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Applications of Compton scattering *

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Abstract: Compton scattering is used very widely. In this article, we depict an overall picture for its applications which are based on two basic theories. The first is the electron densitometry theory related to electron density. According to this theory its applications are in two fields: one is Compton scatter densitometry (CSD), the other is Compton scatter imaging (CSI). The second technique involves the electron momentum distribution and Compton profile. Applications of this technique are mainly the Compton profile analysis (CPA) and the Compton profile or the electron momentum distribution in physics and chemistry. Future research fields are suggested according to the current situation and limits of this technique and a promising prospect is unfolded.

Keywords: Compton scattering; Compton profile; electron density; electron momentum density

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1 Introduction

Compton scattering is well known, and its applications are studied by physicists, chemists and specialists in many fields. Some applications are relatively mature and relevant instruments have been developed such as ComScan; whereas the others are still in research and development stage.

Compton scattering was put forth by Compton [1] and Debye [2]. In definition, it refers to inelastic scattering of incident photons from electrons bound by atoms; it is essentially a result of interaction between photons and atom-bound electrons. In fact, interaction between photons and atom-bound electrons includes scattering, photoelectric effect, elastic scattering and electron pair production. Scattering is composed of elastic scattering (coherent scattering) and inelastic scattering (incoherent scattering or Compton scattering). In the scattering between photons and electrons, coherent scattering of photons depends strongly on the atomic number (Z) of scatterers, whereas the dependence of Compton scattering (or incoherent scattering) on Z is comparatively quite weak. Compton scattering occurs when only part of the photon energy is transferred to an effectively free atomic electron and the photon scatters with lower energy than the incident one. Practically, this means that the energy of incident photons must be larger compared to the electron binding energy. This is in contrast to the photoelectric effect, which depends very strongly on Z and becomes most probable when the energy of the incident photon is equal to or slightly greater than the binding energy of the electron. Thus, as the photon energy increases beyond the binding energy of the electron, the photoelectric effect decreases rapidly and Compton effect becomes more and more important especially in testing material of a small Z.

Compton scattering has advanced quickly since

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1920s. Cooper and Manninen made remarkable contribution to its historical development [3]. In this paper, we will give an overview on the extensive applications of Compton scattering based on electron densitometry, electron momentum distribution and Compton profile, unfold the prospect of Compton scattering applications.

2 Applications of Compton scattering

As time goes by, the applications of Compton scattering become wider and wider. Mainly two principles are involved in those applications. First, the number of scattered photons is in proportion to the number of electrons or the density of electrons, and is also related with the atomic number and the physical density. This is the mechanism to investigate electronic density distribution by measuring the energy spectrum of Compton scattering. Second, Compton's energy shift formula is derived from assuming electrons to be stationary and free; whereas electrons always belong to a certain atom, i.e. they are bound by Coulomb attraction to nucleus. So, a scattered spectrum carries abundant information of scatters, and reconstructing the information of scatters can give an image, namely, Compton profile. We can get the electron information (such as chemical bonds) and the structure of scattered matter by analyzing Compton profile.

2.1 Electron densitometry

2.1.1 Theory of electron densitometry

As we have known, the dependence of Compton scattering on the element number Z is rather weak. Compton scattering occurs when only part of the photon energy is transferred to an effectively free atomic electron and photons scatter with lower energy than the incident ones. Nevertheless, scattered photons are in proportion to the number of electrons or the density of electrons and are related to the atomic number and the physical density. The number of electrons depends on Z. Therefore, if an incident beam is mono-energetic, and it is assumed that the photons scattered through a given angle are mono-energetic [4], the scattering angle delivers information about the energy of Compton scattered photons. Compton scattered photons may exhibit an angularly dependent wavelength shift and essentially random phase change in scattering [5].

As shown in Fig. 1, with certain incident photon energy, the number of photons singly scattering into a fixed solid angle $\mathrm{d}\Omega$ subtended by the scattering volume $\mathrm{d}V$ and reaching the detector collimator is given by

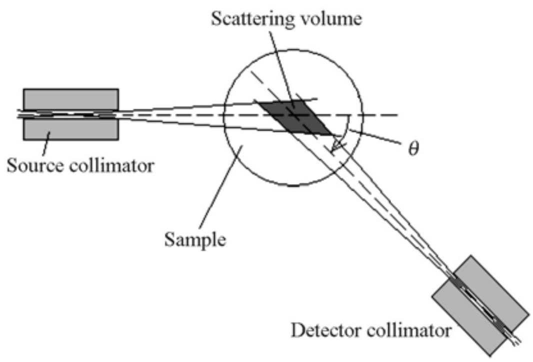

Fig. 1 Illustration of the scatter geometry of Compton scattering

$$\mathrm{d}N = \phi_0 f_1 f_2 \rho_e \mathrm{d}V \frac{\mathrm{d}\sigma_{\mathrm{KN}}(\theta)}{\mathrm{d}\Omega} S(q,Z) \tag{1}$$

where $\mathrm{d}N$ is the number of counts per second; ϕ_0 is the photon flux of the incident beam (photons $\mathrm{m}^{-2}\,\mathrm{s}^{-1}$); f_1 and f_2 are respectively the exponential attenuation factors of the primary beam and the scattered beam; ρ_e is the electron density of the tested material; $\frac{\mathrm{d}\sigma_{\mathrm{KN}}(\theta)}{\mathrm{d}\Omega}$ is the Klein-Nishina differential cross section [6] with σ_{KN} as the total cross section and θ the scattered angle; $S(q,Z)$ is the incoherent atomic scatter function that accounts for electron binding energy effects with q being the photon momentum transfer [7]. Its value is tabulated for all elements [8]. For a certain incident photon energy and flux in a fixed geometry (θ, f_1 and f_2 are fixed), the count rate $\mathrm{d}N$ depends only on the electron density of the tested material.

2.1.2 Applications of electron densitometry

One typical application of Compton scattering is the Compton scatter densitometer (CSD) [9-11], the other is Compton scatter imaging (CSI).

2.1.2.1 Compton scatter densitometer (CSD)

According to Eq. (1), the electron density in certain volume of an object can be obtained by applying Compton scattering. The Compton scatter densitometer (CSD) is a technique that a collimated detector is focused on a thin incident beam to measure the density of a small-volume element, and derive the physical density distribution, the element number or other relative information about an object. Therefore, with the CSD, the physical density of scattered objects can be measured. The objects can be also tested by CSD even if they have defects like flaws, impurity or bubbles. Practically, the technique is used very widely in industry, agriculture, and other fields.

The CSD is used so widely because of its advantages as follows. Compton scattering can give a higher yield of photon counts and can be applied to scattering at conveniently large angles; by scanning the sample it yields 3-dimessional (3D) information about the sample without computational reconstruction; the detected contrast is larger than in transmission imaging, because changes are seen against a much smaller background signal; and it can be used in some applications where geometry constraints make transmission imaging difficult [11]. It measures the electron density of the object directly, with the position of the detector adjustable on the same side as the source rather than on the opposite side as in the case of transmission measurements. This is very favorable in the cases where accesses to two opposite sides of an object are not possible [12]. In short, there has been considerable interest in the industrial use of CSD, such as in metallurgy [13] and charcoal production [14].

2.1.2.2 Compton scatter imaging (CSI)

Theoretically, Compton scattering can be used to obtain the information of a volume element by a detector at the scatter angle in the energy spectrum of a scatter. If the volume information in the detector is encoded (Monte Carlo simulation and Code), the structure of the volume can be reconstructed. By scanning the objects, complete information can be obtained. In addition, computed tomography (CT) provides a way to solve the problem of constructing the image of an object. Thus, in contrast to CT, based on manipulation of projection information, Compton scatter imaging (CSI), which records the scatter signal from a certain volume element, can be done. Scanning is critical to CSI. Lale [15] constructed the image by a point-by-point imaging scheme; Harding and his colleague [11], applied a line-by-line scheme and a plane-by-plane scheme to imaging.

In certain cases, compared with CSD, CSI is a great improvement. So based on CSI, the physical density of scattered objects can be measured.

Apparently, one of the main advantages of CSI is the ability to provide quantitative 3D images of the electron density distribution of an object, without the need for all-round access to the object and without the need of mathematical image reconstruction. Another advantage is the high resolution of CSI, especially for low atomic number material. The disadvantage of CSI is the relatively low scanning rate. Therefore, CSI offers a useful method for non-invasive examination and non-destruction testing in medicine and other industries [16-20], particularly in the food and agricultural industry [21]. In Ref. [21] photons inelastically scattering from a well-defined volume of a sample were employed to implement a non-destructive technique for measuring soil density distribution, and images of soil samples with two very close densities were obtained. In Ref. [22], based on the principle of CSI, ComScan was developed for applications to a backscatter geometry as diverse as aircraft fuselages and frescoes. The technique has been commercially applied to the Philips Industrial X-ray. However, there has yet been relatively little interest from the food industry [23]. Previous work has shown that Compton scatter can give better discrimination among a range of soft X-ray materials than transmission measurements, and suggested application of the technique to foods [24] . Fig. 2 [22] shows a sagittal section image through a Central African mummified body, with several layers of textile by the ComScan parallel to the long axis of the body.

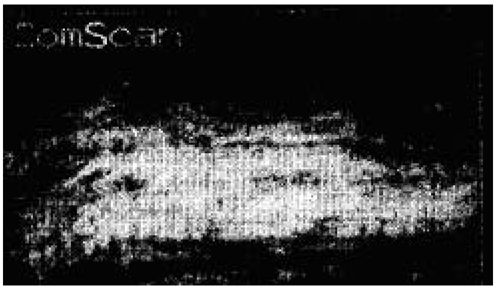

Fig. 2 Sagittal section image of a Central African mummified body obtained through ComScan, showing several layers of textile

2.2 Electron momentum distribution and Compton profile

Compton wavelength shift is derived by assuming electrons stationary and free [1]. The monochromatic characteristic of incident photons should result in a single-line spectrum, but experiments always give a different result. The reasons include: a) electrons belong to a certain atom, i.e. they are bound by Coulomb attraction to the nucleus; b) electrons may be affected by the other atoms; c) there is also interaction between electrons (through chemical bonding, etc.); d) electrons have certain momentum; and e) there exists multiple scattering. Those factors contribute to certain breadth and the shape of spectrum which is defined as Compton profile. Researchers after Compton found that the Compton scattering is related with electron momentum and Compton profile is also associated with electron momentum distribution. Therefore, Compton profile analysis can give information about electron momentum distribution, the structure of Fermi face, and even chemical bonding.

2.2.1 Theory of Compton profile

Electron motion gives rise to a second term in the Compton equation, which depends on p_z, the component of the electron momentum along direction *z* of the scattering vector. The corresponding shift $\Delta\lambda$ is given by [25]

$$\Delta\lambda = \frac{h}{mc}(1-\cos\theta) + 2(\lambda_1\lambda_2)^{1/2}(p_z/mc)\sin\frac{\theta}{2} \quad (2)$$

where the subscripts 1 and 2 refer to the incident and scattered photons, respectively; *h* is Planck's constant; *m* is the rest mass of electron; and *c* is the velocity of light in vacuum. This equation is the starting point for studying electron momentum distributions. Based on the impulse approximation (i.e. the interaction between the photon and the electron takes place impulsively in such a short time that the scattering interaction is over before the electron has a chance to move in the potential well and change its potential energy), the Compton profile $J(p_z)$ is determined by the probability that the scattering electron has a component of momentum p_z, i.e.

$$J(p_z) = \int_{p_x}\int_{p_y} \chi^*(\boldsymbol{p})\chi(\boldsymbol{p})\mathrm{d}p_x\mathrm{d}p_y \quad (3)$$

where $\boldsymbol{p}$ is the electron momentum; $\chi(\boldsymbol{p})$ is the electron wave function in the momentum representation obtained by Fourier transformation of the real space wave function $\psi(\boldsymbol{r})$ in which $\boldsymbol{r}$ is the coordinate in space, and

$$\chi^*(\boldsymbol{p})\chi(\boldsymbol{p}) = n(\boldsymbol{p}) \quad (4)$$

is the momentum density, in which χ^* is the Hermite conjugate, and *n* is the probability density in momentum representation. The Compton profile conforms to normal distribution. Of course, its expression has a different form with different approximation or model [26]. Based on certain principles, Electron momentum and its distribution can be derived from the relationships of Compton profile.

2.2.2 Applications of Compton profile

Application of Compton profile has not been well developed despite the long history of researchers' attempts to employ it as an investigative method in many fields. Anyway, trials of using Compton profile and electron momentum distribution are yet active and extensive. In the following, we describe Compton profile analysis (CPA) and some applications of Compton profile and electron momentum distribution in physics and chemistry.

2.2.2.1 Compton profile analysis (CPA)

As known to us, Compton profile directly depicts the distribution of the energy of photons scattered at a particular scattering angle. The technique of Compton profile analysis (CPA) is based directly on the dependence of the Compton scattered photon energy spectrum (Compton profile) upon the elemental composition of the scattering material. The spectrum is usually measured by using a high-resolution detector and is related directly to the composition parameters of a small *Z* element material. The Compton analyzer is one of the instruments based on the principle. The technique of Compton profile analysis (CPA) has its advantages compared with other techniques such as X-ray fluorescence (XRF). Most existing measurement techniques demonstrate good sensitivity to high *Z* elements, but are relatively insensitive to lower atomic-number components. In contrast, CPA suits well with the measurement of light elements. In particular, CPA offers good discrimination between materials such as water or organic compounds and inorganic material of low *Z* elements, while being relatively insensitive to the exact composition of higher *Z* components. CPA technique has been reported in the medical literature [27-29] and in industry [30] on its characterizing mineral density in the bone and composition in the tissue and measuring ash in coal and solid loading fraction in slurry. With CPA, the error in measuring the elemental composition of a solid fraction can be reduced, particularly in a case of inhomogeneous or poorly mixed matter.

2.2.2.2 Applications of Compton profile in physics

Applications of Compton profile in physics are also extensive. Our discussion mainly focus on two aspects. The first one is the measurement of electron distribution of the scatterer. In comparison with other technologies such as annihilation between electron and positron, diffraction of X-ray and photoelectron spectrum, Compton profile has two advantages: Compton profile is not influenced by the defeat of the scatterer; and it is sensitive to a valence electron. Compton scattering is generally used for a comparison with solid state calculations, and by its definition is sensitive to collective and delocalized features of an electronic structure. Many characteristics of matter are owing to valence electrons, so there are very broad applications in solid physics and material science. For example, Compton profile can measure the structure of Fermi face of a light metal and the high-temperature superconductivity of a material. There is a certain dependence between the structure of Fermi face and correlated electrons, which can be used to research high-temperature superconductivity by Compton profile. Directional Compton profiles can be analyzed in a quantitative way through refining a model wave function of solid [31]. Compton profile can also be applied in combination with synchrotron radiation sources to research. Compared with the other sources such as X-ray, γ-ray and so on, synchrotron radiation sources have a high energy resolution and a high count rate. These can be used to study the structure of Fermi face, strong relevance electrons, and superconductivity of material.

Additionally, Compton profile can be applied to measuring electron momentum; it has restricts compared with other method, though. Compton profile can measure solid samples, but requests a certain thickness of the samples, and the result obtained is an average [32].

2.2.2.3 Applications of Compton profile in chemistry

There are six basic principles [33]: Fourier transform (FT) principle, Virial theorem (VT) principle, bond directional (BD) principle, bond oscillation (BO) principle, hybrid orbital (HO) principle, and expectation value (EV) principle. Based on these principles, Compton scattering is involved in many fields of chemistry. For example, the type of chemical bonds between electrons can be determined by Compton profile because of its sensibility to the effects of chemical bonds. In Ref. [34], two linear twelve-electron systems respectively in beryllium oxide and boron nitride were calculated through average and directional Compton profiles. Electron correlation effects and chemical bonding were predicted with the self-consistent field theory and configuration interaction levels.

3 Summary and prospect

In this paper, we depict an overall picture of the applications of Compton scattering in many fields. Generally speaking, these applications include two aspects involving four techniques: CSD, CSI, CSA and the applications of Compton profile or electron momentum distribution in physics and chemistry.

Because the theory of Compton profile is uncompleted or unperfected and the value of theoretical calculation is not very well agreed with experiment results. The theory of Compton profile and its applications or electron momentum distribution in physics and chemistry are still in development. Anyway, the applications of Compton scattering are active and extensive. In the future, promising exploitation may be distinguishing the type of chemical bonding by analyzing and partitioning the momentum distribution. Compton profiles of mixtures and solutions should be further studied, and thorough understanding of the effects of various degrees of interaction on momentum distribution will be sought because few of such Compton experiments have been carried out.

Obviously, more efforts are needed in developing applicable techniques based on Compton scattering. The resolutions of existing techniques need improving. Profound understanding and best exploitation of Compton scattering will surely expand its usage in more fields, which will be potentially very rewarding.

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