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EXPECTATIONS FOR NEUTRONS AS MICROSCOPIC PROBES

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ABSTRACT

Neutrons have been used as microscopic probes to study structural and dynamical properties of various materials. In this paper I shall give a comparative study of the neutron research in the condensed matter physics with other typical microscopic methods such as X-rays, laser optics, magnetic resonances, Mössbauer effect and μSR. It is emphasized that the neutron study will extensively be important in future beyond the condensed matter physics. Chemistry, biology, earth sciences, material engineerings and medical sciences will become new frontiers for neutron study.

INTRODUCTION

There is an increasing interest in applying neutron diffraction to various materials beyond the condensed matter problems such as chemistry and biology. Historically speaking, the main users for the neutron diffraction were condensed matter physicists who were willing to have structural informations of various crystals or spin configurations of magnetic materials. Soon after the first stage, it was found that the inelastic scattering phenomena provide fruitful information about the elementary excitations in solid, for example, phonons and magnons. The success in the inelastic scattering means that neutron is effective not only in determining the structures but also the microscopic properties of materials and many large facilities of the neutron diffraction study have been constructed. BNL in United States and ILL in France have been ranked as the central laboratories with high neutron flux machines providing various important and influential discoveries. The high flux is necessary because the inelastic scattering corresponds to the Raman scattering in optics and the scattering intensity is weaker than the Bragg scattering.

Japanese researchers have been suffering from lack of the high flux neutron source and they have been forced to visit foreign laboratories to extend their work for many years. Recently, however, the new facilities associated with JRR-3M in JAERI, Tokai have been constructed with nearly equivalent effectiveness with those in BNL and ILL. They consist of an epoch-making machines in Japan and large contribution is expected to all of the applicable branches of basic sciences for both the domestic and international users.

In this occasion, it seems to me most important to note that the neutron diffraction is extremely effective not only for the condensed matter physics but also for other basic sciences, chemistry, biology, earth and space material sciences and even for some industrial technologies. The present paper gives a perspective view of the role of the neutron diffraction technology with special concern to the comparative study with other microscopic tools in basic sciences. The comparison may clarify the objective status of the neutron diffraction and will lead the most efficient use of the new facility in JAERI in coming glorious days.

COMPARATIVE STUDY OF MICROSCOPIC PROBES

There are may ways to have informations in material science and they are classified into two groups. The traditional methods are macroscopic and the typical ways are mechanical, thermal and electro-magnetic studies. The key words through these methods are classical and synthetic. On the other hand, however, several microscopic methods are found in the 20th Century with the key words of modern and analytic. These methods directly present various informations on the atomic, molecular and electronic states in materials and they are listed in Table-1.

Table 1 Comparison of Microscopic Probes

Method	Characteristics	Note
X-rays	Mainly Structure-Analysis	Application of SR
Neutron	Structure-Analysis and Excitation-Anaylsis	Steady and Pulse Sources
NMR	Nuclear Spin Probe	High Resolution and MRI
Mössbauer effect μSR	Supplement of NMR h.f.s. Monitor	RI Science
ESR	Electron Spin Probe	High Resolution and Spin Wave
Resonant optics	Laser-Raman Hole Burnning	Laser and SR Science

The X-ray diffraction was the first microscopic and powerful way for determining atomic arrangement established in the beginning of this century. The key words are Bragg scattering and reciprocal lattice. The related theory strongly promoted the periodicity-physics and the concept is extensively developed to the electronic band theory of solid because the scattering of de Broglie wave of electron is similarly applied in solid.

A weak point of the X-ray diffraction is in the scattering intensity decrease in light atoms, especially hydrogen atom because the intensity is nearly proportional to the number of electrons. In other words, the intensity is too heavy for heavy atoms so that flat scattering intensity is not obtained. In the neutron diffraction, the scattering is not electromagnetic but nuclear scattering and the cross section does not depend on the electron number. We have enough scattering intensity from hydrogen atoms. Moreover, the magnetic scattering due to neutron spin moment enables us to see the magnetic moment distribution in materials. Considering these properties, complementary use of neutron diffraction with that of X-ray is quite desirable for the atomic structure analysis.

A new trend in the X-ray analysis is use of synchrotron radiation (SR) beams. It supplies well controlled high intensity X-rays and clear diffraction pattern is expected by instantaneous irradiation of the beams. Construction of big SR machines is now proceeding in the world.

A characteristic importance of the neutron diffraction is the inelastic scattering as is described in the introduction and the reason is schematically shown in Fig.1, where the dispersion relations of photon, neutron and electron are illustrated by the logarithmic scale.

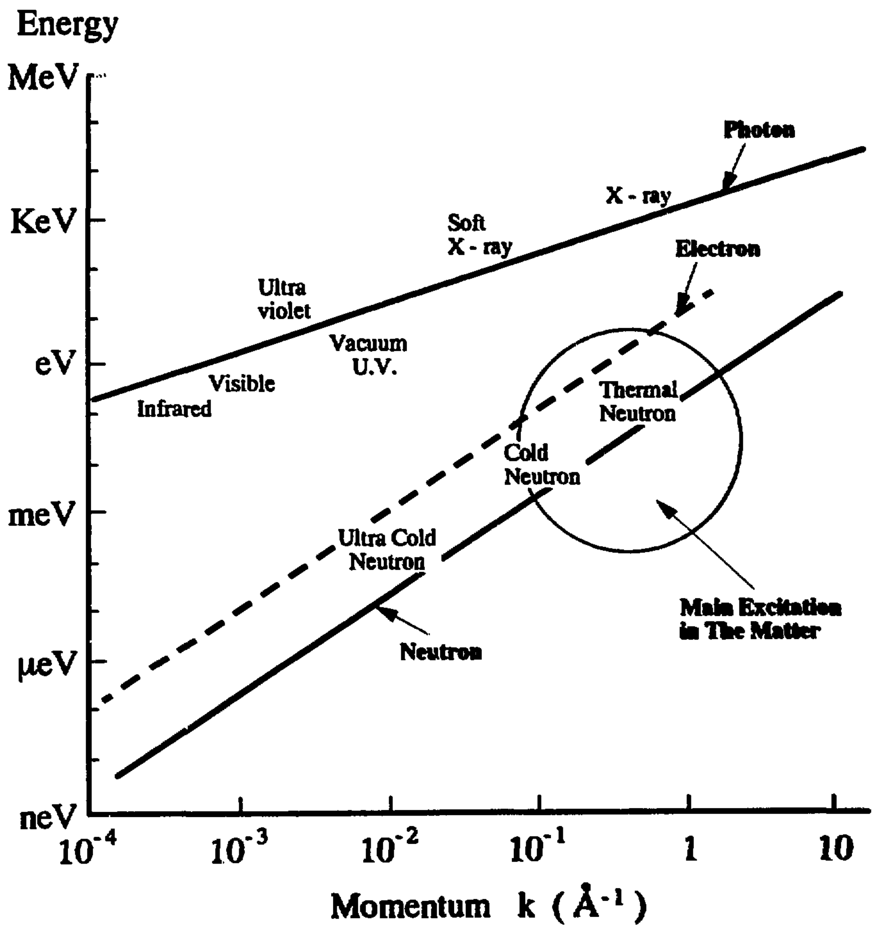

Fig. 1 Dispersion relations of neutron, electron and photon and main excitation in the matter.

A circle in Fig.1 represents the area where phonons, magnons and various excitations in materials are expected. Fortunately, the neutron dispersion line crosses the circle. This means that the neutron is the best particle to see these excitations because the cross section to see the Raman effect i. e. the inelastic effect is large when the excitations are close to the dispersion curve. The dispersion curve of electron is also not so far from the circle but electron is a charged particle and the interaction with matter is too strong so that it is not an adequate test probe. The test probe should be cool from various interactions in matter. X-rays, a kind of photons, are also cool for material interactions but the dispersion curve is rather far from the circle. This is one of the reasons why neutron is indispensable tool for a microscopic probe.

Two important neutron sources are developed. One of them is the steady neutron source obtained from the nuclear reactor and another is the pulsed neutron source generated by high energy proton beam collision to a target. The steady source is effective for various precise diffractometry while the pulse source is easy to cover wide momentum and energy regions and both sources have been considered to be complementary. A new pulsed source complementary to that of JRR-3M is highly needed now in Japan.

NMR, ESR and Mössbauer effect belong to another categories of the microscopic test probes. The common key word is spin and these technologies have been developed after the Second World War. It is noticed that the spin angular momentum can be regarded to be an additional dimension of particles. For example, electron in solid may be described by three-dimensional Schrödinger equation and another freedom of the spin dimension. The nuclear spin is described with similar angular momentum operator but the interaction with matter is very small compared to that of electron spin. The nuclear spin couples with matter through the hyperfine interaction, quadrupole interaction and magnetic dipole interactions and NMR or Mössbauer effect provides electronic information through these couplings. This is the reason why NMR and Mössbauer effect have been widely used not only in physics but also in chemistry and biology. The key words in NMR are spin-echo in physics and high resolution for chemistry while MRI, magnetic resonance imaging or NMR-CT, has become a major CT-scanner for medical use. Electron spin has an intermediate character as a test probe in materials because various interaction with matter is not so weak as in nuclei. Isolated unpaired electron spin in solid offers rich information in materials and has been regarded as a good test probe. In ferro - or antiferromagnetic materials, on the other hand, the spins play an important role on the properties of materials themselves. ESR is thus regarded as a unique microscopic method to have material informations.

Resonant optics in Table-1 is becoming important by rapid progress in laser techniques and SR machines. The resonant optics originally means the atomic and molecular spectra analysis in the beginning of this century. After the discovery of laser oscillation phenomena, however, the light source is highly improved and laser-Raman techniques have been developed widely. It is noted that the hole burning technology, which has been used in the NMR study, is now effective to identify the microscopic analysis of electronic process. Laser is also very effective to follow very fast observation of chemical reactions in time of $10^{-12} \sim 10^{-15}$ sec.

Use of the SR machine to optical spectroscopy is recently developing because VUV and soft X-ray can excite inner shell electrons. Deep electron excitation produces rich variety in the electronic process so that it is effective to determine the band structure of materials.

It should be added finally that there are many other ways of the microscopic analysis out of Table-1. In the surface science, for example, electron microscope, electron diffraction and STM, scanning tunneling electron microscopy, are important method in this field. The details are not given in this paper.

EXPECTED FRONTIERS FOR NEUTRONS

Methodological importance of the neutron diffraction is given in the previous section. The main aim of this section is what is the frontiers of the future neutron diffraction research. The use in the condensed matter physics will extend with much variety but the present paper wishes to give new possibility in chemistry and biology sciences. Application of X-rays in these field gives many epoch-making success for determining the structures of many key-materials such as DNA. The next step is to see the dynamical information of these materials. For example, it is still not clear that how DNA moves to reproduce genetic materials in cells. Proton motion and displacement may be decisive for the action so that neutron diffraction may give important information in future. Moreover, the neutron diffraction is very effective to see the energy transfer mechanism because the inelastic scattering related to the energy transfer in the chemical and biological reaction will be investigated by applying the neutron diffraction. In the field of NMR, the wide application to the biological systems is now discussed in U.S.A. When high magnetic field up to 80 Tesla is achieved, the macromolecular interactions such as the antigen-antibody interaction will be analyzed using high resolution NMR spectroscopy. Neutron diffraction in such a system will be fruitful in future because the expected informations in NMR and neutron diffraction are complementary.

Technical support to realize advanced research in the neutron diffraction study is also important. The central idea is the armament with extreme physical conditions, temperature, pressure and high magnetic field. Millikelvin cryostat with high pressure, high magnetic field is now necessary for standard neutron diffraction work. Recently high pulsed magnetic field above 50 Tesla is becoming available and these facilities will be very effective for future neutron diffractions.

Finally, it is emphasized that the international and interdisciplinary cooperation should be a key to success above new frontiers. Neutron diffraction physicist should be professional but should have wide mind to all of highly qualified physicist, chemist and biologist. The present symposium will offer a good chance to have the cooperation.