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The influence of X-ray wavelength and the simulative human skin and muscle obstruction on the detection of human body-hidden drugs by non-intrusive X-ray diffraction method

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Abstract

In order to detect the body-hidden drugs non-intrusively and rapidly, the influence of the X-ray wavelength and covering of the simulative skin and muscle on the detection of methamphetamine sample by synchrotron radiation X-ray diffraction (SR-XRD) technique have been investigated. Synchrotron radiation based X-ray with three different wavelengths (1.29Å, 1.54 Å, 1.80Å) has been chosen as the X-ray source. The results indicate that the intensities as well as the number of the diffraction peaks of methamphetamine sample covered by simulative muscle decreased with the increasing of the X-ray wavelength from 1.29Å to 1.80Å. In addition, the intensities of the diffraction peaks for methamphetamine will be seriously affected by the covered simulative skin or muscle due to the X-ray absorption. Furthermore, the absorption of X-ray by the simulative muscle seems much stronger than that of the simulative skin. Moreover, the specific molecular structure of the methamphetamine sample has been obtained by X-ray diffraction method.

Keywords: drug detection; SR-XRD; methamphetamine; molecular structure.

1. Introduction

Methamphetamine, also known as the drug “ice,” is one of the most widely consumed illicit drugs in the world today. The diffusion of methamphetamine and related ‘‘de-signer drugs’’ is dramatically increasing on the European illegal market. This trend is confirmed by the European Monitoring Centre for Drugs and Drug Addiction(EMCD-DA), indicating these kinds of drugs are widely spreaded in Europe as cannabis [1]. The National Drug Intelligence Center also reports that (t)- methamphetamine (METH) is the second major drug threat to the United States, only behind cocaine[2]. Furthermore, drug abuse is always associated with crimes, trafficking and mob, which generate

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many social issues. Obviously, for security reasons, practical detection technologies are aspired for the non-destructive and fast detection for those human body-hidden drugs.

Currently, different detection techniques for illicit drugs have been developed, such as acoustic detector technology [3], neutron/gamma-ray scattering analysis[4-6], and different X-ray inspection techniques including X-ray dual-energy transmission and scatter technologies [7,8] and energy dispersive X-ray diffraction method （EDXRD）[9-12].Among them, EDXRD method has been considered to be the suitable non-destructive method to rapidly identify different illegal materials, which can satisfy the above security requests. The details of the EDXRD have been reported otherwise [13]. For the application of EDXRD to detect body-hidden drugs, the influence of X-ray wavelength, the human skin, muscle and bone structures should be considered. However in the EDXRD method, normally an X-ray source with continues wavelength X-ray is adopted, so the X-ray with definite wavelength can only be emitted or removed simultaneously, which could not be used to investigate the influence of the wavelength of the X-ray. Synchrotron radiation (SR) X-rays have the advantages of tunable wavelength combined with the related monochromic beamlines, which can be used as ideal light source to investigate the influence of the wavelength of the X-ray in the EDXRD method.

In this study, the influence of the X-ray wavelength on detection of human body-hidden drugs was investigated. Then the effects of the covering skin or muscle on the methamphetamine sample have been systematically simulated. Moreover, the molecular structure of the methamphetamine sample has been investigated based on the experiments of SR-XRD.

2. Experiment

The experiments in this paper have been carried out at the X-ray diffraction and scattering station in the National Synchrotron Radiation Lab of University of Science and Technology of China. The X-ray diffraction and scattering station has a commercial imaging plate detector system (Mar345), which contains an imaging plate of diameter 345mm and a program selectable pixel size 100 or 150 mm with a maximum readout time of 88s. This station is also equipped with a Huber Ψ diffractometer, which is useful for the general purpose of X-ray diffraction works, including high-resolution diffraction (single-crystal or powder samples), multiple beam diffraction and some surface diffraction [14]. In the current study, the Mar 345 commercial imaging plate detector was used as the detector as shown in Fig.1.

The methamphetamine sample used in the experiments is applied from the first research institute of ministry of public security of the People's Republic of China.

In the experiments, the artificial simulative skin and muscle were used to substitute the true human skin and muscle. The densities, structures and elements of the simulative skin and muscle are similar to true human skin and muscle.

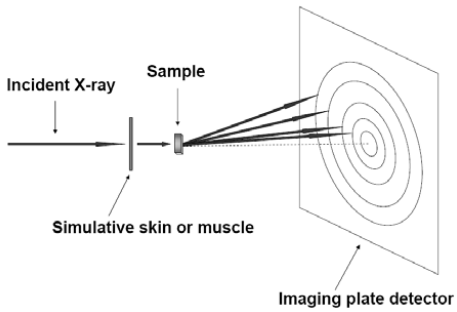

Fig.1 Schematic representation of SR-XRD

2. Results and discussion

2.1. Influence of the X-ray wavelength

In order to investigate the influence of the X-ray wavelength on the detection of human body-hidden drugs by SR-XRD, synchrotron radiation based X-ray with three different wavelengths was chosen as the emitting X-ray sources, the methamphetamine sample was chosen as the sample. The diffraction patterns of methamphetamine sample with covering simulative muscle (thickness is 10mm) emitted by the different wavelength X-ray sources are shown in Fig.2a-c with the X-ray wavelengths of 1.29 Å, 1.54 Å and 1.80Å respectively. The distance between the sample and the detector is 112 mm, and the measurement time for each pattern is 1 min. In the Fig.2a, there are more than twenty diffraction dots in the pattern, namely there are more than twenty diffraction signals, which are enough for discriminating methamphetamine sample from other materials effectively. In the Fig.2b, when the X-ray wavelength was increasing to 1.54 Å, the number of diffraction dots decreased and the pattern showed less than ten diffraction dots with weakened intensity. In the Fig.2c, only two weak diffraction dots could be observed with the X-ray wavelength of 1.80 Å. From the diffraction pattern of Fig.2a, it was clear that the diffraction signals of methamphetamine sample are sharp dots instead of diffraction rings, demonstrating the good crystallinity of the methamphetamine. Even covered by simulative muscle, the diffraction signs could still be clearly observed, thus the SR-XRD is a suitable method for detecting methamphetamine sample and the X-ray wavelength will effect the detection obviously with the simulative muscle covering. Accordingly, in the practical inspection of human body-hidden drugs, it is necessary to reduce the interfere of the muscle and the skin, which can be achieved by choosing the X-ray source with shorter wavelength.

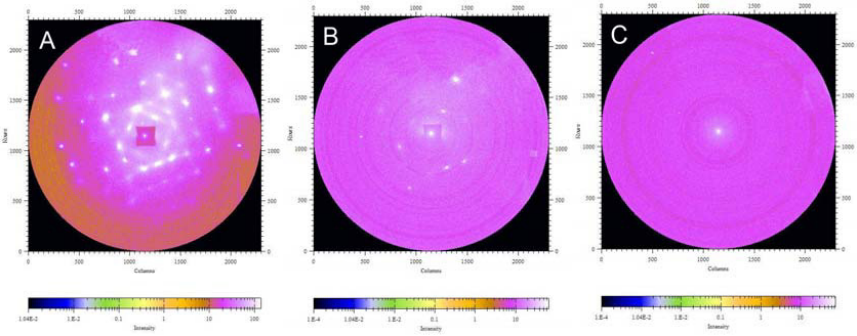

Fig.2 The diffraction patterns of methamphetamine sample with covering simulative muscle emitted by the different wavelength X-ray sources, a：1.29 Å, b：1.54 Å, c：1.80 Å.

2.2. Influence of the simulative skin and muscle

In order to investigate the influence of the simulative skin (thickness is 4mm) and muscle (thickness is 10mm) on the detection of the human body-hidden drugs by SR-XRD, the simulative muscle and skin were chosen to substitute for human skin and muscle, the X-ray wavelength of 1.54 Å was chosen as the emitted X-ray source, the methamphetamine sample was chosen as the sample. The distance between the sample and the detector is 112 mm, and the measurement time for each pattern is 1 min. The diffraction patterns of methamphetamine sample, methamphetamine sample covered with simulative skin, methamphetamine sample covered with simulative muscle and methamphetamine sample covered with simulative skin and muscle are shown in Fig.3 a~d respectively. In the Fig.3a, there are more than ten diffraction dots of methamphetamine sample. Fig.3b shows similar pattern of Fig.3a, which demonstrates that the influence of the skin on the detection of the human body-hidden drugs by SR-XRD is slightly. While in Fig.3c, less than ten weak diffraction dots could be seen distinctly, indicating that the effect of the muscle on the detection of the human body-hidden drugs by SR-XRD is distinctly. Moreover, there are only several diffraction dots in the Fig.3d with much weaker intensities, which shows that when the methamphetamine sample

was covered by simulative skin and muscle simultaneously, the number and intensities of the diffraction dots of the methamphetamine sample decrease more obviously. However, when the wavelength of X-ray source was adjusted from 1.54 Å to 1.29 Å, the diffraction pattern of methamphetamine sample covered by both simulative skin and muscle is changed greatly and shown in Fig.4. More than thirty sharp diffraction dots can be observed. The intensity of the dots is also stronger than that of the dots in Fig.3a, which is recorded with the X-ray with the wavelength of 1.54 Å. So it is found that the influence of the muscle is greater than that of skin on the detection of methamphetamine sample by SR-XRD, while choosing the more short wavelength X-ray as the emit X-ray source can reduce the interfere of the skin and muscle on the detection of the human body-hidden drugs by SR-XRD.

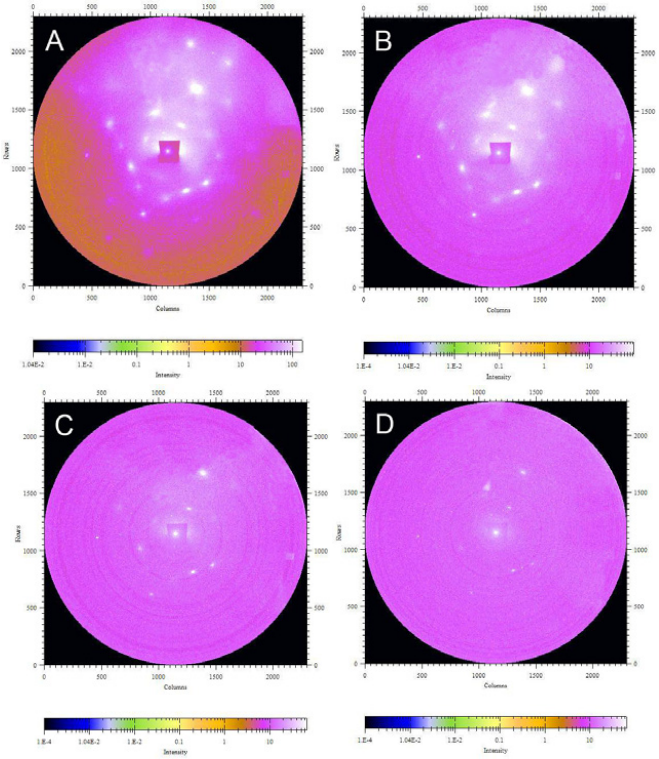

Fig.3 The diffraction patterns of methamphetamine sample, methamphetamine sample covered with simulative skin, methamphetamine sample covered with simulative muscle and methamphetamine sample covered with simulative skin and muscle, a: methamphetamine sample, b: methamphetamine sample covered with simulative skin, c: methamphetamine sample covered with simulative muscle, d: methamphetamine sample covered with simulative skin and muscle.

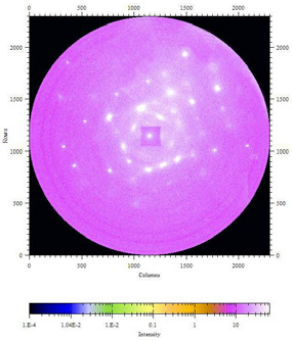

Fig.4 The diffraction pattern of methamphetamine sample covered by simulative skin and muscle at the same time with the emitted X-ray wavelength 1.29 Å

2.3. Investigation on the molecular structure of methamphetamine sample by the X-ray diffraction

The above clear and sharp diffraction patterns recorded based on synchrotron radiation supply the possibility to deeper investigate the specific molecular structures of methamphetamine sample drugs, which should be important for further optimization of the drugs detection system. For the molecular structure of methamphetamine sample investigation by X-ray diffraction method, the diffraction patterns of methamphetamine sample were collected on a MAR345 image plate system. The raw data were processed using AUTOMAR program (release version 1. 3. 0) to yield the reflection files. The structures were solved by direct method (SHELXS-97) and refined on F^2 by full-matrix least-squares using all unique data (SHELXL-97) [15, 16]. All non-hydrogen atoms were refined anisotropically and the hydrogen atoms were included in the calculated positions (riding model). The structures were finally refined to the conventional *R*-values of 0.0342. The crystal data, conditions for the intensity data collection, and important parameters of the structural refinement for methamphetamine sample is listed in Tab.1.Selected bond lengths and angles of the methamphetamine sample are presented in Tab.2.

Tab.1 The crystal data and important parameters of the structural refinement for methamphetamine sample.

formula	C10H16NCl
fw	185.6964
T/ K	290
wavelength/ Å	0.71073
crystal system	monoclinic
space group	P21
a/ Å	7.1806(4)
b/ Å	7.3390(4)
c/ Å	10.8883(10)
α/°	90.000
β/°	97.182(7)
γ/°	90.000
V / Å ^{3}	569.29(6)
density/ (g ·cm $^{-1}$)	1.083
abs. coeff . / mm $^{-1}$	0.289
Z	2
F(000)	200
limit indmethamphetamine samples	-8 =< h =< 9 -9 =< k =< 7 -14 =< l =< 13
total/ unique reflections/ R(int)	5137/2294/0.0316

data/ restraint	2294/1
parameters	111
goodness-of-fit	1.010
*R*1	0.0342
*w R*2	0.0798
highest peak	0.19
deepest hole	-0.32

The molecular structure and atom-labeling schemes of methamphetamine sample are given in Fig.5. From the Tab.1 and Fig.5, it is found that the molecular of the methamphetamine sample is the methamphetamine hydrochloride, rather than the pure methamphetamine. The molecular of methamphetamine sample is consist of two parts, one is anion(Cl^-)and other is cation ($C_{10}H_{16}N^+$) ,the cation $C_{10}H_{16}N^+$ contain a benzene ring and a chain, the benzene ring is consist of C1, C2, C3, C4, C5, C6,while the chain is consist of C7, C8, C9,N1,C10,the C9 connect to C8 by substituting one H atom, the N1 connect to C8 and C10,futher more, the N1 also connect to two H. Generally, the N atom can connect three other atoms, because there are three unpaired electrons around the N atom, however there are four atom (C8,C10 and two H atom) around the N1 in the molecular of methamphetamine sample, which can be explain like NH_4^+ in NH4Cl.In the table2,it is found that the bond length of N1-C8 is1.511(2) Å, the bond length of N1-C10 is 1.484(2) Å, and the bond length of N1-H1A,N1-H1B both 0.9000 Å. Moreover the bond angle of C10-N1-C8 is 116.23(13)°, and the bond angles of C10-N1-H1A, C8-N1-H1A, C10-N1-H1B, C8-N1-H1B are all 108.2°, the bond angle of H1A-N1-H1B is 107.4°.

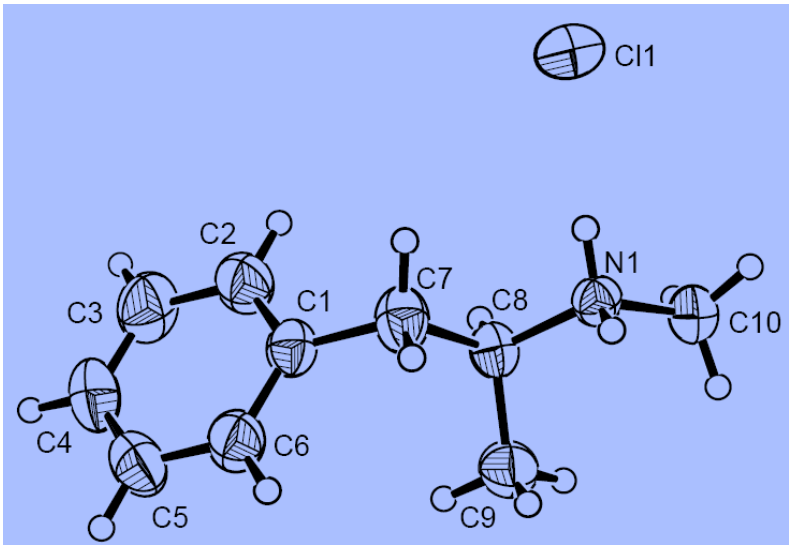

Fig.5 The molecular structures and atom-labeling schemes of methamphetamine sample.

Tab.2 Selected bond lengths and angles of the methamphetamine sample

Bond lengths/Å		Bond angles/°	
C1- C2	**1.369(3)**	**C10-N1-C8**	**116.23(13)**
C1- C6	**1.375(3)**	**C10-N1-H1A**	**108.2**
C1- C7	**1.516(3)**	**C8-N1-H1A**	**108.2**
C2- C3	**1.389(3)**	**C10-N1-H1B**	**108.2**
C2-H2	**0.9300**	**C8-N1-H1B**	**108.2**

C3- C4	1.354(3)	H1A-N1-H1B	107.4
C3-H3	0.9300	C1-C7-C8	113.64(15)
C4- C5	1.367(3)	C1-C7-H7A	108.8
C4-H4	0.9300	C8-C7-H7A	108.8
C5- C6	1.371(3)	C1-C7-H7B	108.8
C5-H5	0.9300	C8-C7-H7B	108.8
C6-H6	0.9300	H7A-C7-H7B	107.7
C7- C8	1.521(3)	N1-C8-C9	109.87(16)
C7-H7A	0.9700	N1-C8-C7	106.35(14)
C7-H7B	0.9700	C9-C8-C7	113.53(19)
C8- C9	1.512(3)	N1-C8-H8	109.0
C8-H8	0.9800	C9-C8-H8	109.0
C9-H9A	0.9600	C7-C8-H8	109.0
C9-H9B	0.9600	N1-C10-H10A	109.5
C9-H9C	0.9600	N1-C10-H10B	109.5
C10-H10A	0.9600	H10A-C10-H10B	109.5
C10-H10B	0.9600	N1-C10-H10C	109.5
C10-H10C	0.9600	H10A-C10-H10C	109.5
N1-C8	1.511(2)	H10B-C10-H10C	109.5
N1-C10	1.484(2)	C2-C1-C6	117.57(17)
N1-H1A	0.9000	C2-C1-C7	121.22(19)
N1-H1B	0.9000	C6-C1-C7	121.21(18)
		C4-C3-C2	120.3(2)
		C4-C3-H3	119.8
		C2-C3-H3	119.8
		C1-C2-C3	121.2(2)
		C1-C2-H2	119.4
		C3-C2-H2	119.4
		C5-C6-C1	121.20(19)
		C5-C6-H6	119.4
		C1-C6-H6	119.4
		C4-C5-C6	120.7(2)
		C4-C5-H5	119.7
		C6-C5-H5	119.7
		C3-C4-C5	119.0(2)
		C3-C4-H4	120.5
		C5-C4-H4	120.5
		C8-C9-H9A	109.5
		C8-C9-H9B	109.5
		H9A-C9-H9B	109.5
		C8-C9-H9C	109.5
		H9A-C9-H9C	109.5
		H9B-C9-H9C	109.5

3. Conclusion

In order to detect the body-hidden drugs non-intrusively and rapidly, the influence of the X-ray wavelength and covering of the simulative skin and muscle on the detection of methamphetamine sample by X-ray diffraction technique have been investigated. Synchrotron radiation based X-ray with three different wavelengths (1.29Å, 1.54 Å, 1.80Å) has been chosen as the X-ray source. The results indicate that the diffraction signals of methamphetamine sample are dots instead of diffraction rings, even covered by simulative skin and muscle, confirming the excellent

crystallinity of the methamphetamine. The SR-XRD is demonstrated to be a suitable method for detecting methamphetamine sample and the simulation results show that the interfere for the detection of methamphetamine sample induced by skin and muscle can be reduced by choosing shorter wavelength X-ray as the light source. Moreover, the specific molecule structure of methamphetamine sample has been also investigated and it is found that the molecular of the methamphetamine sample is the methamphetamine hydrochloride, rather than the pure methamphetamine. The molecular of methamphetamine sample is consist of two parts, one is anion(Cl^-)and other is cation ($C_{10}H_{16}N^+$) ,which like the NH_4Cl molecular.

Acknowledges:

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Reference:

[1] EMCDDA, 2000 Annual Report on the State of the Drugs Problem in the European Union, European Monitoring Centre for Drugs and Drug Addiction, 2000.

[2] NDIC (2008) National drug treatment summary. Johnstown,PA: National Drug Intelligence Center.

[3] George RD, Gauthier RD, Denslow KD, Cinson AM, Diaz AA, Griffin M. Contraband detection using acoustic technology. *Proc. SPIE* 2008;**6934**:693415

[4] Lee HS, Park SR, Lee BY, KO SK, Chung CW. Study on detection technique of illicit materials using pulsed fast white neutron analysis. *Nucl.Instrum.Meth.A* 2006;**562**:1076-1080.

[5] Buffler A, Brooks FD, Allie MS, Bharuth-Ram K, Nchodu MR, Material classification by fast neutron scattering. *Nucl.Instrum.Meth.B* 2001;**173** : 483-502.

[6] Im HJ, Song K, Applications of prompt gamma ray neutron activation analysis: detection of illicit materials.*Appl. Spectrosc. Rev.* 2009;**44(4)** : 317 -334.

[7] Lu Q, The utility of X-ray dual-energy transmission and scatter technologies for illicit material detection, Doctor's Thesis, Virginia Polytechnic Institute and State University, Blacksburg, Virginia, August, 1999.

[8] Singh S, Singh M, Explosives detection systems (EDS) for aviation security.*Signal Processing* 2003;**83**:31-55.

[9] Cook E, Fong R, Horrocks J, Wilkinson D, Speller R, Energy dispersive X-ray diffraction as a means to identify illicit materials: A preliminary optimisation study. *Appl. Radiat. Isot.* 2007;**65(8)**:959-967.

[10] Kämpfe B, Luczak F, Michel B. Energy dispersive X-ray diffraction.*Part. Part. Syst. Charact.* 2005;**22(6)**:391-396.

[11] Cook EJ, Griffiths JA, Koutalonis M, Gent C, Pani S, Horrocks JA, George L, Hardwick S, Speller R. Illicit drug detection using energy dispersive x-ray diffraction, Non-intrusive inspection technologies II. *Proceedings of the SPIE* 2009;7310 :73100I

[12] Cook EJ, Pani S, George L, Hardwick S, Horrocks JA, Speller RD. Multivariate data analysis for drug identification using energy-dispersive X-ray diffraction.*IEEE T. Nucl. Sci.* 2009;**56(3)** : 1459-1464.

[13] Sun B, Li MQ, Zhang F, Zhong Y, Kang NS, Lu W, Liu JH.The performance of a fast testing system for illicit materials detection based on energy-dispersive X-ray diffraction technique. *Microchem. J.* 2010; **95** :293- 297.

[14] Pan GQ, Xu CY, Fan R, Gao C, Lou XH, Teng MK, Huang QQ, Niu LW. Design and performance of U7B beamline and X-ray diffraction and scatteringstation at NSRL and its preliminary experiments in protein crystallography.*Nucl. Instrum. Meth. A* 2005;**540**: 480-486.

[15] Sheldrick GM.Phasing annealing in SHELXL290 :direct methods for larger structures.*Acta. Cryst . A* 1990;**46** :1102119.

[16] Sheldrick GM.SHELXL9722 ,Version 10. 31 [EB/ OL].Tech. Kep . , University of GÊttingen ,Germany ,2001.