Confirm of the optimum detection angles of several substances using energy dispersive x-ray diffraction

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Abstract

Energy dispersive X-ray diffraction (EDXRD) is proposed as a suitable non-destructive method to rapidly identify substance. In this study, 4 samples (i.e., methamphetamine, TNT, sugar and salt) have been investigated using EDXRD at different scattering angle for 300 second. The measured peak positions of EDXRD profiles can be regarded as a ‘fingerprint’ of the substance. The aim is to find out the optimum detection angle and provide a simple and practical solution to rapidly confirm substance. Furthermore, the data collected of all kinds of substances could be taken a series of process in computer to consist data base, such as Background Deduction, Feature Extraction. On that basis, the automatic, instant and accurate detection substance could be achieved in the near future.

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Key words: EDXRD; Non-destructive detection; Rapidly confirm;

1. Introduction

Energy-dispersive X-ray diffraction (EDXRD) has been used for many years as a method to measure the atomic planar spacings in a crystalline substance [1]. This method is a suitable technique as the shapes and positions of diffraction peaks in the measured spectra are characteristic of the scattering substance. The data collection time can be reduced by selecting optimum detection degrees to collect as many scattered photons as possible whilst maintaining a sufficiently high momentum transfer resolution to identify substances [2].

This paper describes the work done to characterise methamphetamine, TNT, sugar and salt using EDXRD at different angles. The aim is to find out the optimum detection angle and provide a simple and practical solution to rapidly confirm substance. Furthermore, the data collected of all kinds of substances could be taken a series of process in computer to consist data base, such as Background Deduction, Feature Extraction. On that basis, the automatic, instant and accurate detection substance could be achieved in the near future.

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2. Theory and Method

The principle of operation is to irradiate the sample using a pencil beam of polychromatic X-rays and to measure the X-ray photons scattered under a fixed angle, allowing the detection of several peaks which are differentiated by their specific energy and corresponding d-spacing within the material. In EDXRD, a polychromatic X-ray source is used, the scatter angle is fixed by a diffraction cell and the diffraction profile is measured using an energy resolving detector [2].

The corresponding diffraction features appear at discrete angular values, as defined by the Bragg relation:

\[
\frac{\Delta E}{E} = \frac{\Delta \theta}{\theta} = \frac{\lambda}{2d}.
\]

Where \(\Delta \theta\) is the angular-dispersive of the system.

When the scattering angle is low, the angular-dispersive of collimator must be reduced in order to keep the collimator angle resolution. In addition to that the increase of the angular-dispersive will cause the decrease of the energy of diffraction peak, which results in the decrease of the penetrability of the X-ray. So, the choice of scattering angle is of critical importance as it will affect the resolution, energy and intensity of the diffraction profiles [3].

3. Experimental results and discussion

The choice of scattering angle is of critical importance as it will affect the resolution, energy and intensity of the diffraction profiles. The EDXRD profiles obtained for methamphetamine at different scattering angles were shown.
in Fig. 2. It can be seen from Fig. 2 that the most distinctive patterns occur at 5°, 7° and 8° scattering angles producing a series of peaks. Compare to other scattering angles, the diffraction profile of methamphetamine at 8° scattering angle shows five well-resolved peaks between 340 and 800 channels. So, a scatter angle of 8° was chosen to identify methamphetamine as this gave the highest signal-to-noise and good energy resolution. Furthermore, it is useful to detect methamphetamine within shortly time in the future work.

The Fig. 3. shows the EDXRD diffraction peaks profiles of TNT at different scattering angles. It indicates that single diffraction peak appears at 6°, 7° and 8° scattering angles. It shifts to left with the angle increase. Furthermore, it can be seen from the Fig. 3. that the relative intensity of diffraction peak is the highest at 6°scattering angles. The 6°scattering angles is regarded the optimum detection angle of TNT. The Fig. 4. indicates that the most distinctive EDXRD diffraction peaks of sugar occur mainly at 7° and 8° scattering angles. Compare to 7°scattering angles, the diffraction profile of sugar at 8° scattering angle shows three well-resolved peaks. Below 6° the diffraction profile is degraded to such an extent to probably be unusable for identification purposes. So, a scatter angle of 8° should be chosen to identify sugar. There are two well-resolved peaks at 8° scattering angle in the Fig. 5. It can be confirmed according to No 28-1945 PDF card that it is the diffraction peaks of salt. Although there are two – three peaks of salt at other scattering angles, the relative intensity of diffraction peaks is weak. So, the optimum detection angle of salt is 8°.
4. Conclusion

Position, intensity and number of characteristic peak could be changed with the detection angle. The proper detection angle and time should be chose in practical application so that the most abundant diffraction profile information of target samples can be obtained rapidly. The EDXRD diffraction profile of five substances above show that there are several diffraction peaks of substance at suitable detection angle. It can be regarded as a ‘fingerprint’ of the substance. In this study, optimum detection angle of methamphetamine, TNT, sugar and salt are 8°, 6°, 8° and 8°, respectively. Furthermore, the data collected of all kinds of substances could be taken a series of process in computer to consist data base, such as Background Deduction, Feature Extraction. On that basis, the automatic, instant and accurate detection substance could be achieved in the near future.

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Conferences

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