RESEARCH PAPER | Science | Volume : 4 | Issue : 8 | August 2014 | ISSN - 2249-555X

Analysis of Small Angle Scattering Method

KEYWORDS: photon flux, coherence volume, scattering cross section, modular tool box, position sensitive detectors (PSD), electron density, dead time corrected counts 2D and 3D phase, gamma correction.

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ABSTRACT *In this work, we present on some extent to experimental and theoretical study on the small angle scattering. Theoretical study of small angle scattering is explained more effectively. When the radiation is incident on the specimen, it deviates from its path is known as small angle scattering (SAS). SAS is very important technique to obtain detail information of bulk sample. In the SAS, partially crystalline or amorphous solids, liquids or gases are used as target. Moreover electrons, gamma rays, X-rays, are incident and target should be point object. But I consider only X-ray, so it is known as small angle scattering (SAXS). The improvement in the SAS instrumentation has recently enabled to get easy collection of datas. Distortion due to the X- ray detection system can be removed. The transverse dimension t of the coherence volume is also defined and discussed, as coherence volume is important to analyze datas. Out of three aspects like shape, polydispersity and packing, two properties must be known in order to explain rest of above properties.Characteristics of nanoparticles like gold can be known, if TEM method is included with the SAXS method, we will get best performance like information on morphological features ranging from micro structure to macro structure. Explanation of pin-hole collimated instruments, Bose- Hart instruments, slit collimated instruments are very popular due to their flexibility in terms of samples and easy availability suddenly increases. SAXS is used in multi phase system to explain scattering. There is also drawback of SAXS related to scattering intensity will be explained in paper.*

Introduction:

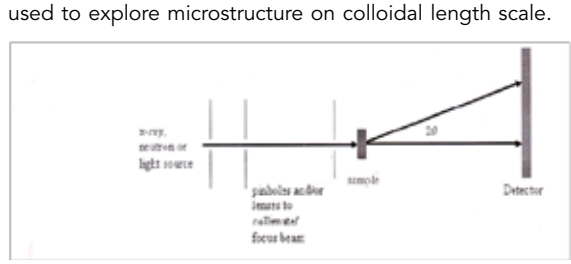
Condensed matter approaches to quantum gravity that space time emerges in the low energy sector of a fundamental condensate.Small angle scattering (SAS) is very important method for the nano structural particles. SAS is developing at a high step over the past two decades. All the theoretical datas pass under this method so that improvements in data correction steps are corrected. Mathematical descriptions are also given where it is necessary. An introduction is also explained here for a SAS.

Irradiate a sample with a well collimated beam of some type of radiation (X-Ray, neutrons or light), measure the resulting intensity as a function of angle between the incoming beam and scattered beam, then determine the structure that caused the observed pattern. Scattering patterns are caused by the interference of the secondary waves that are emitted from various structures when irradiated. Scattering of X-Ray is caused by difference in electron density, scattering of neutrons is caused by difference in scattering power of different nuclei and scattering of light is caused by difference in refractive index.

If at any instant there are n particles in a beam with a velocity v, the flux of the beam is nv and if N be the number of nuclei exposed to the beam at any instant of time, then the rate of react or scattering is expressed as…….proportional to nv and N.

In 20 thcenturies, Rontgen discovered radiation with wavelength much smaller than that of visible light. Rontgen named this high energy radiation X-ray because of their unknown nature. Soon after this discovery, Von Laue and his associate discovered that scatter X-ray in distinct pattern. It was quickly recognized that these patterns give direct insight into the structure of the materials that caused the scattering. Since these early discoveries, many technical advances made X-ray scattering one of the most powerful characterization tools available for both homogeneous and heterogeneous materials.

In fig (1), irradiate a sample with a well- collimated beam of some type of radiation (X-rays, neutrons or light), measure the resulting intensity as a function of angle between the incoming beam and scattered beam, then determine the structure that caused the observed pattern. Scattering patterns are caused by the interference of secondary waves that are emitted from various structures (electron for X-rays and light, nuclei for neutrons) when irradiated. Scattering of X-ray is caused by differences in electron density, scattering of neutrons is caused by differences in scattering power of different nuclei and scattering of light is caused by difference in refractive index. Since the larger the diffraction angle the smaller the length scale probed, wide angle X-ray scattering (WAXS) is used to determine crystal structure on the atomic length scale while small angle X-ray scattering (SAXS) or small angle scattering (SANX) is used to explore microstructure on colloidal length scale.



SAS has many drawback but still this method has many important information, for example, experiment of gold nanoparticles, krypton bubbles in copper, coated silica particles, zerolite precursor particles are exactly agreement

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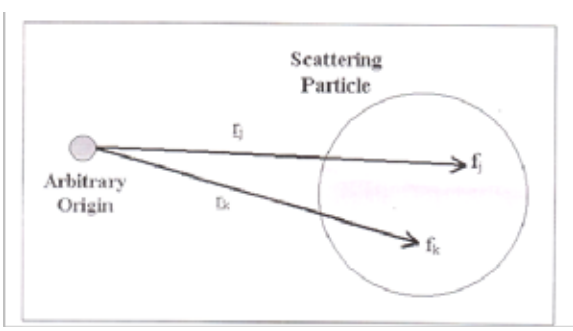
between SAXS and TEM analysis. Small angle X-Ray scattering requires combined techniques of TEM and AP. When two main contrasting phases are involved in these methods, we get best performance of the sample. When someone use these two conditions are coincide, hence we will get information on morphological features ranging from sub nanometer region to several micron. This information is valid for the entire range of radiation.

One more drawback of SAXS, even it is more used in the phase system, SAXS measures only the scattering intensity is collected. This method cannot measure phase of photons. And critical information of the originals structure is also lost. According to latest research, distribution of electron density is responsible for the scattering. This means many solutions may be equally valid for a particular set of collected intensities which may only be resolved by obtaining structural information from other technique such as transmission electron microscope (TEM). This is unexpected correction.

Compton Scattering, which is virtually nonexistence at small angles, refers to scattered waves that have changed phase and wavelength as shown below figure (2). The coherent scattering of X-rays by a single fixed particle is explained. As shown fig (2),$f_j$and f_k are the scattering powers of the j^{th} and k^{th}atoms respectively. Also in fig (2), r_j and $r_k$are vectors from some arbitrarily chosen origin to the centre of the j^{th} andk^{th} atoms respectively.



The increasing availability of intense short pulse X-ray sources allows a measurement of a type not possible before, namely angular fluctuations of intensity about mean values on rings of constant q from snapshots of a relatively small number of identical particles differing only in random positions and random orientations. In an SAXS instrument a monochromatic beam of X-rays is brought to a sample from which some of the X-rays scatter, while most simply go through the samplewithinteracting with it. The scattered X-ray from a scattering pattern which is then detected at a detector which is typically a three dimensional flat X-raydetector situated behind the sampleperpendicular to the direction of the primary beamthat initially hit the sample. The purpose here is not to familiarize the reader with all these methods but rather to describe the most commonly used approaches. An important is that Monte-Carlo methods can be used to calculate entire scattering patterns.

Consider X-ray scattering from identical molecular in solution. If the scattering is from radiation of pulse length longer than the rotational diffusion time, τ of the atoms. The signal from each molecule will be its vibrational average and signal amplification is provided by the addition of such vibrationalsaveragesfrom all illuminated atoms, as given by the SAXS.

Nowadays, there are many instruments like SAXS, and variety of flavors and colours. There are three parts (1) pin holecollimate instruments (2) slit collimated instruments (3) Boson-Hart instruments. Pinhole collimated instrument is very popular due to their flexibility in terms of samples and easy availabilityin the market. This part of instrument is very useful and also dominates the SAXS field and for neutron sources.

Slit collimated instrument is much more compact than the pin hole collimated systems. Slit collimated instrument is less expensive and illuminates a larger amount of sample to collect more scattering. SAXS is capable of delivering structural information of macro molecules between 10 to 35 nm of repeat distance in partially ordered systems of up to 160nm. USDAX (ultra small angle X-ray scattering) can resolve eve larger dimensions.

SAXS instruments can be divided into two main groups point collimation and line collimation instruments. Point – collection instruments have pin holes that shape the X-ray beam to a small circularspot that illuminates the sample. Due to the small illuminated sample volume and the waste fullness of collimation process- only those photons are allowed to pass that happens to fly in the right direction. Moreover the scattered intensity is small and therefore the measurement time is in the order of hours or days in case of very weak scatterers. And second type of instrument is much larger compared to point collimation. Line collimation is of great benefit for any isotropic nanostructured materials like proteins and particle dispersion.

Monte-Carlo method is a technique to solve a complex problem by the observation of a random process whose parameters are based on the complex problem. Consider the task of choosing points in space to simulate a sphere with a radius equal to 5 cm. The points in space, once chosen, will then be used as scattering points. However, there are problems with the shell and grid method, the problem is that the discrete shells cause artifacts in the scattering pattern. Also it is very difficult to get a constant point density with this method. So the t of choosing random points to simulate the sphere is by far the most appropriate choice.

In order to reduce scattering, more focusing and monochromatization crystals, high intensities X-ray sources and total reflective mirrors, three collimators are used. These types of inventions led to adoption of all of these elements in, subsequent instruments to improve the flux and signal to noise ratio. Due to X-ray sources we can increase brightness, increase in photon flux 10^7 photons per second, photons are generated from micro source tubes. SAXS tomology experiment, 10^{11} -10^{13} photons per second arenecessary. This is only happening when synchrotron based instruments are used.

"Bonse Hart" camera is suitable for ultra small angle scattering purposes which are used for high angular selectivity of crystalline reflections to single out a very narrow band of cattering angles for observations.

Actually, there are three important parameters to know a structure properties (1) polydisperity (2) shape (3) packing. Out of these three, two properties must be known for the structural properties. With the help of particle size distribution and shape, we know an arrangement of particles in the space. A unique particle size distribution can be obtained by making a low density packing assumption and

Volume : 4 | Issue : 8 | August 2014 | ISSN - 2249-555X

from particle shape. Particle shape is determined by TEM method. This essay investigates what could be meant by this claim.

In the case of SAXS application, the materials can be solid or liquid and they can contain solid, liquid or gaseous domains of the same or another material in any combination. Not only particles, but also the structure of ordered systems likes lamellae, and fractal- like materials can be studied. The most important outcome of this part of the research is in learning how to properly perform these simulations. The existence of analytical solutions allowed me to pinpoint error in the code, allowed for the determination of simulation times required, and also aided in the choice of a random number generator.

Conclusion:

The ultimate goal of this research to develop a SAXS method that is able to fit real experimental data. For the simplest systems, i.e. identical single particles that are infinitely symmetric or identical single particles with perfect alignment, this goal could currently be reached if a suitable least square routine aredeveloped. The former could probably be cooled and run on a fast PC, while the latter is obviously more time consuming because an entire two dimensional pattern is necessary.

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