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Effect of geometrical parameter's uncertainty of BIXS experimental setup for tritium analysis

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ABSTRACT

In this paper, the effect of geometrical parameter's uncertainty of experimental setup in β-decay induced X-ray spectroscopy (BIXS) method has been studied. By varying deliberately the distance between the X-ray detector and the sample surface, the change of the tritium content and the tritium depth distribution obtained by the BIXS method has been observed. Both Monte Carlo simulations and experimental measurements were carried out for our BIXS experimental setup. It is found that the BIXS method will not give reliable tritium content and depth distribution of the sample if the sample-detector distance of the experimental setup is not measured accurately, i.e., the deviation of 1 mm of the sample-detector distance will cause ~10% error of total tritium content besides of the distortion of the shape of tritium depth distribution. This indicates that the geometrical parameters of the experimental setup in the BIXS method must be accurately determined, especially the internal configuration of the X-ray detector used in the BIXS method. The measurement of the internal configuration of an X-ray detector used in the BIXS method by an industrial computed tomography (CT) has been shown in this paper.

1. Introduction

Measurements of tritium content and depth distribution in materials play an important role in nuclear fusion studies and in applications of nuclear technology. A number of tritium analysis methods have been developed [1], each method has its own advantages and disadvantages. In 1998, Matsuyama et al. proposed a method for tritium analysis, which is based on the tritium β-decay induced X-ray spectroscopy (BIXS) [2]. This method can distinguish the tritium retained on the surface and in the bulk quantitatively and non-destructively, and it can easily be used in *in situ* measurements. The BIXS method can also detect deeper tritium distributions (~0.1 mm and ~1 mm for high-Z and low-Z materials, respectively). The BIXS method has been used to analyze the tritium contents and depth distributions in solid and liquid materials which are relevant to nuclear fusion studies by Matsuyama et al. [3–7]. In recent years, our group has devoted to develop the BIXS method as a reliable routine examination method for T–Ti films, which are often used as the target of a neutron generator. In Refs. [8,9], An et al. improved the BIXS method by incorporating Monte Carlo simulations and Tikhonov regularization into this method. The Monte Carlo simulations could take into account more accurate physical processes in complicated practical situations. The Tikhonov regularization was employed to treat the ill-posed inverse problem in the BIXS method. Based on Monte Carlo simulations, An et al. also discussed the effects of internal bremsstrahlung of tritium β-decay, sample surface roughness and contents of tritium in the analyzed samples in the BIXS method for the first time [10]. In Ref. [11], we applied the BIXS method, which incorporated the Monte Carlo simulations and the Tikhonov regularization, to the tritium analyses of T–Ti films, the tritium contents obtained by the BIXS method were in very good agreement with the values obtained by the PVT method.

In the present BIXS method, we think that if the Monte Carlo simulations are performed correctly and with sufficient sampling particle number to obtain a reasonable statistical uncertainty, and the ill-posed inverse problem in the BIXS method is treated with an appropriate regularization method, the BIXS method could give reliable tritium content and depth distribution of the analyzed sample. Among all the factors that affect the results of the BIXS method, the accuracy of the geometrical parameters of the BIXS experimental setup, including the internal configuration of the X-ray detector used in the BIXS method, is important. If the geometrical parameters used in Monte Carlo simulations are inaccurate, the BIXS method will give unreliable results. In Ref. [12], Mesradi et al. have shown that the actual internal geometrical parameters of an X-ray detector may be very different from that

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given by the manufacturer. In the previous work of our group, the internal geometrical parameters of the X-ray detector used in Monte Carlo simulations were also obtained from the manufacturer's specifications. Up to now, the effect of geometrical parameter's uncertainty of BIXS experimental setup has not yet been discussed. In this paper, this effect will be discussed based on Monte Carlo simulations and experiments. The measurement of the internal geometrical parameters of the X-ray detector used in the BIXS method by an industrial computed tomography (CT) has also been shown in this paper.

This paper is organized as follows. Section 2 briefly introduces the basic principle of BIXS and the methods for discussing the effect of geometrical parameter's uncertainty, including Monte Carlo simulations and experimental measurements. Section 3 shows the results and discussion. The conclusions are given in Section 4.

2. Methods

The principle of BIXS method has been described in detail in Refs. [2,9,10]. That is, if the total X-ray spectrum is measured experimentally and the bremsstrahlung and characteristic X-ray spectra emitted from different depths in a sample are calculated by Monte Carlo code, the tritium contents and depth distributions of the sample can be obtained by solving the following equation,

$$S(E) = \sum_{i=1}^{n} a_i f_i(E), \tag{1}$$

where $S(E)$ represents the experimental X-ray spectra measured by an X-ray detector, $f_i(E)$ is the calculated X-ray spectrum recorded by an X-ray detector when the sample is divided into n layers and only the ith layer contains unit tritium content. The X-rays generated by tritium β-rays at the ith Ti layer are attenuated by the Ti layers before the ith Ti layer, Ar gas between the sample and the X-ray detector and the Be window of the X-ray detector when these X-rays reach the sensitive volume of X-ray detector. A layer of argon gas is usually filled between the sample and the X-ray detector in order to detect the tritium content that concentrates on the top surface of the sample. The obtained a_i values by solving Eq. (1) are exactly the tritium content and depth distribution in the sample. It is known that Eq. (1) is usually a discrete ill-posed inverse problem, it must be solved by using a so-called regularization method. In our previous papers [8,9], we made use of Monte Carlo simulations to generate experimental spectra by assuming four kinds of tritium depth distribution in samples with different statistical uncertainties, and then by using the Tikhonov regularization method [13] we satisfactorily reconstructed the assumed tritium depth distributions.

2.1. Monte Carlo simulations

In this paper, the Monte Carlo simulations are based on the PENELOPE code [14], which can perform simulations of coupled electron–photon transport in arbitrary materials for an energy range from 50 eV to 1 GeV. The detailed description for the PENELOPE code can be found in Refs. [14,15]. The PENELOPE code simulates the coupled electron–photon transport by using a combination of numerical and analytical physical models to describe the interactions of electrons and photons with matter. The electron interactions included in the PENELOPE code are elastic collision, inelastic collision and bremsstrahlung emission, and the photon interactions included are Rayleigh scattering, Compton scattering, photoelectric effect and electron–positron pair production. The PENELOPE code simulates the emission of characteristic X-rays and Auger electrons that originate from the vacancies in K, L and M shells produced by electron impact, by photoelectric absorption and by Compton scattering of photons. The relaxation of these vacancies is continued until all vacancies have transferred to N and outer shells. The PENELOPE code automatically follows the secondary particles (such as knock-on electrons, characteristic X-rays and Auger electrons) generated in the interactions of electron and photon with matter, therefore the PENELOPE code provides a detailed description for X-ray generation in targets, including self-absorption and fluorescence effects [14,15]. In the PENELOPE code, the bremsstrahlung scaled differential cross sections [16–18] and corresponding shape functions [19,20] are employed to simulate the external bremsstrahlung photons produced by incident electrons. The atomic inner-shell ionization cross sections calculated by the distorted-wave Born approximation theory [21–23] are used to simulate the characteristic X-ray photons. The internal bremsstrahlung photons emitted by the tritium β-decays are simulated by the KUB theory [24,25]. All the above inputs for our Monte Carlo simulations were experimentally verified and described in detail in Ref. [10]. For example, for the characteristic X-rays and bremsstrahlung that are the most important in the BIXS method, the comparison between experiments and PENELOPE simulations can be found in Refs. [15,26] and the agreement is very satisfactory. As described in Ref. [11], we have made use of a message passing interface to parallelize the PENELOPE code to accelerate the speeds of Monte Carlo simulations.

In this study, the geometry of BIXS experimental setup used in the PENELOPE code is the same as Fig. 1 in Ref. [11]. The distance between the sample surface and the X-ray detector was 21.5 mm. The collimator with a diameter of 1.85 mm was employed to measure the surface homogeneity of tritium contents. A layer of argon gas was filled between the sample and the X-ray detector. The sample consisted of a tritium-containing Ti film (5.63 μm) and Mo substrate (1 mm), and the diameter was 16 mm. The internal geometrical parameters of the X-ray detector were given by the manufacture, i.e., the active diameter and thickness of the Ge detector were 11.3 mm and 10 mm, respectively, and the distance between the Be window and the active Ge crystal is 5 mm, the thickness of Be window is 25 μm. For calculating the $f_i(E)$ spectra, the sample was arbitrarily assumed to be divided into 20 layers equally, and the distribution of tritium in each layer was supposed to be spatially homogeneous, and the distance between the sample surface and the X-ray detector was assumed to be 21.5 mm. Besides, the total X-ray spectra $S(E)$ with sample-detector distances of 19.5 mm, 21.5 mm, 23.5 mm were also calculated by Monte Carlo simulations and the tritium distributions were assumed to be uniform in the sample. The total X-ray spectra $S(E)$ with different sample-detector distances obtained by the Monte Carlo simulations will be used to reconstruct the assumed uniform tritium distribution in order to observe the effect of different sample-detector distances, i.e., the effect of geometrical parameter's uncertainty. In this paper, we focus our attention to the sample-detector distance because that the uncertainty of the sample-detector distance in the BIXS method will affect not only the total tritium contents but also the tritium depth distributions.

2.2. Experimental

In this paper, the $S(E)$ spectra with different sample-detector distances were also obtained experimentally and used for discussing the effect of different sample-detector distances. The experimental setup was also the same as Fig. 1 in Ref. [11], the distance between the sample surface and the X-ray detector was 21.5 mm. The FWHM of the X-ray detector used in our study for ^{55}Fe 5.9 keV X-rays is 150 eV. The internal geometrical parameters of this X-ray detector was given by the manufacturer and described in Section 2.1 of the present paper. The sample was prepared as described in Ref. [11] and its structure was also given in Section 2.1 of