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Identification of Liquid Materials Using Energy Dispersive X-ray Scattering

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Abstract

Energy dispersive X-ray scattering (EDXRS) has been successfully applied for the identification of liquid materials for the first time. Three liquid systems of primary alcohols, ketones compounds and acids are carefully investigation and the scattering spectra are described. Based on structural and compositional differences of compounds, the scattering profiles of all samples exhibit characteristic shapes, indicating that EDXRS profile is unique to each specific liquid material. These findings imply that EDXRS would be promisingly applied as a non-invasive inspection for liquid identification.

Keywords: liquid materials; energy dispersive; X-ray scattering; detection; identification

1. Introduction

Energy dispersive X-ray scattering (EDXRS) is the measurement of the energy-dispersive low angle scattering of photons from a polychromatic incident beam. Under low energy and low angle conditions, coherent scatter plays a dominant role among scatter models. The physics of EDXRS and its potential as a tool for material identification has been described in detail elsewhere [1-3]. Over the passed decade, EDXRS has been widely developed as a technique for structural characterization of explosive, illegal drugs, and biological systems [4-7]. It has been recognized to be a suitable tool in the investigation of liquid systems because of its high speed and good reliability compared with those of a traditional angular scanning diffractometer [1, 8, 9]. More recently, intermolecular structure of pure liquid and solution has already been investigated extensively at different conditions by means of EDXRS methods, in order to study the local structure of H-bonding, hydration and molecular aggregation [10-12].

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Liquid materials such as hazardous liquid fuel, liquid explosives and precursor chemicals are deserved special attention by security screening. Many different approaches have been proposed to address the challenge of liquid identification for security screening [13-18], Unfortunately, a part of such methods are costly and require sophisticated instrumentation; some approaches require direct contact with the liquid samples generally hidden in wine or liquor bottles that can not be opened routinely for inspection. EDXRS as a powerful tool that provides a very good structural insight of disordered systems, would be potentially used to identify and detect liquid substances [19, 20]. EDXRS is a method to noninvasively inspect unopened liquid containers, its scattering spectra can be collected much faster by using only a few reflection angles, though momentum transfer q ranges obtainable are equal to or larger than those of traditional diffraction [21]. Moreover, most of experimental equipments are cost-low, and the operating procedures of EDXRS are convenient due to its geometric properties allowing the placement of liquid samples stored in sealed cells.

It is well-known that liquids do not possess sharp Bragg peaks which are generally presented by crystalline specimen. In contrast, they show more or less amorphous XRD patterns consisting of weaker and broader features, and the strength of which depends on the degree of molecular order in the material concerned [22]. It has prompted the facetious comment that liquid XRD patterns all look alike [19]. Under the same probe conditions, each liquid exhibits a unique scattering profile, including the position, shape, width and intensity of a series of peaks which are governed by the liquid properties. To the best of our knowledge, EDXRS as a tool for liquid material identification has never been reported.

In the present work, some pure liquids were employed to investigate the X-ray scattering profiles using EDXRS. The profile features were analyzed systemically. The purpose of this article is to describe how liquid materials can be identified by EDXRS in spite of their lack of crystalline structure. A further goal of this work is to show that the experimental tool is intrinsically reliable, which enables it to be potentially developed as a feasible method to identify hazardous liquid fuel, liquid explosives and precursor chemicals.

2. Experimental Section

2.1. Liquid samples

A total of 12 liquid samples were measured for this study. The samples were as follows: methanol, ethanol, 1-propanol, 1-butanol, 1-pentanol, oil of vitriol, acetic anhydride, acetic acid, 3,4-methylenedioxyphenyl-2-propanone, acetone, 2-butanone, distilled water. Except distilled water, all reagents used in our experiments were analytically pure grade, purchased from Shanghai Chemical Reagents Company, and used without further purification.

2.2. EDXRS experiments

We performed our experiments using the non-commercial energy-scanning diffractometer built in the Institute of Intelligent Machines, Chinese Academy of Sciences. The diffractometer consisted of (1) a Seifert X-ray generator, (2) a watercooled tungsten X-ray source with 3.0 kW maximum power and a nominal focal spot of 1×10 mm, (3) a Silicon Drift Detectors (XR-100SDD), connected to a multichannel analyzer (AMPTEK PX4, 1024) channels by an electronic chain for diffraction spectra collection, has an energy detection of 0.14 keV at 5.9 keV (^{55}Fe), (4) a collimator system which focuses the X-ray beam in front of and behind the sample, (5) a step motors for moving the arms supporting the detector, whose minimum step movement leads to a minimum angle incrementum and reproduction of 0.01°, and (6) an adjustable sample holder that was positioned in the optical center of the diffractometer.

A schematic diagram of the experimental system is shown in Figure 1, the source to sample distance is 180 mm, and sample to detector distance is 120 mm. The tungsten tube works at 55 kV and 20 mA, thus producing a white spectrum in the low energy range (the bremsstrahlung component of the X-ray source was used). Two vertical slits 15 mm in height and of variable slit width collimate a parallel beam onto the sample, a horizontal soller silt and a 0.02 mm in width and 15 mm in height receiving slit, which improve the angular resolution, collimate the scattered beam. We can perform our measurements at a fixed scattering angle θ, having a white incident polychromatic beam.