Introduction to Neutron Scattering and Description of ORNL Facilities

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Solid State II, Spring 2009

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March 4, 2009

This paper begins with a brief introduction to Neutron Scattering; the second part discusses some theory about neutron scattering, we will compare neutron scattering with other methods such as synchrotron radiation and x-ray to show the differences and advantages. Next, we will introduce some basics way to get neutrons and introduce the neutron scattering facilities in ORNL. Finally, conclusion and outlook are made towards the future research on Neutron Scattering.
Keywords: neutron scattering, neutron source, HFIR, SNS

I. Brief Introduce of Neutron Science

The 1994 Nobel Prize in Physics is awarded to Bertram N. Brockhouse who is working at the Chalk River Laboratory in Ontario and Clifford G. Shull at the Graphite Reactor at Oak Ridge National Laboratory (ORNL) in Tennessee[1], the award was given for their developments in studying both the structure and dynamics of materials, their pioneering contributions to the development of neutron scattering techniques. Bertram N. Brockhouse and Clifford G. Shull used a new way to help people know some more detail about where atoms "are" and what atoms "do." The saying "neutrons see where atoms are and what they do" has become the motto of neutron scattering science. Just as Bertram N. Brockhouse mentioned in his Nobel Lecture [2], from 1932, people already identification that neutron can emitted in some radioactive processes and show that the supposition of neutrons would exhibit wave-particle duality. The use of neutrons to investigate the fundamental properties of materials began from the 1940s. Neutron applications were explored in the 1950s, from this time, some studies had been made of the elastic scattering of monochromatic slow neutrons by specimens in the form of powdered crystals; then, research further can use well-defined beams of the "slow neutrons" to study the properties of material specimens; people put a lot of energy to study to neutrons and began more and more use it as a very advance method in research[6].

II. Neutron Scattering

Now, neutron is become a very useful tool for studying condensed matter in general. For example, people use neutron scattering method to examination the structure of new materials: such as high- temperature superconductor and magnetic materials. Scientist can also use it to clarification of still unknown phenomena in processes such as recharging of electric batteries. Now, we need to introduce some detail about Neutron scattering both from its own properties and the advantages compared with other traditional studying way[3].

1. The Advantages of Neutron Scattering

When people examination the structure of a new material, they always combine various method to study the materials. Such as x-ray, neutron scattering, STM, AFM and SPM. In resent year, people found that neutron scattering have a lot of advantages compare with x-ray [4]. There are some reasons for it. First, for x-ray, it always interacts with the electron cloud outside the nucleus, so it can only see some heavier elements and the atom that has more electrons outside its nuclear, however, for some light elements, especially at the time when heavier elements are present, X-ray can not see them. But for neutron [5], they have no charge, their dipole moment is nearly zero or too small to be measured, the neutron beams can interactions with the nucleus, so it can effectively see those light elements such as hydrogen and its isotopes. Second, x-ray has very small penetration depth, so it can only be use to do some surface studies of samples. For neutron, it is an electrically neutral particle, neutron interact with atoms via nuclear force which is very short range –of order of only a few fermis, thus, in neutron's eyes, solid matter is not very dense, the distance between nuclear is 100,000 times bigger than the scattering center, so neutron can penetrating the material very highly and with out scattered or absorbed, this properties make neutron can be used to study bulk samples to examine the spatial distribution of stress and texture, for this good property, neutron can also often be used in a wide range of sample environments which is very difficult to use with x-ray, such as high temperature, magnetic field, high pressure and so on. Third, Neutrons also interact with the magnetic moment of unpaired electrons, so the neutrons can be scattered by all elements, this allowing their use for studying magnetic order in materials. Forth, the neutron has a very weak interaction with other matter. The weak interaction between matter and neutrons can let us use born approximation to interpret the scattering cross-section. [7]Thus neutrons can be used for a sensitive, nondestructive study, to study some low atomic numbers, such as proteins and surfactants. But for x-ray or synchrotron, their very high intensities may cause the structures of those sensitive materials to be changed[14]. Figure 1 is a cartoon shows the differences between neutron scattering with x-ray and synchrotron.

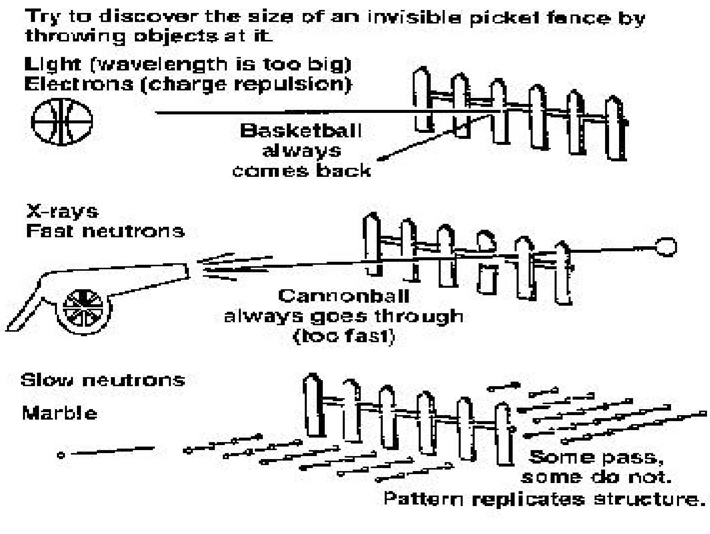

FIG. 1: How does neutron scattering work

2. The Principles of Neutron Scattering
    a. Elastic and Inelastic Neutron Scattering

As the 1994 Nobel Prize's winner, [1] Shull made use of elastic scattering of neutrons, during the elastic scattering, when neutron collide with an atoms, it will changes its direction but didn't losing its energy. People can through examine the change in momentum and angle of the neutrons to study the materials. So through the way neutrons scatter off gases, liquids and solid matter gives us information about the structure of these materials. On the other hand, Brockhouse made use of inelastic scattering of neutrons, during this process, when neutrons collide with an atoms, it will change both direction and energy. So when we study a material, we can not only measuring the change in wave vector, but also can from the dependencies of momentum and energy, use the change in momentum and energy to characterize a systems vibration, magnetic, lattice excitations and other dynamics, and the neutron excitation of atoms gives information about the binding energy within matter [8]. Figure 5 shows the Schematic diagram about both elastic scattering and inelastic scattering.

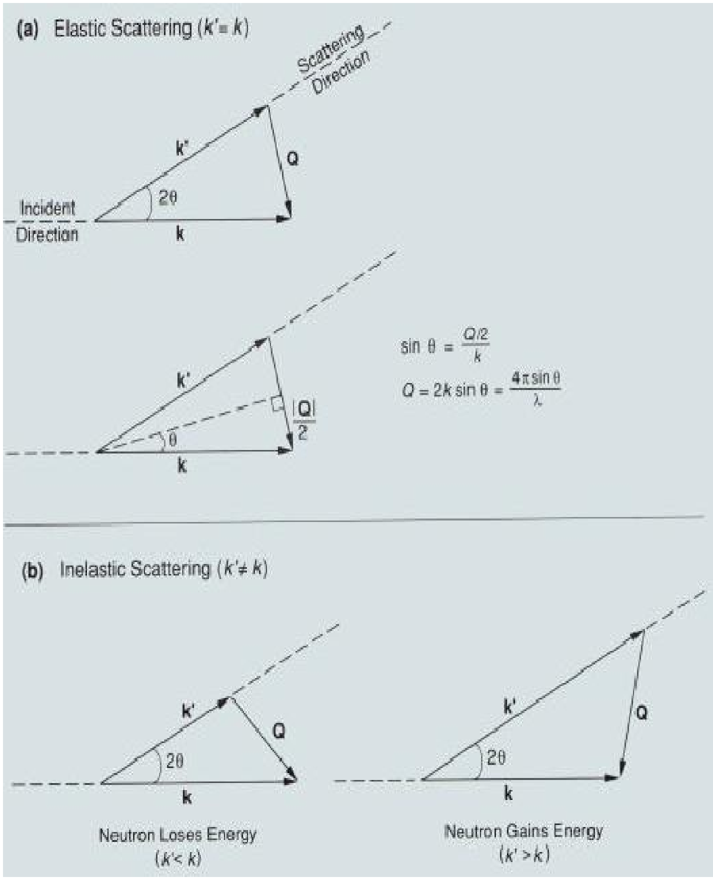

FIG. 5: process of elastic scattering and inelastic scattering

b. When people use neutron scattering to study the properties of materials, the scattering of the neutron can be measured in terms of a cross section σ(in barns) [12].

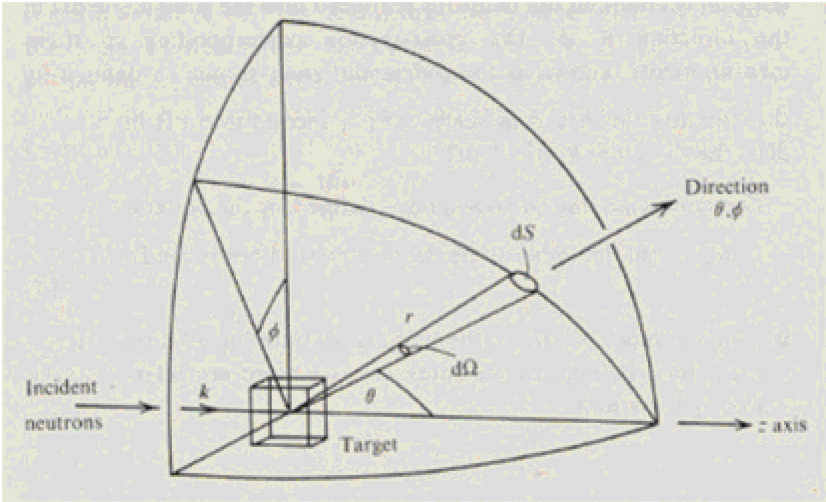

FIG. 2: cross section

Φ = number of incident neutrons per cm square per second
Σ = total number of neutrons scattered per second

number of neutrons scattered per second into $d\Omega$:

$$\frac{d\sigma}{d\Omega}=\frac{d\Omega}{\Phi d\Omega}$$

number of neutrons scattered per second into $d\Omega$ and dE

$$\frac{d^2\sigma}{d\Omega dE}=\frac{d\Omega \,\&\, dE}{\Phi d\Omega dE}$$

For the point scattered[11], because the range of the nuclear potential is very small compared with the wave-length of the neutron, so the nuclear is effectively can be seen as a point, and it is scattered isotropically. Because the energy of neutron is too small to change energy of nucleus, so neutron can not transfer kinetic energy to a fixed nucleus, the scattering is can be seen as elastic. If v is the velocity of the neutron (not change during the scattering), the number of neutrons passing through an area dS per second after scattering is :

$$vdS\left|\Psi\right|^2 = vdSb^2/r^2 = vb^2 d\Omega$$

Since the number of incident neutrons passing through unit areas is :

$$\Phi = v\left|\Psi_{incident}\right|^2 = v\text{ , }\quad \frac{d\sigma}{d\Omega}=\frac{vb^2 d\Omega}{\Phi d\Omega}=b^2$$

So $\sigma_{total} = 4\pi b^2$

Figure 3 is shows the Schematic diagram about the scattering by a single Nucleus

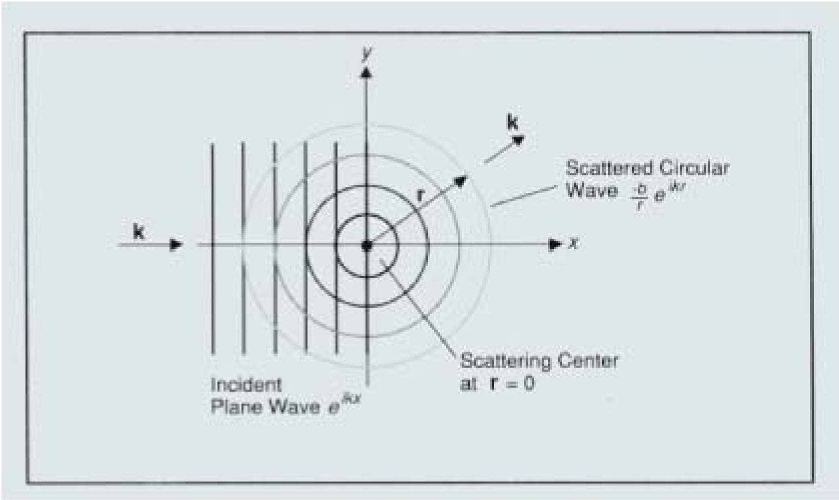

FIG. 3 scattering by a single Nucleus

In majority of cases, when people do research, they see b is a real and energy-independent quantity, b has to be determined through experiment for different nuclear isotope. Because the neutron's interaction with a nucleus of an atom varies from isotope to isotope, that can be use to do some isotopic-labeling techniques. For example, we can not use x-ray to distinguish hydrogen and deuterium, because those two atom are very light and interact weakly with x-ray, but when we use neutron scattering, we can found the large differences in scattering length of those two atom. Figure 4 is shows the intrinsic cross section of different atoms, which can be used to study distinguish isotope[11].

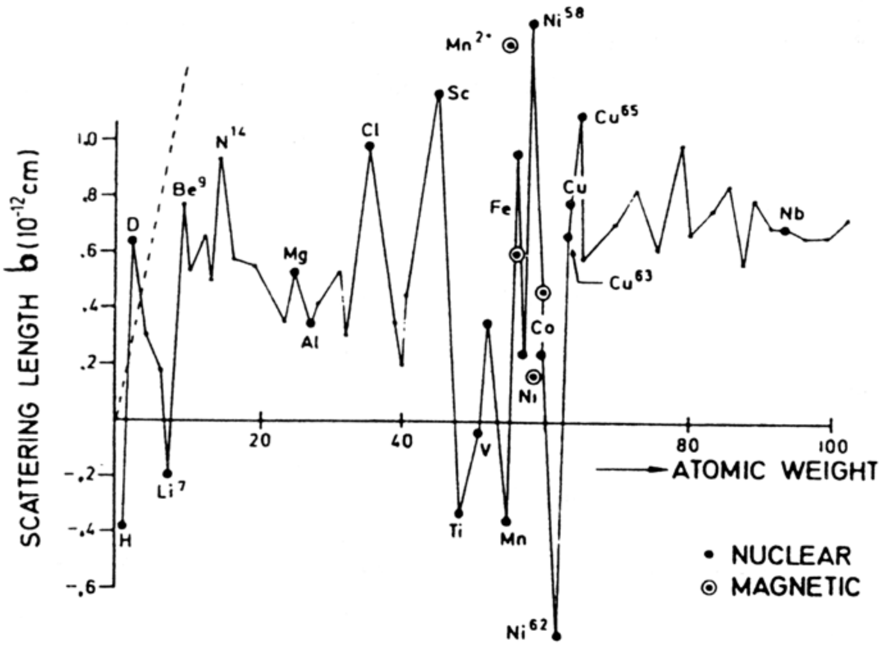

FIG. 4: intrinsic cross section

When people want to know how neutrons are scattered by matter, the scattering from each individual nucleus should be add up. During the process, both the momentum and the energy should be changed, we can not go on to see it as an elastic process because the atoms in matter are free to move, they can recoil during the collision, Because the total momentum and energy should be conserved, so the energy lost by the neutron should be gained by the sample. We have the function for both momentum and energy(with Q in the equation), k is the incident wave and k' is the scattered neutrons. Q is known as the scattering vector, during the experiment, people measure the intensity of neutrons scattered by the sample as a function of the Q and E, then through the intensity of the neutron scattered, people can know the relative positions and relative motion of atoms in matter. There are two part of this scattering[13], the first part is named coherent scattering, in this scattering, the neutron wave interacts with the whole sample as a unit, the scattered waves from different nuclei can interfere with each other. The relative distances between different atoms will determine this, so it can give us information about the structure of materials. Elastic coherent scattering can give us information about the materials equilibrium structure. The intensity of elastic coherent neutron scattering is proportional to the spatial Foutier transform of the pair correlation Function G(r), it is the probability of finding a particle at position r if there is simultaneously a particle at r=0. The intensity of inelastic coherent neutron scattering is proportional to the space and time Foutier transforms of the time dependent pair correlation function G(r,t), it is proportional the probability of finding a particle at position r at time t when there is a particle at r=0 and t=0 . Inelastic coherent scattering can show some information about the collective motions of the atoms, for example: the vibration in crystal lattice. The second part is named incoherent scattering, the neutron wave interacts independently with nucleus in the sample, and the scattered wave from different nucleus don't interfere. For inelastic incoherent scattering, the intensity is proportion to the space and time Fourier transforms of the self-correlation function Gs(r,t), it is the probability of finding a particle at position r at time t when the same particle was at r=0 at t=0, which means incoherent scattering is due to the interaction of a neutron wave with the same atom at different time and different position, so it can provide some information about atomic diffusion. Through the experiment, we can get G(r,t) [11]:

$$G\ (\vec{r},t)=\frac{1}{N}\int\left\langle\rho_N(\vec{r},0)\rho_N(\vec{r}+\vec{R},t)\right\rangle dr$$

$$G_s(\vec{r},t)=\frac{1}{N}\sum_j\ \int\left\langle\delta(\vec{r}-\vec{R}(0))\delta(\vec{r}+\vec{R}-\vec{R}_j(t))\right\rangle dr$$

then, use the above equation, we can get S(Q, **ω**):

$$S(\vec{Q},\omega)=\frac{1}{2\pi\hbar}\iint G(\vec{r},t)e^{i(\vec{Q}x-\omega t)}d\vec{r}dt$$

$$S_i(\vec{Q},\omega)=\frac{1}{2\pi\hbar}\iint G(\vec{r},t)e^{i(\vec{Q}x-\omega t)}d\vec{r}dt$$

next, we can get the result that:

$$\left(\frac{d^2\sigma}{d\Omega dE}\right)_{coh}=b_{coh}^2\frac{k^{'}}{k}NS(\vec{Q},\omega)$$

and $$\left(\frac{d^2\sigma}{d\Omega dE}\right)_{inc}=b_{inc}^2\frac{k^{'}}{k}NS_i(\vec{Q},\omega)$$

S(Q, **ω**) is the dynamical structure factor of the crystal, this is a structure factor which is totally determined by the crystal itself without reference to any properties of the neutrons

III. Facilities of Neutron Scattering in ORNL

1. How to Get Neutrons

In general, in the condensed matter research, there are two ways to get the neutron source, one is produced by nuclear reactor, which is used by the facility named of High Flux Isotope Reactor (HFIR), and another one is produced by spallation source, which is named Spallation Neutron Source (SNS). Both of those methods and their associated instrumentation have their own advantages and disadvantages for such measurements [15].

2. Reactor Sources

Through the fission of U-235 in a chain reaction, this reactors produce neutrons, the advantages for the reactors is that it is have more neutron flux and have better developed instrumentation for the use of polarized neutrons[16]. Figure 6 shows the reaction about how to get reactor sources.

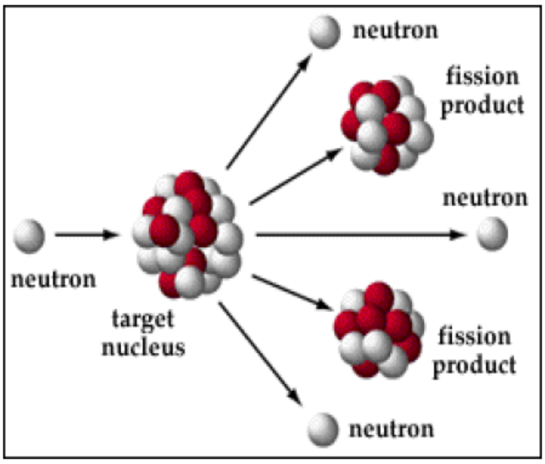

FIG. 6 fission reaction

The reactor source uses nuclear fission to create neutrons, so it can get continuous neutron flux, and the flux is dependent on fission rate. That is a very important advantage for reactor source. However, this way also have some disadvantages like it creates radioactive nuclear waste, at the same time, because the nuclear fission can also create some other isotopes, so it make the neutron unclean and we need further method to purify the neutron source.

When we get neutrons from the way of spontaneous fission, the neutron have very high energy, the wavelength of neutron is to short to be used to investigate the structure of condense matter, for another reason, the high energy neutron will damage the sample, because it may kicking the atoms out of their initial position. So we need use some method to cool down those neutrons, we put neutron in to a thermal contact with moderator, the moderator are always made by some materials which has very big scattering cross section. In the moderator, the neutron collide with the atoms and lose energy, at last, the neutron attain the thermal equilibrium. When the neutron emerging from the moderator, it has very low energy and the wavelength are long enough which has the same order compare with the position between the atoms in the sample. However, the thermal neutron which we get from the moderator have different energy and different wavelength, we can not use them directly into our experiment. we need the monochromatic neutron beam which has neutrons in a single, narrow energy band. Here, we use a method named triple-axis spectrometer to get the monochromatic neutron beam. Monochromator is made by some materials which has high reflection, such as germanium and copper. The basic theory about this method is Bragg reflection, we know the reflection angle and the spacing of the reflection plane, and then, through the Bragg equation, we can get the exactly wavelength which we want, the energies of the monochromated and scattered neutrons are determined by Bragg reflection.

Figure 7 shows a schematic diagram of a triple-axis spectrometer[13], this is used for inelastic experiments on single crystals at reactor sources. Neutrons are detected by a He-3 ionization chamber.

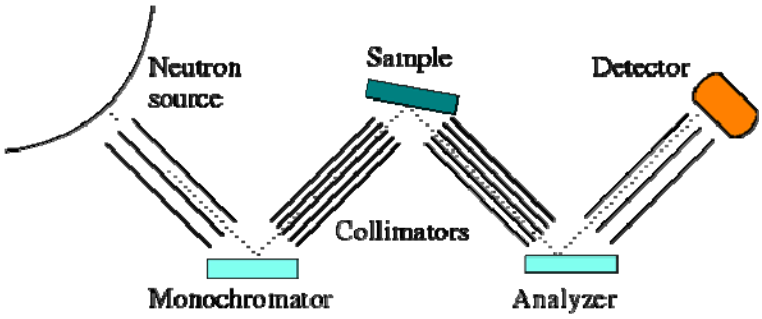

FIG. 7 Schematic diagram of a triple-axis spectrometer, which is widely used at reactor sources for measuring excitations. The incident wave vector of the neutrons is selected by a monochromator (M) crystal (typically graphite). Neutrons scatter at the sample (S). The final wave vector (energy) of the scattered neutrons is selected by an analyzer (A) crystal. Neutrons are detected in a He-3 ionization detector

3. Spallation Sources

When a high-energy proton beam hits a heavy metal (such as Ta, Hg, U) target, driving nertrons our of the nuclei of the target, we can get spallation source[17]. That is a kind of effect named cascade effect. Because we get spallation source through the proton hits the target, so the source is pulsed; this allows the neutron's energy to be measured by time-of-flight methods. In this cases, the proton is supplied by the accelerators. The advantage of this method is we can get low energy neutrons. Spectrometers with a low intrinsic background can be built at pulsed neutron sources. Those kinds of neutron sources have high intensity and the heat production is relatively low[18]. Figure 8 shows a schematic diagram of the process of how to get spallation sources.

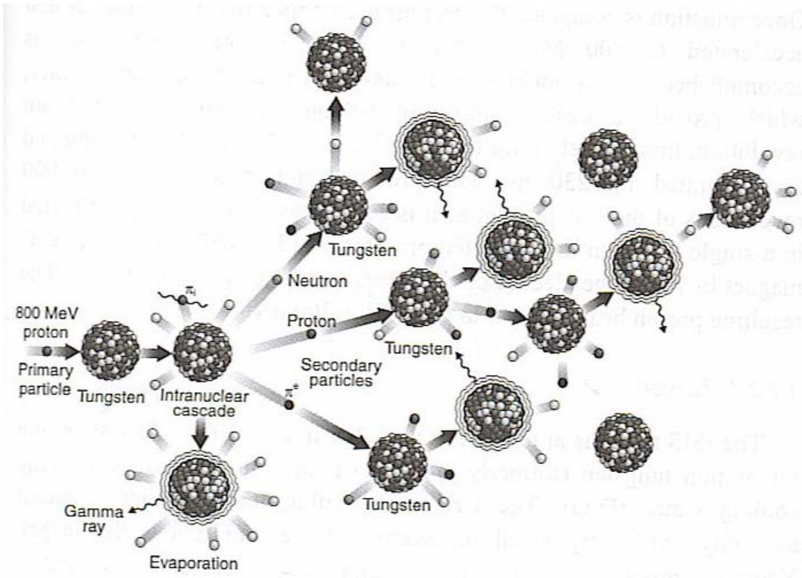

FIG. 8 Spallation Sources

From the analysis above we can find the different between nuclear reactor and spallation source[8] Fig 9 is a diagram show this differences

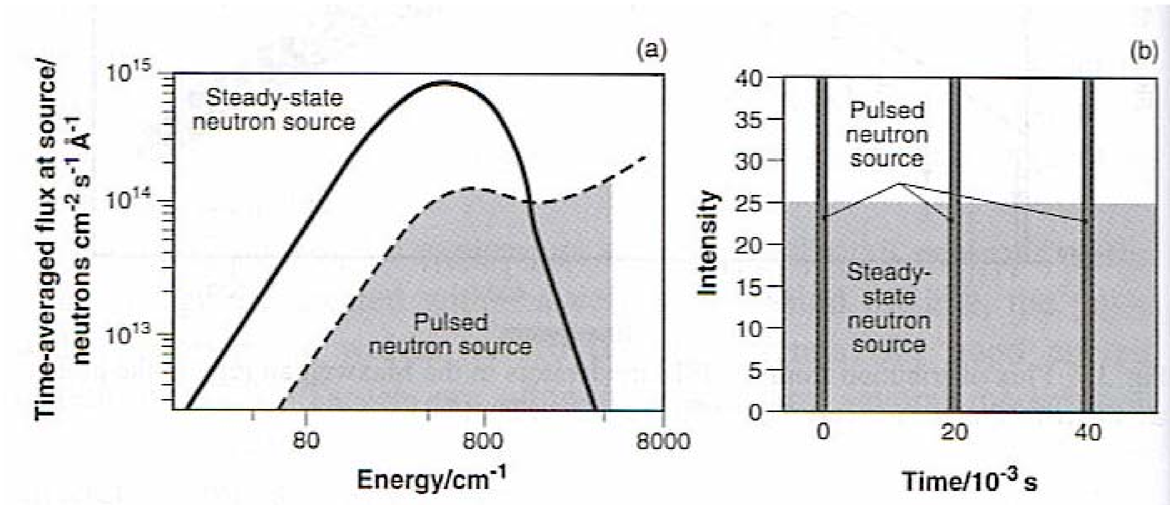

FIG. 9 the different between the nuclear reactor and spallation source Facilities

4. HFIR

ORNL High Flux Isotope Reactor is the highest flux reactor-based source of neutrons for condensed matter research in the United States, it use reactor source, it can provides one of the highest steady-state neutron fluxes of any research reactor in the world. Actually , it is a very expensive facility, because we use spontaneous reaction of U235 to get the neutron source, so in this auxiliary equipment, the facilities are always contained in a sealed vessel with very thick of wall, people use this way to avoid the escape of radioactive material into the environment, during the process of reaction, the pressure inside the building is always lower than outside to insure the leakage is inward rather than outward [13]. The thermal and cold neutrons produced by HFIR are used to study in various areas such as physics, chemistry, materials science, engineering, and biology. The intense neutron flux, constant power density, and constant-length fuel cycles are used by more than 200 researchers each year for neutron scattering research into the fundamental properties of condensed matter [19]. Figure 10 (a),(b) is a simulated picture for the HFIR.

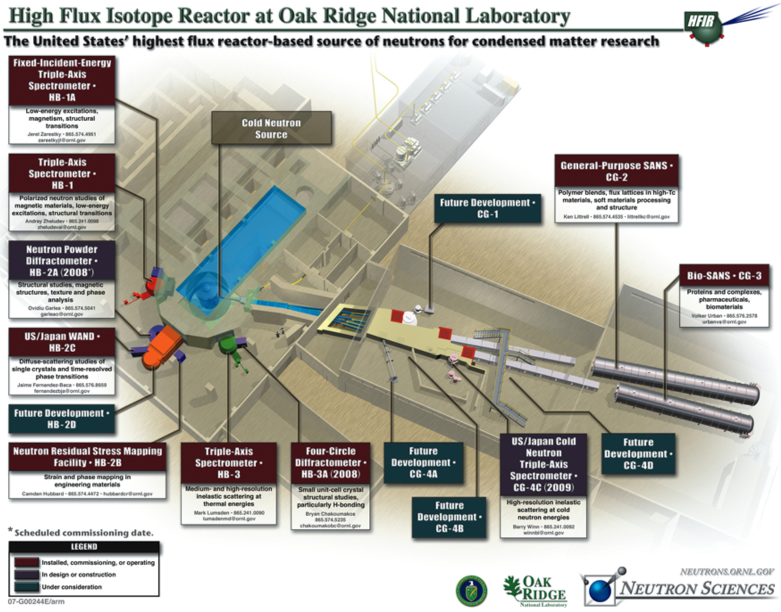

FIG. 10(a) HFIR at ORNL

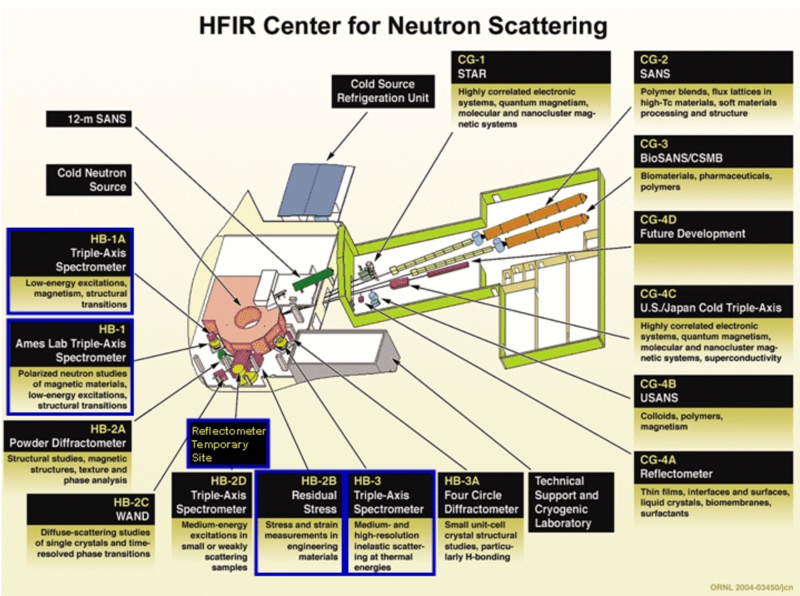

FIG. 10 (b) HFIR Center

5. SNS

ORNL Spallation Neutron Source (SNS) is a kind of facility to provide spallation source, it will offer unprecedented performance for neutron-scattering research. The SNS in Oak Ridge can provided more than an order of magnitude higher flux than any existing facility, and become one of the most powerful facility than the most intense existing pulsed (non-fission) spallation source. The beams of this facility suited to the needs of users in different research areas. Instruments will be available to researchers with varying degrees of experience[20]. Figure 11 is a simulated picture for the SNS.

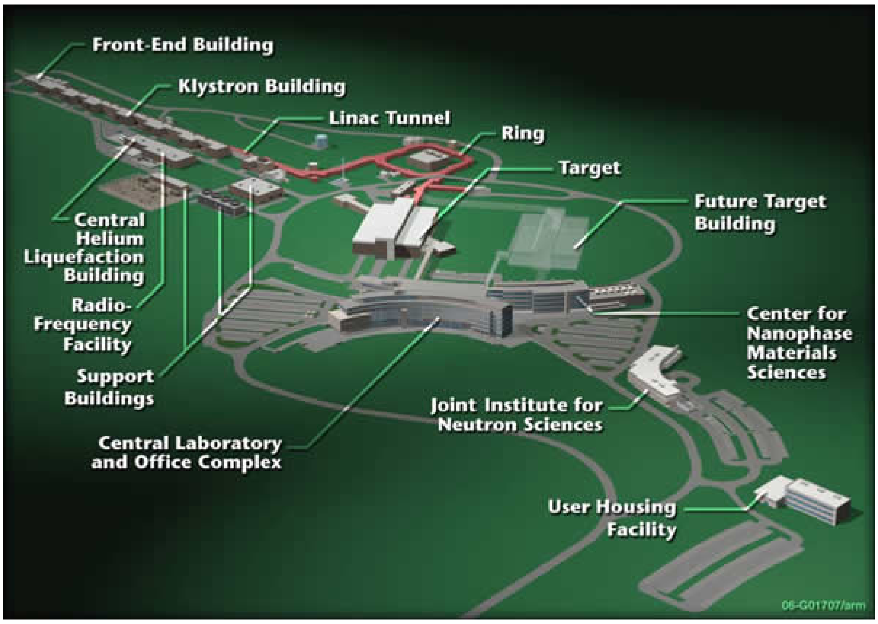

FIG. 11 Conceptual drawing of the SNS facility showing all completed buildings, as well as the planned second target building and the Joint Institute for Neutron Sciences. Items in red—the linear accelerator and ring systems—are underground[21]

IV. Conclusion and Outlook

Over the years since Bertram N. Brockhouse and Clifford G. Shull made the contributions for which they are now being awarded the Nobel Prize, neutron scattering methods have found widespread applications. As everyone know, neutron scattering is a very expensive method to study the different materials, however, nowadays, thousands of scientists are using neutron scattering to help them for their research, they study the structure and dynamics of the high temperature superconductors; some of them use neutron scattering to study the molecule movements on surfaces for catalytic exhaust emission control, some biologist use this advance method to study the interaction between proteins and the genetic material of viruses, the connection between the structure and elastic properties of polymers[3]. In view of the above, one might expect that neutron scattering would have made a significant impact on our future science research.

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