MSE 205 Lecture 27

INTRODUCTION TO NEUTRON DIFFRACTION

Recap

- The electron probe micro-analyzer (EPMA), uses X-ray spectrometry to identify and measure concentration of elements in microscopic volumes of the specimen.

- Scanning Electron Microscopy (SEM) with Energy Dispersive X-Ray Analysis (EDX) provides detailed high resolution images of the sample by rastering a focussed electron beam across the surface and detecting secondary or backscattered electron signal.

- When electrons are accelerated up to high energy levels (few hundreds keV) and focused on a material, they can scatter or backscatter elastically or inelastically, or produce many interactions, source of different signals such as X-rays, Auger electrons or light. Some of them are used in transmission electron microscopy (TEM).

Diffraction

Diffraction, the spreading of waves around obstacles. Diffraction takes place with sound; with electromagnetic radiation, such as light, X-rays, and gamma rays; and with very small moving particles such as atoms, neutrons, and electrons, which show wavelike properties.

Diffraction

X-Ray Diffraction

Electron Diffraction (SEM, TEM)

Neutron Diffraction

X-ray diffraction : The atomic planes of a crystal cause an incident beam of X-rays to interfere with one another as they leave the crystal. The phenomenon is called X-ray diffraction.

Electron diffraction: the diffraction of a beam of electrons by atoms or molecules, used especially for determining crystal structures.

Neutron diffraction : **Neutron diffraction** or elastic **neutron scattering** is the application of **neutron scattering** to the determination of the atomic and/or magnetic structure of a material

Neutron Diffraction

- Neutron diffraction or elastic neutron scattering is the application of neutron scattering to the determination of the atomic and/or magnetic structure of a material: A sample to be examined is placed in a beam of thermal, hot or cold neutrons to obtain a diffraction pattern that provides information of the structure

- Or Neutron diffraction is a form of elastic scattering where the neutrons exiting the experiment have more or less the same energy as the incident neutrons. The technique is similar to X-ray diffraction but the different type of radiation gives complementary information.

Neutron Diffraction

- Neutron scattering is the technique of choice for condensed matter investigations in general because thermal/cold neutrons are a non-invasive probe; they do not change the investigated Sample since they do not deposit energy into it.

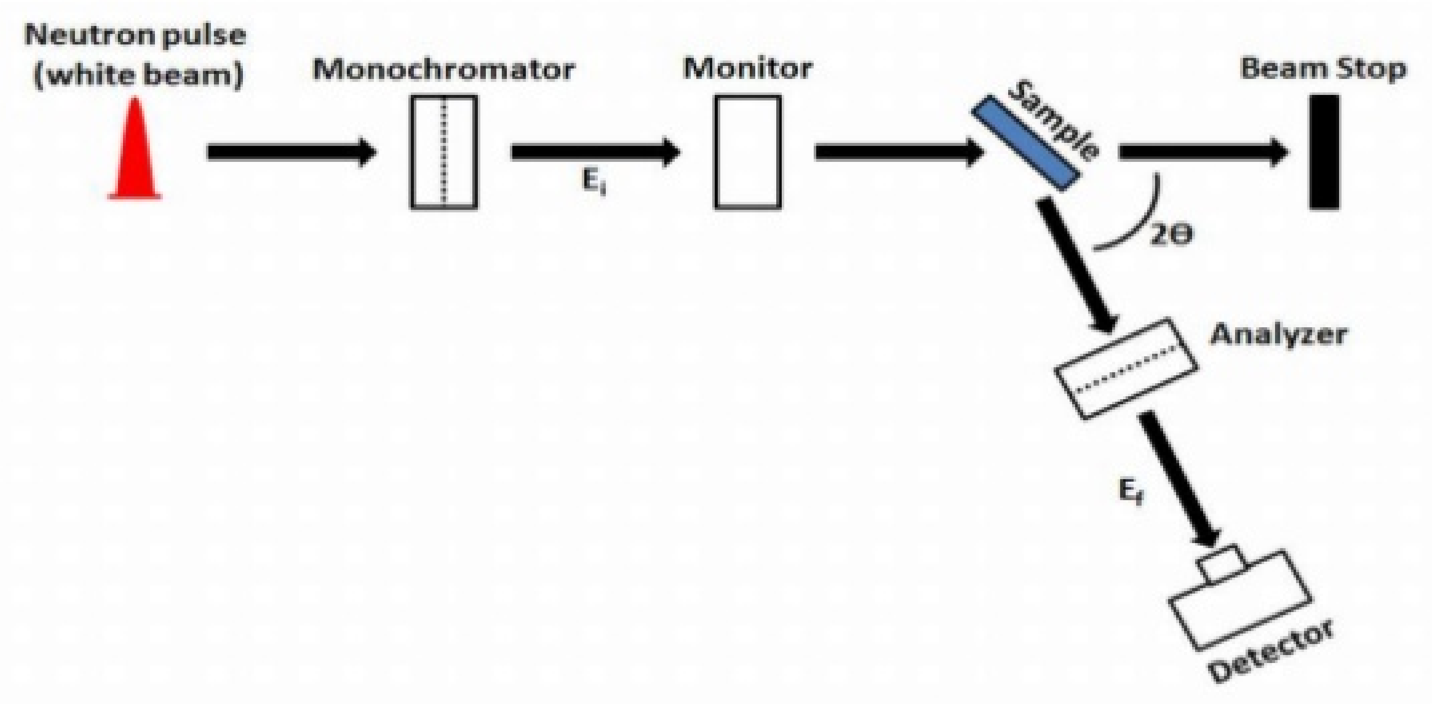
- Neutron does not interact with the elctron of the crystal. Thus unlike the X-ray, which is entirely diffracted by electron, the neutrons is entirely scatterd by the nuclei.

- Although uncharged, neutrons has an intrinsic magnetic moment, so it will interact strongly with atoms and ions in the crystal which also has magnetic moments.

- Neutron sources in the world are limited , so it is a very special tool.

INSTRUMENTATION

It consists mainly of neutron source, monochromator and detector.



16

Instrumentation and working

- The technique requires a source of neutrons. Neutrons are usually produced in a nuclear reactor or spallation source.

- At a research reactor, other components are needed, including a crystal monochromator, as well as filters to select the desired neutron wavelength. Some parts of the setup may also be movable.

- The technique is most commonly performed as powder diffraction, which only requires a polycrystalline powder. Single crystal work is also possible, but the crystals must be much larger than those that are used in single-crystal X-ray crystallography. It is common to use crystals that are about 1 mm^3.

- The technique also requires a device that can detect the neutrons after they have been scattered.

Instrumentation and working

Like all quantum particles, neutrons can exhibit wave phenomena typically associated with light or sound.

Diffraction is one of these phenomena; it occurs when waves encounter obstacles whose size is comparable with the wavelength. If the wavelength of a quantum particle is short enough, atoms or their nuclei can serve as diffraction obstacles.

When a beam of neutrons emanating from a reactor is slowed and selected properly by their speed, their wavelength lies near one angstrom (0.1 nanometer), the typical separation between atoms in a solid material.

Such a beam can then be used to perform a diffraction experiment. Impinging on a crystalline sample, it will scatter under a limited number of well-defined angles, according to the same Bragg's law that describes X-ray diffraction.

Neutrons and X-rays interact with matter differently. X-rays interact primarily with the electron cloud surrounding each atom. The contribution to the diffracted x-ray intensity is therefore larger for atoms with larger atomic number (Z).

On the other hand, neutrons interact directly with the *nucleus* of the atom, and the contribution to the diffracted intensity depends on each isotope; for example, regular hydrogen and deuterium contribute differently.

It is also often the case that light (low Z) atoms contribute strongly to the diffracted intensity, even in the presence of large Z atoms. The scattering length varies from isotope to isotope rather than linearly with the atomic number.

An element like vanadium strongly scatters X-rays, but its nuclei hardly scatters neutrons, which is why it is often used as a container material.

Instrumentation and working

- The nuclei of atoms, from which neutrons scatter, are tiny. Furthermore, there is no need to describe the shape of the electron cloud of the atom and the scattering power of an atom does not fall off with the scattering angle as it does for X-rays.

- Diffractograms therefore can show strong, well-defined diffraction peaks even at high angles, particularly if the experiment is done at low temperatures. Many neutron sources are equipped with liquid helium cooling systems that allow data collection at temperatures down to 4.2 K.

How does neutron scattering work?

With each collision, the fast **neutron** transfers a significant part of its kinetic energy to the **scattering** nucleus.

And with each collision, the "fast" **neutron** is slowed until it reaches thermal equilibrium with the material in which it is scattered.

Advantages

- One of the key advantages of neutron crystallography is the ability to visualize hydrogen and deuterium atoms.

- Neutrons are more useful than X-ray for determining the crystal structures of solids containing light elements.

- Neutrons have high penetration (low absorption) for most elements making neutron scattering a bulk probe.

- Neutron diffraction is also a very important tool for the study of the structure of non-crystalline forms of matter, such as liquids and glasses.

- Neutrons are very penetrating, they do not heat up or destroy the sample, .

Disadvantages

- Usually in order to prepare the samples that are being examined in **neutron diffraction** it is needed large crystals rather small ones as the one needed for X-ray studies. This is one of the main **disadvantages** of this instrument.

- The main disadvantage to neutron diffraction is the requirement for a nuclear reactor. Neutron sources are very expensive to build and to maintain.

- Neutron sources are characterized by low flux compared to x-ray sources. Relatively large amounts of sample (gram amounts) are required for neutron scattering measurements

Difference between X-Ray, Electron and Neutron Diffraction

X-Ray	Electron	Neutron
Wavelenght needed for diffraction of the crystal order of 1 Å which is same as size of an atom	Wavelenght needed for diffraction of the crystal order of 1 Å which is same as size of an atom	Wavelenght needed for diffraction of the crystal order of 2Å
X Ray have energy E= 10^4 eV	Electron have energy E = 40 eV	Neutron have enrgy E = 0.08 eV
X-ray is the cheapest widely used method	Electron beam can easily obtained by cathode tube, easily available	Neutrn source in the world are limited so it is en expensive and very special tool

X-Ray	Electron	Neutron
X-ray interacts with the spatial distribution of the valence electrons	Electrons are charged particles and interact with matter through Coloumbic forces	Neutrons are scatterd by the atomic nuclei through strong nuclear forces
Normal Penetration	Less penetration	High Penetration
Uncharged	Charged	Uncharged
Scatterd by atomic charge densities	Scattered by electronic and nuclear charge densities	Scattered by atomic nucleus
X-rays interact with matter through electromagnetic interactions with the electron cloud of atoms.	Electron beams interact through electrostatic interactions	Neutrons interact through nuclear interactions

Summary

- The main disadvantage to neutron diffraction is the requirement for a nuclear reactor.

- For single crystal work, the technique requires relatively large crystals, which are usually challenging to grow.

- The advantages to the technique are many - sensitivity to light atoms, ability to distinguish isotopes, absence of radiation damage, as well as a penetration depth of several cm

Summary

- X-ray and electrons are scattered by atomic electron whereas neutrons are scattered by atomic nulei. This results in number of differences, perhaps the most important being in the scattering of light elements..Whereas one electron on a hydrogen atom can be hard to find by x-ray or electron diffraction, the hydrogen nucleaus scatters neutrons strongly and is easily found in neutron diffraction method.

- The magnetic structure of the material can be determined by neutron diffraction method , electron and x-ray diffraction method does not give any information about any magnetic property.