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Validation study of a ray-tracing simulator for focal construct geometry

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HIGHLIGHTS

- X-ray diffraction produced by scanning a sample through an annular beam is simulated using ray-tracing.
- Simulated results are validated analytically and empirically.
- Rapid optimisation and prototyping of focal construct technology is achieved.
- Analytical imaging applications include security screening for explosives and narcotics.

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ABSTRACT

We present the results of a computer modelling package designed to simulate X-ray diffraction imaging employing focal construct geometry. The paths of coherently diffracted X-rays are modelled by ray-tracing. The results of the study show good agreement between simulated and measured data obtained in the laboratory. The validation of the modelling package permits the rapid optimisation and prototyping of focal construct technology, which has wide applicability in security X-ray imaging.

1. Introduction

Recent efforts have focused on developing a variety of material specific screening techniques that complement conventional systems already employed by the aviation industry for trace and bulk threat detection (Harding et al., 2012; Singh and Singh, 2003; Price and Forrest, 2013). These systems must adhere to the strict security requirements of high sensitivity, specificity and throughput if they are to reduce the annual false alarm cost incurred by airports (which in the USA alone is estimated to be 10^9 USD) (Harding et al., 2012; Speller, 2001; Oster and Strong, 2008). Dual-energy X-ray imaging is the mainstay screening tool for checkpoint security providing non-invasive images of sample morphology and colour-encoding based on "effective" atomic number and density. However, it lacks the ability to obtain unique 'finger print' signals that identify explosives with high specificity (Singh and Singh, 2003; Speller, 2001; Eilbert, 2009).

X-ray diffraction has been investigated as a complementary approach with various authors demonstrating its ability to identify illicit materials (Crespy et al., 2010; Sun et al., 2010), perform mineral analysis (Ruan and Ward, 2002), detect cancerous tissue (Pani et al., 2010; Chaparian et al., 2010) and measure bone mineral density to identify osteoporosis (Farquharson and Speller 1997). However, analytical diffraction techniques produce relatively low intensity signals due to the low coherent scatter cross-section. Also, traditional narrow beam topologies define relatively small gauge volumes, which limit the total number of crystals having the correct orientation to contribute to Bragg scatter (Eilbert, 2009; Evans et al., 2010). In security scanning systems this situation is exacerbated by the clutter routinely found in luggage/cargo masking threat signatures, which significantly reduces sensitivity and specificity. A conventional solution is to employ brighter X-ray sources and increase the scanning integration time. This approach inexorably leads to bulky, expensive systems with low throughput. For this reasoning X-ray diffraction has previously not been widely implemented by the security

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industry and its applications are limited to organic explosives (Wells and Bradley, 2012; Singh and Singh, 2003).

An alternate angular-dispersive configuration, namely focal construct geometry (FCG) has been previously employed by Rogers et al. (2010) and Evans et al. (2010). This configuration utilises an annular X-ray beam of monochromatic radiation incident on a polycrystalline sample that yields diffraction caustic patterns of increased intensity. The potential advantages of FCG to the security industry include: high data acquisition speed, the use of commercially available X-ray sources, reduced hardware complexity and reduced radiation shielding (Evans et al., 2010; Rogers et al., 2010; Prokopiou et al., 2013). FCG has also been successfully applied to discriminate between threat liquids and mitigates against structural complexities such as large grain size and preferred orientation (Prokopiou et al., 2013; Rogers et al., 2010).

It is beneficial to be able to rapidly optimise and prototype different system configurations based on the FCG principle. *In silico* methods are best suited for this purpose. A convolution based simulator for FCG was previously investigated by Rogers et al. (2010) to understand the role of a number of fundamental parameters. In this analysis the interrogating cone opening angle (φ) was set to 0°. Therefore, each generated Debye cone was normally incident at the detection surface and produced a circular footprint. This convolution based approach served as a good first approximation to FCT patterns as a function of the diffraction angle (i.e. half opening angle of the Debye cones (2θ)) and the separation between the source, sample and detector. However, an annular beam originating from a point source i.e. $\varphi > 0°$ will produce elliptical Debye rings when incident upon a sample, which makes this approach impractical for optimising FCG. Winslow et al. (2005) show that ray tracing (combined with Monte Carlo simulation) to be the superlative for realistic radiographical simulations. For example, Monte Carlo based ray-tracing simulation packages such as SHADOW (Liu, 2006) and McXtrace (Knudsen et al., 2013) have been developed to accurately model and optimise X-ray beam instrumentation. The flexibility offered by the latter means that McXtrace is able to model our optical arrangement precisely by employing a monochromatic lab source (distributed by 4π) and a configuration of beam stops and apertures to create a divergent hollow or annular cone. However, even when 'directional sampling' is employed (i.e. reducing the direction that X-rays are emitted to a predefined aperture at some distance) our geometry is such that ~97% of the modelled rays are terminated at the optic, amounting to significant wasted computational effort. This feature significantly increases the total simulation time. In contrast, our bespoke ray-tracing package has been produced as a tool for accurately modelling FCG and only simulates rays that pass through a specified annular aperture. This study validates the results of the simulator analytically and also against measured results obtained in the laboratory.

2. Experimental system and methods

2.1. FCG principle

FCG is a novel method of obtaining increased coherent diffraction signatures from poly or semi-crystalline materials

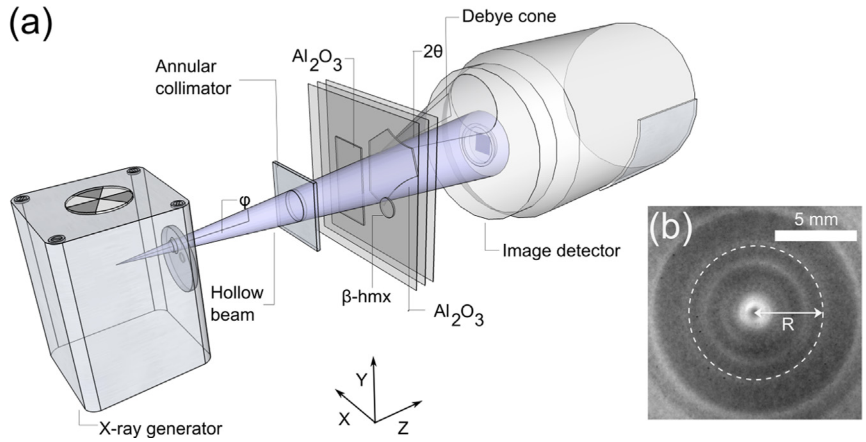

Fig. 1. Schematic diagram of FCG. An annular beam is incident on a phantom containing alumina and β-hmx components. Only one Debye cone is illustrated (a). An example image illustrating a ring of radius *R*, generated by FCG diffraction from an alumina sample.

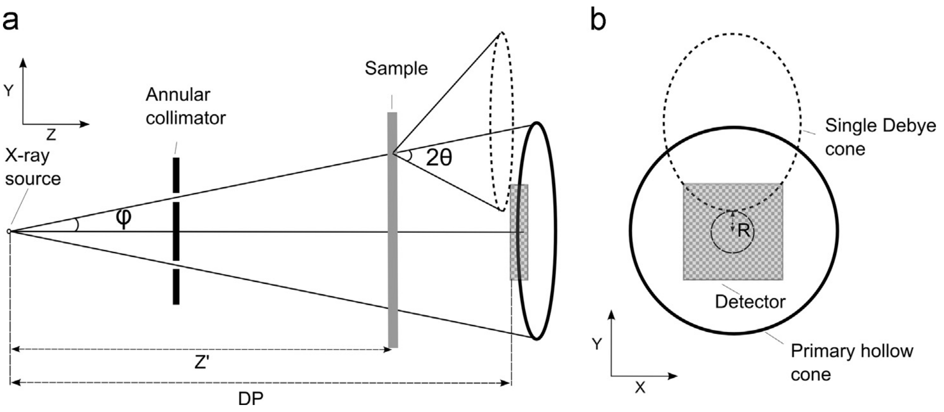

Fig. 2. The annular X-ray beam is defined by a half opening angle (φ). The position of a Debye cone, of half opening angle (2θ) along a caustic is given by (R). The symmetry or principal axis of the annular beam is incident normally upon the detector, which produces elliptical Debye rings in the plane of the detector.