relating the intensity of the scattered neutrons to the relative positions and the relative motions in matter. This reveal scattering effects of two types. One is coherent scattering, in which the whole sample as a unit so that the scatterd waves from different nuclei interfere with each other. This type of scattering depends on the relative distances between the constituent atoms and thus gives information about the structure of materials. Elastic coherent scattering tells us about the equilirium structure whereas in inelastic coherent scattering provides information about the collective motion of the atoms, such as those that produce vibrational waves in a crystalline lattice. In the second type of scattering, incoherent scattering, the neutron wave interacts independently with each nucleus in the sample so that the scattered waves from different nuclei dont interfere. Incoherent scattering may due to the interaction of a neutron wave with the same atom but at different positions and different times, thus providing information about atomic diffusion.

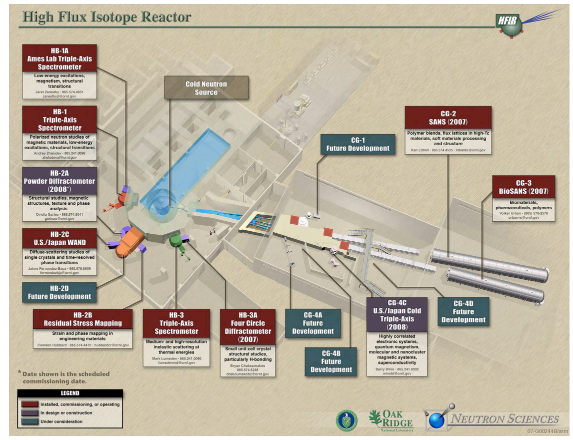

FIG. 6: Layout of HFIR in ORNL

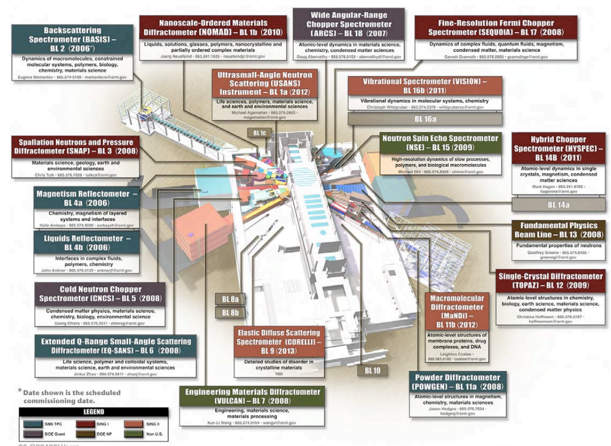

FIG. 7: Layout of SNS in ORNL

III.NEUTRONS RESOURCE

Neutron scattering facilities throughout the world generate neutrons either with nuclear reactors or with high energy particle accelerators.[5] These neutrons produced usually have energy as high as tens or even hundreads mega-electron which is damage to sample and the corresponding wavelength is too short. So we need to cooled down the neutrons first.This cooling is done by bring the neutrons into thermal equilirium with a moderating material which has a large scattering cross section, such as water or liquid hydrogen.There are two fundamental mechanisms provide neutrons for slow-neutron scattering purposes in present day research facilities: fission (in research reactors) and spallation (in accelerator-driven spallation neutron sources).

The reactor source is research grade nuclear reactor where the fission of uranium produce a continous flow of neutrons. The overall physics is the same and they use a chain reaction of the fission of uranium. However, because of the heat limit, these research reactor are limited in the overall flux neutrons produced.

Then we have spallation source. In a spallation, source a neutron rich, heavy metal target is bombarded with pulses of protons. As the protons collide with the target, this creates a cascade effect that produces a large number of neutrons per pulse. The cascade of neutrons are only produced during the pulse and therefore does not allow for a continuous flow of neutrons.

Many countries have worked together to provide different reactor and spallation sources. In Oak Ridge National Laboratory, TN, USA, a new source is the Spallation Neutron Source(SNS)[6] which is hoped to compliment the High Flux Isotope Reactor(HFIR)[7] already at ORNL. This HFIR is the highest flux reactor-based source of neutrons for condensed matter research in the United States, and it provides one of the highest steady-state neutron fluxes of any research reactor in the world. And for SNS, When it is operating at full power, it will offer unprecedented performance for neutron-scattering research, with more than an order of magnitude higher flux than any existing facility. Figure 6 and Figure 7 is the layout of the HFIR and SNS respectively.

China also has a neutrons spallation source project in process. Chinese Academic of Science join hand with local government to construct Chinese Spallation Neutron Source (CSNS) begin at 2007. It is designed to accelerate proton beam pulses to 1.6 GeV kinetic energy at 25 Hz repetition rate, striking a solid metal target to produce spallation neutrons. The future CSNS will be a world-class facility for a new generation of neutron sources, which is characterized with high-flux, broad-wavelength, and is safer and more efficient.

IV.RESEARCH AREA

Neutron science is involved in many research areas as follows,

1. Chemistry
2. Complex Fluids
3. Crystalline Materials[8]
4. Disordered Materials
5. Engineering
6. Magnetism and Superconductivity
7. Polymers
8. Structural Biology

However, these areas mainly use neutron scattering to show where atoms are and what atoms do which is referred in elastic-scattering and inelastic scattering. First, let us get to know where atoms are. As we know, The cross section for light atoms like hydrogen, in X-rays case, is much small than in neutron case. This gives us a idea about research in structural biology. Neutron scattering plays two different roles in biological research, both arising from the special properties of hydrogen. At high resolution, neutrons are used in conjunction with electron density maps established by x-ray studies, and in which hydrogen atoms are not visible, to complete the structure determination. At lower resolution, small angle neutron scattering (SANS) experiments utilize the different scattering power of hydrogen and deuterium to selectively reveal particular aspects of complex biological assembly. Figure 8 shows the surface structure of acarboxymyoglobin derived in this way[9][10]. All of the bound water molecules are associated with polar or charged groups on the skeletal surface of the protein. In figure 6, the oxygen-binding heme group is in purple, the main amino acid chain in blue, with acidic and basic side chains in orange and green, respectively. Neutron scattering results have allowed the determination of the position of 87 weakly bound surface water sites indicated by space-filling dotted clusters. Access to the heme site is not blocked by the surface water.

Next, let us see what atoms do. Neutron scattering helps scientists determine the positions and interactions of "magnetic" atoms in different materials of importance. Because neutrons have a magnetic moment and behave as tiny magnets, they are scattered by an interaction with the unpaired electrons that cause magnetism in materials. It was also called magnetic neutron scattering. Magnetic neutron scattering plays a central role in determining and understanding the microscopic properties of a vast variety magnetic systems.[11] Neutron scattering is the only technique that can directly determine the complete magnetic excitation spectrum, whether it is in the form of the dispersion.

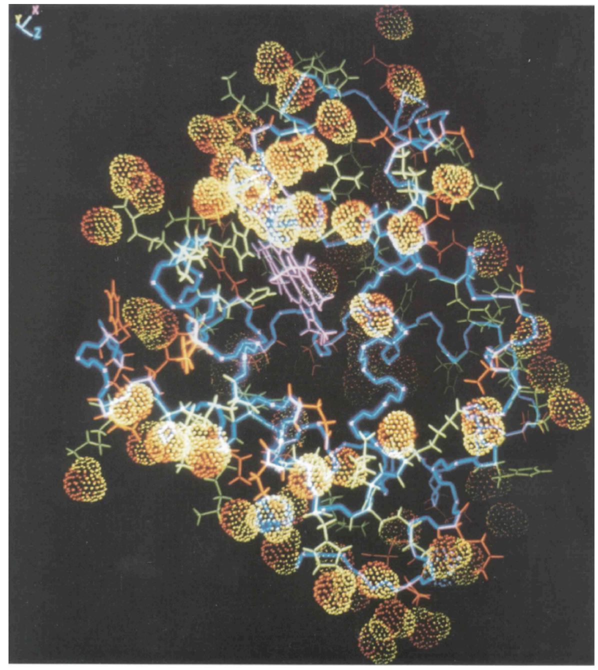

FIG. 8: Surface structure of acarboxymyoglobin by using SANS

Pengchen Dais group have done much work about magnetic excitation termed Resonance in high Tc superconductors with the help of neutron scattering[12]. One of their results can be show in Figure 9.They first probed the low-energy magnetic excitations of $Pr_{0.88}LaCe_{0.12}CuO_{4-\delta}(Tc = 24K)$ using the so-called Spin-Polarized Inelastic Neutron Scattering Spectrometer(SPINS). Considering we are only interested in how neutron scattering method are used, so we are only concentrating the experiment itself. Figure 9a,9b,9c is a Momentum transfer Scan along $Q = [1/2, 1/2, 0]$ at an constant energy transfer $E = 3.5, 8.0, 10\ meV$ respectively. Figure 9d is an Energy Transfer Scan at an constant Momentum Scan $Q = [1/2, 1/2, 0]$ at different temperature $T = 2K, 30K, 80K$ which is covering their Tc. Figure 9e suggests a resonance-like enhancement at $11\ meV$. It is easy to see that the neutron scattering experiments are conventionally conducted through energy transfer and momentum transfer with changing other conditions like temperature and applied-magnetic field.

V.SUMMARY

In summary, neutron will always be an indispensable tool for studying atomic structure and dynamics in condensed matter. Because of its unique properties. However the value of neutron data can be considerably enhanced by the use of complementary data obtained with

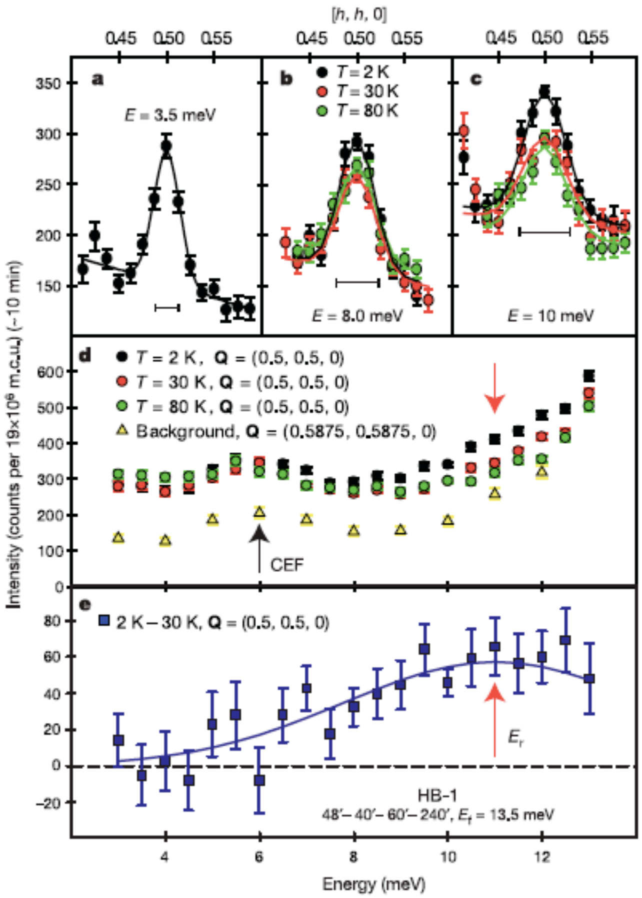

FIG. 9: Magnetic excitation in electron-doped superconducting $Pr_{0.88}LaCe_{0.12}CuO_{4-\delta}(Tc = 24K)$

other methods, and similarly data obtained with other methods are enhanced by the use of neutron data. There is no single experimental technique[13] that can provide us with all the information we need to know about materials. Neutrons scattering do play an implacable role in science.

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