Energy-dispersive X-ray diffraction system with a spiral-array structure for security inspection

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ABSTRACT
Energy-dispersive X-ray diffraction (EDXRD) is a promising technique for detecting drugs and explosives in security inspections. In this study, we proposed an EDXRD structure with a spiral-array of detectors that can be used for the detection of thick objects. The detectors are configured to share the same diffraction angle, and the detection area of the system is multiplied along the optical axis. Based on the spiral-array structure, an experimental system with 5 CdTe detectors was established. Experimental results demonstrate that the accurate data can be acquired at different positions within the 250-mm detection area, and the data measured by 5 detectors have a good consistency. This work may provide a new and commercial method for the detection of thick luggage in the field of security inspection.

I. INTRODUCTION
In recent years, the smuggling of explosives, drugs, and other contraband has become a major threat to modern social security. There is a growing need to provide rapid, nondestructive material characterization of objects hidden inside baggage and parcels. The main method of security inspection, based on X-ray transmission imaging, suffers from a relative difficulty in detecting low-Z materials, such as explosives, drugs, and commonly used organics, because of their similar densities and atomic numbers. Energy dispersive X-ray diffraction (EDXRD) is a promising technique for material characterization, as it produces a diffraction pattern that provides a unique fingerprint of the diffracting crystal. As drugs, explosives, and most contraband are crystalline, the diffraction technique is suitable for material identification in security inspections. According to Bragg’s law, the interplanar spacing $d$ of the crystal can be calculated from the wavelength $\lambda$ of the radiation and the diffraction angle $\theta$. If a sufficient subset of the spacing $d$ can be derived, then material characterization becomes possible.

EDXRD uses a polychromatic source to generate X-rays with a wide range of $\lambda$ and keeps the detector at a fixed angle to receive the photons at a specific diffraction angle. In this method, energy resolution of the diffraction spectrum (equivalent to the angular resolution of the system) is the most important feature for the identification of materials. To improve the energy resolution, the angular spread should be decreased. Thus, narrow collimators are used to provide the collimation of incident and diffracted beams. However, the collimation reduces the flux of the beam and limits the detection area of the system. To improve the efficiency of the detection, several organizations have developed diverse array-detector EDXRD systems. For the prototype DILAX system from UCL, 20 cadmium zinc telluride (CZT) crystal semiconductor detectors are organized into a sector array, with the detection areas of the individual detectors arrayed sequentially along the Y-axis (set the X-, Y-, and Z-axes to represent the length, width, and thickness of the object, respectively). This arrangement gives the DILAX system the capability to cover objects up to 200 mm wide. The diffraction image of the detected object can be obtained with a linear scan movement along the X-axis. This system can detect objects with a thickness less than 60 mm, such as laptops and handbags. For the thicker objects, such as luggage, GE Security proposed the XDI system with a 2D pixilated energy-resolving detector. The pixilated detector can analyze the voxels lying on the YZ planar of the object simultaneously. This system has high detection efficiency and can detect objects of...
large thicknesses with the object movement along the X-axis. However, the 2D pixelated detector is difficult to manufacture and very expensive. For the detection of thick objects, an economical detection method is using the transmission imaging to determine the region of interest (ROI) on the XY plane of the suspicious luggage, and then using EDXRD method to cover the detection along the Z-axis of the material in the ROI for further inspection. Therefore, it has much potential to develop the array-detector system with commercial off the shelf (COTS) and low-cost detectors that can cover a large-thickness detection area.

In this paper, we propose an EDXRD system with a spiral-array structure to solve the problem of thick object detection in the field of security inspection. Experimental results show that the effective diffraction profiles of materials can be obtained at any positions within the 250-mm detection area. The energy resolution of the detector is 1.5 keV at 122 keV. The energy resolution of the spectra measured by the spiral-array system is about 2.5 keV at 24.9 keV (equivalent to the system angular resolution of 0.5°), and the spectra measured by the 5 detectors have a good consistency.

II. THEORY OF EDXRD

When coherently scattered photons interfere within a material, X-ray diffraction occurs, and a series of peaks is produced, according to Bragg’s law,

$$n\lambda = 2d \sin \left(\frac{\theta}{2}\right),$$  

(1)

where \(\lambda\) is the X-ray wavelength, \(d\) is the interplanar spacing in the material, \(\theta\) is the diffraction angle, and \(n\) is a positive integer specifying the order of diffraction. Since \(d\) depends on the structure of the material, the diffraction profile has a characteristic pattern, and identification of the material becomes possible when a sufficient subset of interplanar spacing \(d\) can be obtained.

In the EDXRD method, a polychromatic X-ray source is used, the scattering angle is fixed by a diffraction cell, and the diffraction profile is measured using an energy-resolving detector. Thus, Bragg’s law can be converted to the following equation in terms of the X-ray energy:

$$E = \frac{nhc}{2d \sin \left(\frac{\theta}{2}\right)},$$  

(2)

where \(h\) is Planck’s constant, \(c\) is the velocity of light, and \(E\) is the energy of the incident X-rays. In an EDXRD spectrum, the combination of all the peak positions and intensities provides a unique spectroscopic “fingerprint,” from which the material can be identified.

III. DESIGN OF THE EDXRD SYSTEM

A. Single-detector system

For security applications, the single inspection of the system with a larger detection area enables inspection of more materials, which makes the system more efficient. To achieve a large detection area, the EDXRD system usually employs array detectors. The detection area of the whole system is composed of the detection area of each detector. Thus, the size of the detection area of a single detector is the major factor that affects the size of the detection area of the whole EDXRD system.

An experimental setup of a single-detector EDXRD system is shown in Fig. 1. The X-ray beam emitted from a source is incident upon the sample through the primary collimators. The scattered photons interfere within the sample, and the diffracted beams are radiated. An energy-resolving detector acquires the diffracted photons through the secondary collimators. The overlapping region between the incident beam (green area) and the accepting area of the detector (red area) is the effective detection area of the EDXRD system (yellow area). The approximate size of the detection area can be calculated using the geometrical parameters of the system,

$$L_D \approx \frac{W_{S1}}{\sin \theta} + \frac{L_{S1}}{\sin \theta} (W_{S1} + W_{S2}),$$  

(3)

$$W_D \approx W_{P2} + \frac{L_{P2}}{L_{P1}} (W_{P1} + W_{P2}),$$  

(4)

where \(L_D\) is the length of the detection area along the Z-axis and \(W_D\) is the width along the Y-axis. \(W_{P1}\) and \(W_{P2}\) are the aperture widths of the primary collimators \(P_1\) and \(P_2\); \(W_{S1}\) and \(W_{S2}\) are the aperture widths of the secondary collimators \(S_1\) and \(S_2\); \(L_{P1}\), \(L_{P2}\), \(L_{S1}\), and \(L_{S2}\) are the distances between \(P_1\) and \(P_2\), \(P_2\) and the diffraction center, the diffraction center and \(S_1\), and \(S_1\) and \(S_2\); and \(\theta\) is the nominal diffraction angle.

The width of the detector crystal \(W_{det}\) is commonly larger than the aperture widths of the secondary collimators. Thus, we used a set of Soller-slit collimators as the secondary collimators to utilize the detector fully. As shown in Fig. 2, the length of the effective detection area of the primary collimators is determined by the X-ray source and the crystal spacing of the detector.

![FIG. 1. Geometrical structure of a single-detector EDXRD system.](image-url)
area $L_{\text{det}}$ can be approximately increased to

$$L_{\text{det}} \approx \frac{W_{\text{det}}}{\sin \theta}.$$  

(5)

For a single-detector EDXRD system, the length of the detection area $L_{\text{det}}$ is generally around 60 mm (when the width of the detector crystal $W_{\text{det}}$ is 5 mm and the diffraction angle is 5°). Using this system, thin objects such as laptops and handbags can be detected easily. However, the complete examination of thicker objects (such as luggage) requires multiple scans at different thicknesses. For security applications, high throughput is a major requirement and the scanning time must be minimized. Therefore, there is a need for a system capable of detecting large-thickness objects.

B. Array-detectors system

In this paper, we describe an EDXRD system to examine large-thickness objects. This system employs a set of detectors arranged in a spiral array, each detector sharing the same diffraction angle $\theta$. As shown in Fig. 3, by placing the detectors at different distances from the optical axis, the corresponding effective detection areas are located at different positions along the optical axis. As the number of detectors is increased, the detection area of the whole system increases, enabling the array to achieve large-thickness detection.

Because the mechanical size of a conventional detector is larger than the detector areas (the size of the crystal), setting the detectors at different distances from the optical axis in a straight line would cause the gaps in the detection area. To use as many detectors as possible, the detectors are arranged in a spiral pattern around the optical axis in 3D space (i.e., around the Z-axis), while the distance between an individual detector and the optical axis is increased gradually, as shown in Fig. 4(a). If the total number of detectors is $N$, the angle between the working planes of two adjacent detectors is $\alpha = \frac{360^\circ}{N}$. Assuming that the perpendicular distance between the first detector and the optical axis is $L_1$ and that the distance along the optical axis between the centers of the detection areas of adjacent detectors is $D$ ($D$ should be slightly less than $L_{\text{det}}$, since there is hardly any signal from the material at the edge of the detection area), the perpendicular distance between the $i$-th detector and the optical axis is

$$L_i = L_1 + (i - 1) \times D \tan \theta.$$  

(6)

Let us establish a coordinate system in the plane in which the individual detectors are located and take the intersection of the optical axis and that plane as the origin of coordinates. In this system, the coordinates of the first detector’s position in the XY plane are $(L_1, 0)$ and the coordinates of the $i$-th detector are $(L_i \times \cos[(i - 1)\alpha], L_i \times \sin[(i - 1)\alpha])$. The length of the whole system’s detection area is $N^\circ D$.

Because the EDXRD system with spiral-array detectors uses multiple independent detectors to detect the diffraction spectra, the consistency of the spectra measured by these detectors is a key factor in the system. The consistency of the spectra depends on the energy resolution and collecting efficiency of each detector. Using the simulation model established in the previous study, we can calculate the energy resolution and collecting efficiency of each detector separately and obtain the simulated diffraction spectra of materials.

C. Experimental setup

We conducted our experiments using a tungsten-target X-ray tube (Varian, NDI-225-22). The diameter of the focal spot of the source was 5.5 mm, and the radiation coverage was 40°. The source was operated at a voltage of 80 kV, generating a polychromatic beam with energies in the range from 0 to 80 keV. The source current was 25 mA. As shown in Figs. 3 and 4, primary collimation of the incident beam was provided by the two collimators $P_1$ and $P_2$, with $P_1$ (having a 1-mm diameter aperture) placed next to the source collimator and $P_2$ (with a 1.3-mm diameter aperture) placed at a distance of 355 mm from $P_1$. The collimated X-ray beam was directed onto the sample, which was placed at a distance of 165 mm from $P_2$.

We employed 5 detectors to acquire the diffracted photons (Amptek, AXR/PA-230), and we arranged the detector configuration as shown in Fig. 4. Each detector consisted of a $5 \times 5 \times 1$-mm$^3$ CdTe crystal, a preamplifier, and a housing. The typical energy resolution was better than 1.5 keV full width at half maximum (FWHM).
at 122 keV ($^{57}$Co). Each detector was mounted on a two-stage thermoelectric cooler, and it can operate in a conventional environment without an external cooler. We used five sets of Soller-slit collimators to collimate the diffracted beams. The Soller-slit collimators contained 10 internal tungsten-steel plates, 100 mm long and 0.5 mm thick, with 0.5-mm spacing between them. Each set of Soller-slit collimators was closely connected to the corresponding detector, and both were mounted on a base plate. We placed each detector and its Soller-slit collimators inside a lead enclosure to reduce background noise. As shown in Fig. 5, we designed a pentagonal prism according to the distances between the detectors and the optical axis. The distance between the orthocenter and the bottom edge of the prism satisfied the functional values $L_i$ ($D = 50$ mm; $L_i = 31.70, 36.07, 40.45, 44.82,$ and $49.20$ mm, respectively). Each detector was connected to the prism by a wedge, which fixed the diffraction angle of the EDXRD system. In this setup, the diffraction angle was $5^\circ$. Thus, the length of each detector’s detection area $L_{\text{det}}$ was about 57 mm, and the length of the system’s detection area was about 250 mm. The center of the prism was placed along the optical axis. The distance between the bottom of the sample and the front of each Soller-slit collimator was 800 mm.

IV. RESULTS AND DISCUSSION

A. Performance of the EDXRD system

In order to verify the performance of the EDXRD system, we measured a drug simulant placed at different positions in the effective detection area. We chose paracetamol ($\text{C}_8\text{H}_9\text{NO}_2$) as the simulant for its complex crystalline structure, with several main peaks in the energy range from 20 to 50 keV, which is similar to many drugs. The paracetamol is in the form of pills, about 20 g in weight and packed in a plastic bag. We measured the diffraction profiles at different positions along the Z-axis (20, 70, 120, 170, and 220 mm from the front edge of the detection area). The integration time was 30 s. Figure 6 shows the spectra measured by each corresponding detector at different positions (black line), and the simulated spectra corresponding to the positions (red line). We applied an FFT smoothing filter to each measured profile and filtered out the portion with a relative intensity less than 0.1 to reduce the background noise. The intensity of each profile was normalized to the intensity of the highest peak.

As shown in Fig. 6, the spectra measured at different positions have good consistency in the positions of the diffraction peaks. The full width at half maximum (FWHM) of the two main peaks (at 24.9 keV and 37.8 keV) of each diffraction profile is shown in Table I. Assuming that the energy resolution of the diffraction profiles is $\Delta E/E$, $E$ is the energy corresponding to the position of the diffraction peak, and $\Delta E$ is the FWHM of the peak. The average
The energy resolution of the diffraction spectrum measured at 20 mm is 0.085, and the average energy resolution of the simulated spectrum is 0.070. The average energy resolution of the spectra measured at 70 mm, 120 mm, 170 mm, and 220 mm is 0.108, 0.089, 0.108, and 0.103, respectively. The average energy resolution of the corresponding simulated spectra is 0.070, 0.073, 0.075, and 0.079. The farther from the front edge of the detection area, the lower the energy resolution of the simulated profiles, but the change is small. For the measured profiles, the energy resolution is lower than the value of the simulated profiles. The average energy resolution of the 5 detectors is 0.099, and the variance is 0.93, which means that the energy resolution of the EDXRD system is relatively stable and the spectra measured by the 5 detectors have relatively good agreement. The difference in the diffraction spectrum is mainly affected by the incomplete integral, the incoherent scattering photons, and the background noise. Overall, the EDXRD system with the spiral-array detectors can effectively obtain the diffraction spectrum of the material within the 250 mm detection area.

FIG. 6. The EDXRD profiles of paracetamol measured at (a) 20, (b) 70, (c) 120, (d) 170, and (e) 220 mm from the front edge of the detection area.
### TABLE I. FWHM of the main peaks (≈24.9, 37.8 keV) in each EDXRD spectrum (unit: keV).

| Profile | Measured data | Simulated data |
|---------|---------------|----------------|
|         | Peak at 24.9 keV | Peak at 37.8 keV | Peak at 24.9 keV | Peak at 37.8 keV |
| a       | 2.28          | 1.61           | 1.61          | 2.81          |
| b       | 3.19          | 1.67           | 1.76          | 2.84          |
| c       | 2.31          | 1.67           | 1.76          | 2.92          |
| d       | 2.86          | 1.85           | 1.85          | 2.95          |
| e       | 2.12          | 1.97           | 1.97          | 3.04          |

#### B. Detection of concealed object

For security applications, the detection of concealed objects is very important for an EDXRD system. The general EDXRD equipment requires multiple scans along the thickness of the baggage to obtain the diffraction spectrum of the material hidden in the baggage. Instead, the EDXRD system with spiral-array detectors only needs a single point detection on the ROI of the baggage. A 10 cm thick suitcase with drugs and common powders inside was used to verify the ability of the EDXRD system for concealed objects’ detection. A layer of clothes was put in the suitcase to increase the background complexity. The detected samples were (a) flour, (b) methcathinone, (c) red-bean powder, and (d) milk powder. The ROI was manually set for the sample detection, and the detection time was 30 s. (In practical applications, the ROI can be determined by transmission imaging technique.)

The diffraction profiles of the samples in the suitcase are shown in Fig. 7. The diffraction spectrum of the methcathinone, which has distinct pattern of peaks, is significantly different from the others. The EDXRD system can obtain the

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**FIG. 7.** The diffraction spectra of the concealed samples in the suitcase. The samples are the following: (a) flour, (b) methcathinone, (c) red-bean powder, and (d) milk powder.
diffraction spectra effectively with the occlusion and scattering of the background. For the 10 cm thick suitcase, the EDXRD system with spiral-array detectors can cover the detection of the entire materials within the ROI, which improves the efficiency of the inspection.

V. SUMMARY

In this study, we proposed an EDXRD system with a novel spiral-array structure, which was capable of inspecting thick luggage. The CdTe semiconductor detectors were selected in this system, which were COTS and more low-cost than the pixelated detector. The detection area of the system was multiplied by arranging the detection area of each detector sequentially along the optical axis based on the spiral-array structure. The experimental system which can cover the 250-mm detection area along the Z-axis was established with 5 detectors. We performed experiments using paracetamol to simulate an illicit drug, and the results show that the system can obtain the diffraction spectra effectively and accurately anywhere within the detection area. The energy resolution of the system was about 0.099, and the spectra measured by the 5 detectors had a good consistency. Experimental results with concealed samples showed that the system can detect objects hidden inside luggage effectively. The detection method is promising and commercial in the field of security inspection.

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REFERENCES

1. B. Sun, M. Q. Li, F. Zhang, Y. Zhong, N. S. Kang, W. Lu, and J. H. Liu, "The performance of a fast testing system for illicit materials detection based on energy-dispersive X-ray diffraction technique," Microchem. J. 95(2), 293–297 (2010).
2. D. O’Flynn, H. Desai, C. B. Reid, C. Christodoulou, M. D. Wilson, M. C. Veale, P. Seller, D. Hills, B. Wong, and R. D. Speller, "Identification of simulants for explosives using pixellated X-ray diffraction," Crime Sci. 2(1), 4 (2013).
3. K. Wells and D. A. Bradley, "A review of X-ray explosives detection techniques for checked baggage," Appl. Radiat. Isot. 70(8), 1725–1746 (2012).
4. J. Srodon, "X-ray powder diffraction identification of illicit materials," Clays Clay Miner. 32(5), 337 (1984).
5. A. J. Dicken, J. P. O. Evans, K. D. Rogers, C. Greenwood, S. X. Godber, D. Prokopiou, N. Stone, J. G. Clement, I. Lyburn, R. M. Martin, and P. Zioupos, "Energy-dispersive X-ray diffraction using an annular beam," Opt. Express 23(10), 13443–13454 (2015).
6. D. O’Flynn, C. B. Reid, C. Christodoulou, M. D. Wilson, M. C. Veale, P. Seller, D. Hills, H. Desai, B. Wong, and R. Speller, "Explosive detection using pixellated X-ray diffraction (PixD)," J. Instrum. 8(03), P03007 (2013).
7. I. Drakos, P. Kenny, T. Fearn, and R. Speller, "Multivariate analysis of energy dispersive X-ray diffraction data for the detection of illicit drugs in border control," Crime Sci. 6(1), 1 (2017).
8. G. Harding, "X-ray diffraction imaging—A multi-generational perspective," Appl. Radiat. Isot. 67(2), 287–295 (2009).
9. G. Harding, H. Streeker, D. Kosciesza, and J. Gordon, "Detector considerations relevant to x-ray diffraction imaging for security screening applications," Proc. SPIE 7306, 730619 (2009).
10. E. Cook, R. Fong, J. Horrocks, D. Wilkinson, and R. Speller, "Energy dispersive X-ray diffraction as a means to identify illicit materials: A preliminary optimisation study," Appl. Radiat. Isot. 65(8), 959–967 (2007).
11. Y. F. Chen, X. Wang, Q. H. Song, J. Xu, and B. Z. Mu, "Development of a high-energy-resolution EDXRD system with a CdTe detector for security inspection," AIP Adv. 8(10), 105113 (2018).