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NEUTRONS AS A PROBE - AN OVERVIEW -

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ABSTRACT

As an introduction to the symposium a brief overview will be given about the features of neutrons as a probe. First it will be pointed out that the utilization of neutrons as a probe for investigating the structural and dynamical properties of condensed matters is a benign gift eventuated from the release of atomic energy initiated by Enrico Fermi exactly half century ago. Features of neutrons as a probe are discussed in accordance with the four basic physical properties of neutrons as an elementary particle; (1) no electric charge (the interaction with matter is nuclear), (2) the mass of neutron is 1 amu, (3) spin is $1/2$ and (4) neutrons have magnetic dipole moment. Overview will be given on the uniqueness of neutrons as a probe and on the variety in the way they are used in the wide research area from the pure science to the industrial applications.

INTRODUCTION

As a speaker of the keynote lectures I understand that it is my role to speak something about the research utilizing neutrons as a probe especially from the users' point of view. Unfortunately I am an "ex-user" and hence not appropriate to talk about the present status and the frontier of the neutron research.

In this sense I am not the qualified person to deliver the keynote lecture in the opening session of this symposium. However I think I can make good use of this half-layman's point of view to speak to the non-experts on how neutrons are useful and how they are used as a probe.

In this opening session a lot of non-experts are in presence and there are variety of experts from the different fields since this symposium covers a wide variety of research fields related to the utilization of neutrons as a probe. Some attendants are the experts on the neutron sources which provide neutrons for the probe-use.

Therefore I think it may be useful to give an overview for the non-experts leaving the most advanced topics to be delivered by the speakers of the sessions to follow. I hope I can

give you a general view ,or guide map , by which you can place the detailed talks you are going to hear in a unified framework.

ATOMIC ENERGY AND NEUTRONS

Before going into the main subject I would like to make a brief comment on the relationship between the neutron utilization and the development of the atomic energy.

As you are aware neutrons as a probe are an indispensable tool in the basic as well as applied sciences. Everyone will admit that without neutrons the basic science especially the condensed matter physics has not reached the present status. The point I would like to emphasize is that the science developed by neutrons is a benefit of the release of the atomic energy and the development of nuclear engineering.

Soon after neutrons were discovered by Chadwick in 1932, the possibility of utilizing neutrons in a way similar to the X-rays as a probe were pointed out because of the wave nature of the neutron as a quantum particle and a few pioneering works followed. However real use of neutrons as a probe had not been possible until the dawn of the atomic energy.

Enrico Fermi succeeded to demonstrate the self-sustaining chain reaction in December 1942, just half century ago. He carried out some measurements on the wave nature, interference and mirror reflection of neutrons just after he realized the chain reaction and plenty of neutrons became available. This was the beginning of the use of neutrons as a probe.

Since then the research reactors were built in Oak Ridge, Brookhaven and in Great Britain and France and thus the neutron research became in full bloom. In accordance with the development of the atomic energy higher and higher neutron beams became available and this has brought the science utilizing neutrons to the present status.

The atomic energy is primarily the release of the nuclear energy through nuclear fission reactions and the nuclear reactors are the device for energy production. However from another point of view they are the sources of neutrons and very intense one at that. Then we can use them as probes which are the issue in the present symposium and also to produce radio-isotopes.

Therefore the release of the atomic energy has not only given us humankind a new means of energy generation instead of usual chemical energies but also bestowed us intense sources of neutrons which we can utilize as probes to develop various fields of science.

WHAT IS A PROBE ?

I think you know what the probe is, but a brief mention will be due here as a step in my talk.

A probe is something to be introduced into a sample in order to investigate properties of the matter by its response to the probe. The probe introduced into the sample encounters the entities of matter and they are partly scattered, partly absorbed emitting secondary radiation, or partly penetrates without interaction. The way how the sample responds to the probe tells us the internal state of the matter.

There are various items we want to know about the state of matter. What items we are interested in decides what the suitable probe to be used is.

As Prof. Date mentioned earlier we have various kinds of probes in hands and there are a great variety in the ways the probes are used.

It may be useful to compare features of the probes with each other but here I am just going to emphasize the uniqueness of the neutrons as a probe without going into details of that kind of comparison.

The synchrotron radiation is the strongest rival of the neutrons since the applied fields are overlapping with each other. Fujii is going to talk about the comparison of both in this symposium.

FEATURES OF THE NEUTRONS AS PROBES

Basic physical properties of a neutron are

- a) it has no electric charge and then the interaction with matters is nuclear,
- b) its mass is about 1 atomic mass unit, i.e. almost equal to the hydrogen nucleus,
- c) its spin is $1/2$ and
- d) it has magnetic moment.

In the followings we are going to see how these properties are useful as probes.

NEUTRONS AS A ZERO-CHARGE PROBE

First let's pay attention to the property that the neutron does not have electric charge and it is neutral. This means that neutrons do not interact with electrons in the matter. The interaction with matters is that with nuclei which are in the core of atoms. This is entirely different from the light or electrons as probes. The latter two probes interact with electrons comprising the outer shell of atoms.

Nuclear, not electromagnetic, interactions are favorable as probes in two respects. First the microscopic sensitivity to each atom does not have any systematic dependence on the atomic number. Secondly the macroscopic penetrability through matter is generally very good.

Let's compare neutrons with X-rays with respect to the visibility, namely the sensitivity of the probes when they encounter with the specific atoms. In case of X-rays atoms with larger number of electrons, that is, the heavier atoms, are more visible. On the contrary lighter atoms have less visibility; especially the hydrogen atoms are hardly visible in comparison with heavier atoms.

By contrast neutrons shows diverse visibility which changes unsystematically from one nuclide to another. The visibility of hydrogen is not bad, which is important as mentioned later. In some cases the scattering strength is negative. In case of hydrogen the normal hydrogen has negative and the deuterium has positive and fairly large scattering strength. This fact is important in the application for the biological systems.

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The good visibility of light elements for neutrons gives rise to the precise determination of the positions of light elements such as hydrogen and oxygen in the crystal-structure determination by neutrons.

For example neutrons are quite important in determination of the oxygen atoms in the crystals of high-Tc superconducting oxides in which the deviation or vacancies of oxygen atoms are likely to play some essential roles in the appearance of the superconductivity. The crystal structures of the oxides were determined promptly after the discovery of each oxide by the high resolution powder neutron diffraction methods.

The sensitivity of neutrons for light atoms and the distinction between different isotopes are especially valuable in studying the biological systems.

Hydrogen is one of the constituent elements which are contained in biological molecules with large numbers and the precise knowledge of the positions of each atom in the three-dimensional structure is quite important in relation to the function of the molecules.

The importance of neutrons as a structural probe with high sensitivity for the light atoms is obvious in this regard. Moreover there is one more unique aspect of utilizing the neutrons as the structural probe for hydrogen atoms. This comes from the difference between normal hydrogen and deuterium in regard to the scattering nature: namely, hydrogen has small and negative scattering amplitude in contrast to the positive one with the normal size for deuterium. Substitution of hydrogen with deuterium, or light water with heavy water, changes the scattering of the biological molecules themselves or those molecules in contrast to the solvent, which can be used in a very ingenious way for studying the structures of biological molecules. The details will be shown in the paper by Zaccai in this symposium.

Neutrons, as a zero-charge particles, can penetrate deeply through materials under investigation. This property is very favorable in the nondestructive testing of industrial products by neutrons in comparison with that by the X-rays. This aspect will be emphasized by Hutchings in his paper on commercial applications of neutrons.

The high penetrability and the selective absorption of neutrons for respective elements are the keys in the neutron radiography and the prompt-gamma-ray analysis which are the aspects covered by Barton and Jervis, respectively in this symposium.

PROBE AS A QUANTUM WAVE WITH MASS 1 AMU

The second feature of neutrons as a probe is their mass with 1 amu.

According to the de Broglie relations a moving particles with momentum p and energy E has wave nature with the frequency ν and the wavelength λ given by

$$\nu = E/h, \quad \lambda = h/p.$$

Neutrons, like electrons which show wave properties demonstrated by, e.g., electron microscope, have wave properties with the frequency-wavelength relationship quite different from that for electrons because of the different mass of the particles.

The wave properties are most evidently demonstrated by the interference effect: the wave, once split into two paths, interferes when it put together again. The interference of the light was demonstrated by, e.g., Michelson interferometer.

The neutron's version of the interferometer was invented by Rauch, who is going to tell us directly in this symposium on the recent advances made in this field. It is marvelous to know the quantum effect manifesting itself in our daily scale, not in the atomic scale.

The neutron interferometer is important in investigating the fundamental problems in the quantum physics. Tonomura is going to discuss the related problems in connection with his recent achievements by the electron holography.

One of the interference phenomena in the atomic scale is the neutron diffraction. Neutrons incident on condensed matters are scattered collectively as waves, that is, the scattered waves from atoms interfere with each other and give rise to a diffraction pattern. The analysis of the pattern gives an information on the arrangements of the scattering centers, that is, the structure of the condensed matters in the atomic scale.

It is essential to have the wave-probe with wavelength which is the same order of magnitude as the typical size of the structure under investigation. Thermal neutrons extracted from the research reactors or pulsed sources are quite favorable in this respect, since they have energy of about 0.025 eV which corresponds to the wavelength of about 0.18 nm. This turns out to be the same order of magnitude as the interatomic distances in condensed matters.

The neutron diffraction method is used very widely to investigate the structure of condensed matters. The uniqueness of neutrons is most remarkable when they are used to determine the light atom positions in the crystals or macromolecules. Neutrons are indispensable in determining the arrangements of magnetic atoms in the various kinds of magnetic materials. This is because of the strong interaction between neutrons and magnetic dipoles as described later.

Neutrons are also useful to study the disordered structures of the condensed matters. The most disordered structure is the liquids which is the subject discussed by Ohno in this symposium.

The small-angle scattering is suitable to investigate the structures one level higher than those of atomic scale, such as density fluctuation in alloys or biological structures. Since larger wavelength is favorable for this purpose, the cold neutrons extracted from the cold sources through neutron guide tubes are used for the small-angle neutron scattering. Availability of the long wavelength neutrons is one of the favorable points of neutrons as a structure probe.

Various examples of the small-angle scattering will be given by Zaccai on the application to the biological systems and by Hashimoto on the application to the polymers.

NEUTRONS AS A PROBE TO SEE ATOMIC MOTIONS

In addition to the feature as the structural probe in the atomic scale thermal neutrons have another important feature in exploring condensed matters. It is the possibility of measuring the energy change when neutrons interact with condensed matters.

The energy of neutrons extracted from the research reactors distributes around 0.025 eV which is almost the same as the energy of elementary excitations in condensed matters, such as lattice vibrations or spin waves.

Neutrons incident on a condensed matter can either give energy to or get energy from the vibrating atoms and we can measure the energy of neutrons after scattering which is different from the energy of incident neutrons. This type of scattering is called the inelastic scattering by which we can get information about the excited states in the condensed matter. This gives us a detailed knowledge on the dynamics of condensed matters at the atomic level.

The feature of neutrons as a dynamic probe does not merely lie on the possibility of measuring the energy change upon scattering. The combination of the two features that the wavelength of neutrons is comparable with the size characterizing the structure of condensed matter in the atomic scale and that the energy of neutrons is comparable with the energy of thermal motions of the condensed matters in the atomic scale reveals nature of collective motions in the condensed matters. This is the most marvelous feature of neutrons as a microscopic probe.

Atoms in a condensed matter do not move individually but they move in a mutually connected way. This is a collective motion. It consists of waves propagating on the three-dimensional array of atoms in various directions with various wavelength.

When a neutron is scattered inelastically by the condensed matter, it usually excites or deexcites one of the propagating waves. The neutron does not hit a single atom but interacts with an array of atoms as a whole and exchange energy by exciting or deexciting the propagating wave. This comes from the wave nature of neutrons. The neutron can excite or deexcite more than two propagating waves. But the chance is less and the scattering does not give useful information but forms just a background.

The propagating atomic motions are characterized by the wave vector q and frequency ν . The wave vector is a vector pointing the direction of propagation of the wave and having the magnitude of the reciprocal of the wavelength. The wave vector is determined by the momentum conservation relation of the scattering and the frequency by the energy conservation relation of the scattering. Thus the inelastic scattering of neutrons exciting or deexciting a propagating wave determines the wave vector and frequency simultaneously. Different configurations of the scattering give different sets of wave vector and frequency.

Thus we can obtain full information of the wave-vector versus frequency relations, namely the dispersion relations, of the elementary excitations in the condensed matters, such as phonons or magnons. This is one of the most essential information to understand the dynamical nature of the condensed matters. The dispersion relations are only part of the more general dynamical characteristics of the condensed matters studied by the neutron scattering.

The phase transition phenomena is closely related to the dynamical nature of solids revealed by the neutron scattering. An instability of a certain type of collective motion, that is the decrease of its frequency as a function of a state variable such as temperature, gives rise to a phase transition. This aspect of the phase transition is extensively disclosed by the inelastic neutron scattering. Shirane, one of the pioneers in this field, will tell us the recent advance in this symposium and Morii is also going to tell us his results on the relationship between the

martensitic phase transitions in a certain type of alloys and the lattice-dynamics observed by the neutron scattering.

Some remarks on the accuracy of measuring the energy change will be due here. The energy resolution of common neutron spectrometers is of the order of 0.1 meV which is enough to measure the thermal vibration of atoms in condensed matters.

In order to observe the atomic dynamics with lower energy, such as the motion of polymer chains related to the viscoelasticity of the polymers or spin fluctuations in the very vicinity of the critical temperature, we are in need of far better energy resolution, say 1 μ eV or lower. Recent advance of the neutron spectroscopic technology provides us an ultimate resolution in the range of 1 μ eV to 1 neV.

Richter will tell us how the high energy resolution machines contribute to reveal the dynamics of polymer in very detail.

One of the methods to improve the energy resolution is to lower the incident energy of neutrons used as the dynamical probe. An extreme in this direction is the utilization of ultra-cold neutrons which is important not only to improve the energy resolution but also to broaden the application of neutrons as a probe as Utsuro will mention in this symposium.

NEUTRONS AS A PROBE WITH SPIN

The property that the neutrons have spin 1/2 makes the scattering dependent on the nuclear spin; the probability of scattering for neutrons with spin in parallel with the nuclear spin is different from the one for anti-parallel alignment. This property introduces the distinction between coherent and incoherent scatterings. The former causes interference among the scattering from all the scattering centers, e.g. nuclei, and the latter is just a superposition of the scattering from each center and forms just a background to the coherent scattering. Most of the abundant information on the structures and dynamics in the atomic scale mentioned thus far is obtained by the coherent scattering.

The nuclear-spin-dependence can be used to study the nuclear magnetism, namely the alignment of nuclear spins on solid state lattices at very low temperature.

NEUTRONS AS A PROBE WITH MAGNETIC MOMENT

Neutrons have a magnetic moment, which means that a neutron is a microscopic magnet. When an atom has a magnetic moment, that is, when the electrons of the atom leave unpaired spins, neutrons are scattered through the magnetic interaction between dipole moments of neutrons and atoms. The magnitude of the interaction is of the same order as the nuclear interaction between neutrons and nuclei.

This property makes the neutrons as a unique probe to investigate the magnetic properties of solids at the atomic level. All the descriptions in the sections "PROBES AS A QUANTUM WAVE WITH MASS 1 AMU" and "NEUTRONS AS A PROBE TO SEE ATOMIC MOTIONS" on the neutrons as a structural and dynamical probe can be applied to the magnetic

structure, that is, the three-dimensional alignment of microscopic magnetic moments, and the spin dynamics.

The neutron scattering method has been instrumental and indispensable in the development of magnetism in the latter half of 20th century. The recent advance in this field will be reviewed by Endoh in this symposium.

One of the especially useful way of using the neutron-magnets as a probe is to align the direction of their magnets. The neutron beam with aligned neutron-magnets is called the polarized neutron beam and very useful not only for the magnetic studies by making it possible to separate the magnetic scattering from the nuclear scattering but also for more general neutron scattering research by separating various components of scattering by analyzing the directions of neutron-magnets after scattering.

An innovative method of utilizing the polarized neutron beam to measure the energy change upon scattering very accurately was invented by Mezei who is one of the invited speakers of this symposium.

A neutron spin under magnetic field makes a precessional motion. The Mezei's method is to measure the number of precession during the time of flight for a certain distance instead of measuring neutron's energy itself. By inverting the direction of neutron-magnets just after the scattering he can ingeniously introduce the echo effect in which the broadening of the precession angle due to the energy broadening of the incident neutrons can be canceled out by traveling the same distance after the inversion of the direction of neutron-magnets. By this method one is able to get rid of the energy broadening entirely and to measure a very fine energy change as a change of the precession angle. Mezei will tell us directly recent progresses of the method and applications.

CONCLUDING REMARKS

We have seen how the basic physical properties of neutrons are used as the features of neutrons as a probe. I tried to emphasize the uniqueness and diversity of the utilization of neutron probe. The details of the various application of neutron probe will be discussed in this symposium by the leading experts of the respect field.

The application of neutrons as a probe is still expanding very rapidly. The future trends of the neutron research will be mentioned in the special invited talk by Lander.

Some of the problems I could not cover are measurement techniques and the source problems. As for the former point Haytor will mention some recent progress and for the latter Taylor is going to discuss advantage of the pulsed source and Lander will tell us prospect towards the 21st century. A panel discussion is going to be dedicated to the future of neutron research including the source problem.

I hope that this symposium is successful to reconfirm the importance of the neutrons as a probe and to exchange opinions on what should be done to develop further the neutron research towards the coming 21st century.