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Motivations and methods for the analysis of multi-modality X-ray systems for explosives detection

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ABSTRACT

Transmission-based imaging and X-ray diffraction-based material analysis have largely developed independently. However, for a variety of applications ranging from in-vivo soft tissue analysis to concealed explosives detection, it is necessary to realize high-fidelity, spatially-resolved material discrimination. We therefore seek to understand to what degree transmission and X-ray diffraction (XRD) complement one another and can be implemented practically, particularly in the case of explosives detection in aviation security. Using a combination of simulated and experimental data, we identify the relative value of the X-ray signatures available to transmission and XRD measurements, and explore how the measurement fidelity can impact these results.

Keywords: X-ray diffraction, material characterization, tomography, aviation security

1. INTRODUCTION

Multi-view, transmission-based X-ray scanners have a successful track record in aviation security for detecting shape-based threats (e.g., weapons) and certain explosive materials. However, transmission measurements alone lack the material specificity necessary to distinguish between certain threat and benign materials with sufficiently low false alarm rates. The challenge to performing accurate, material-based threat detection via transmission measurements stems from the fundamental X-ray-matter interaction physics coupled with the inherent variability of materials.^{1,2} These two elements conspire to create a considerable overlap between threat and non-threat materials in ‘transmission space.’ Orthogonal technologies, such as X-ray diffraction tomography (XRDT), provide complementary, material-specific information that has been shown to provide additional features by which threat and non-threat materials can be better separated.^{3,4} As a result, XRDT can help reduce false alarm rates significantly, relative to a transmission-only measurement, while maintaining or improving detection.⁵ Stand-alone XRDT systems, however, have historically been challenging to implement in a practical, cost-effective manner.

To balance performance and practical implementation, we employ a multi-modality approach that combines the strengths of both transmission and XRD imaging to offset their respective weaknesses. Previous examples of such hybrid transmission + scatter systems have been heavily biased toward either transmission (e.g., a computed tomography, CT, front-end with pencil beam XRDT for alarm resolution⁶) or diffraction (e.g., whole-bag XRDT with supporting radiographic imaging⁷). While these systems have demonstrated impressive threat detection capabilities,⁸ an optimal hybrid system must be fully integrated both in design and implementation at both the hardware and software levels in order to fully exploit the information available. Designing and analyzing such systems, however, is difficult both for fundamental reasons (e.g. performance dependencies on architecture, hardware choices, algorithm details, object details, etc.) and practical reasons (e.g. large computational resource requirements, an expansive trade space, etc.). In this paper, we discuss our methods for attacking this challenging problem, which include rapid, flexible high-fidelity X-ray simulations, the ability to model large ensembles of realistic bags, an information theoretic analysis framework, and system-level experimental studies to inform and validate the results of numerical analyses.

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2. MOTIVATION FOR HYBRID MEASUREMENT: A TOY PROBLEM

Transmission X-ray imaging has long been used to create images (i.e., spatial maps) of the attenuation properties of objects throughout their volume. Whether one uses a single transmission projection measurement (i.e., radiography) or multiple measurements that enable some degree of tomographic, volumetric estimation (e.g., CT), the contrast mechanism is the same: the energy-dependent X-ray attenuation coefficient (denoted here as $\mu(E)$, see Fig. 1 a). Physically, μ represents the loss of X-rays from the incident beam due to a combination of physical effects, such as photoelectric absorption, coherent scatter, and incoherent scatter, and, as such, indirectly probes these interactions. Because the dominant interactions in the energy range of 20 - 200 keV are loss due to photoelectric absorption and incoherent scatter,⁹ most X-ray transmission-based material discrimination systems represent materials in terms of only two key features that are reflective of these distinct processes. Examples include describing materials in terms of their photoelectric and incoherent contributions or according to their density and effective atomic number, Z_{eff} . While these two features can be readily estimated using a combination of multi-view and multi-energy measurements, in what follows we consider a material to be represented by its complete energy-dependent attenuation coefficient in transmission space.

Figure 1: a) Attenuation coefficient (left, from the NIST XCOM database) and XRD form factor (right, obtained used a commercial diffractometer) for honey and glycerol. b) Schematic representation of the variability model in transmission (left) and scatter (right) space, where the red arrows correspond to the amount of variability present in the model (due to a combination of noise, intrinsic variability, etc.). c) Histogram showing the number of material pairs with a particular Bhattacharyya distance (BD) ratio BD_{ratio} . The histogram is divided into three regions: the leftmost region (for $\log(BD_{ratio}) \ll 0$), middle region (for $\log(BD_{ratio}) \sim 0$), and rightmost region (for $\log(BD_{ratio}) \gg 0$) correspond to the case where transmission provides better discrimination than scatter, where they are matched, and where scatter provides better discrimination, respectively.

In contrast to transmission-based imaging, X-ray diffraction is well-known for non-imaging assessment of the molecular structure of materials. X-ray diffraction involves the measurement of X-rays that undergo coherent scatter within a material with some degree of spatial order. The distribution of scattered X-rays as a function of angle and energy act as a unique fingerprint of the material and provide a means for determining the identity (and therefore threat status) of the material. In its simplest representation, a material can be described in 'XRD space' in terms of its coherent form factor, $f(q)$, where $q = E \sin(\theta/2)/hc$ is the momentum transfer, θ and E are the X-ray deflection angle and energy, respectively, h is Planck's constant, and c is the speed of light. Figure 1 a) shows an example of the form factors for glycerol and honey. Scatter at a particular momentum transfer value indicates that the corresponding inter-molecular separation is present in the material, and each momentum transfer value can represent a distinct degree of freedom. Thus, while we represent a given material in both transmission and XRD space with a one-dimensional vector (i.e., $\mu(E)$ and $f(q)$, respectively), the XRD form factor has the capacity to contain significantly more information about a material and its properties than the attenuation coefficient.

To investigate the relative value of transmission and XRD material representations at a fundamental level, we analyze a toy problem. At this stage, we explicitly want to avoid any considerations about the manner in which the material-specific information is obtained; we therefore ignore the system architecture, measurement cost (in terms of dollars, time, power, etc.), measurement/data processing uncertainty, etc. that might arise in extracting $\mu(E)$ and $f(q)$ from the measurement of a target material. Instead, we assume access to these X-ray material properties, but allow for material variability to exist.^{1,2} This variability may be due to variations in processing, history, temperature, packing, chemical composition, etc. which may arise naturally as well as noise or related statistical uncertainty that may be present in the measurement. We describe quantitatively the amount of variation in transmission and XRD space in terms of the parameters α_μ and α_{fq} , respectively: larger values of α correspond to larger variability of the representation in terms of either $\mu(E)$ or $f(q)$. In many ways, these α variability parameters play the role of defining the “region of responsibility” that any given material subtends within a given representation space. Figure 1 b) shows schematically how any one material can have a range of different, slightly perturbed representations in transmission and XRD space. We therefore consider a probability distribution for each material, as defined in terms of $p(x|Y)$, where x is the material property (e.g., $\mu(E)$ or $f(q)$) and Y describes the class of interest that the material belongs to (e.g., a threat T or non-threat NT).

Armed with these probability distributions based on the fundamental physical representations of a variety of materials, we proceed by quantifying the similarity between the distributions associated with our two classes. For this analysis, we consider over 60 unique materials that include liquid/solid, crystalline/non-crystalline, threat/non-threat, etc. materials that are relevant to and likely to be found in baggage at the airport. We choose to use the Bhattacharyya distance (BD) as our proximity metric, which is defined between the threat and non-threat distributions as

$$BD[p(x|T), p(x|NT)] = -\ln \int dx \sqrt{p(x|T) p(x|NT)}. \quad (1)$$

The BD is particularly useful because of its relevance to measuring the separability of classes in classification problems as well as its natural connection to mutual information and related bounds on classifier performance (e.g. probability of error in two-class classification problems).¹⁰ Thus, by calculating the BD between different pairs of materials using their $\mu(E)$ and $f(q)$ representations separately, we can gain insight into the ability for each X-ray material property representation to distinguish between classes of interest. For each pair of threat and non-threat materials, we calculate the BD for transmission, BD_T , and XRD, BD_S , where larger numbers correspond to a larger separation (i.e., easier discrimination). We then calculate the ratio $BD_{ratio} = BD_S/BD_T$ between each pair of materials within each class to compare the relative separations in transmission and XRD space. For $BD_{ratio} \gg 1$ ($BD_{ratio} \ll 1$), XRD (transmission) is better able to distinguish between the particular choice of materials, whereas $BD \approx 1$ indicates that the representations are equally capable of distinguishing the materials.

Figure 1 c) shows the results of our BD analysis. The plot is a histogram showing the number of materials that we find to have a particular BD_{ratio} , where we have chosen equal amounts of variation in transmission and scatter space such that $\alpha_\mu = \alpha_{fq} = 0.3$. We have highlighted three regions of interest; some materials are equally distinguishable by either transmission or scatter (those near $\log(BD_{ratio}) = 0$), a handful are better distinguished by transmission (those for which $\log(BD_{ratio}) \ll 0$), and a significant number of materials are best distinguished by XRD (those for which $\log(BD_{ratio}) \gg 0$). While we note that considering only the BD_{ratio} does not quantify the absolute separation of any pair of materials (i.e., does not indicate that the separation is or is not sufficient for classification with a particular accuracy), the relative value of each feature set does provide insight into the role that transmission and scatter can play in a system intended to perform material-based classification. Without any concern about how to measure these quantities (a point that will be discussed in more detail in the next section), the skew of the data toward positive values of $\log(BD_{ratio})$ indicates that XRD is inherently better suited to providing material discrimination than transmission-based measurements. This may be unsurprising, given that XRD is routinely used to perform structural analysis of materials at the atomic level; however, it is interesting to note how many materials can be separated with comparable fidelity using transmission only, given that $\mu(E)$ is generally smooth and featureless (i.e., lacking k-edges in the energy range of interest) for most materials.

3. BEYOND FUNDAMENTALS: PRACTICAL CONSIDERATIONS

The previous analysis based on BD provides useful insights into the fundamental capabilities and limitations of X-ray transmission-based and XRD-based features to distinguish between materials of different classes. We explicitly did not consider, however, the resource costs associated with realizing a system that can actually measure $\mu(E)$ and $f(q)$ with the fidelity associated with the data used above. For example, measuring $\mu(E)$ requires one to perform hyperspectral CT with ~ 1 keV energy resolution at high signal to noise ratio (SNR) and in the absence of data processing artifacts. Similarly, the XRD form factors used above were measured using a commercial diffractometer (Bruker D2 Phaser) with a momentum transfer resolution of $\Delta q = 0.004 \text{ 1/\AA}$, which puts stringent requirements on any XRDT system intended to extract this information in a real-world environment with complex objects. Thus, while the fundamental analysis above is important in that it indicates the best possible performance that could be realized from any transmission or XRD system, it does not enable one to draw any direct conclusions about how to design an optimal X-ray scanner. To go beyond this idealistic study, one must consider some of the auxiliary aspects of each system.

Table 1 shows a comparison between conventional transmission-only and XRDT-only systems in terms of several key parameters for consideration. For each system, we indicate key parameters, such as scan speed, image quality, detection performance, etc., and indicate whether the attributes represent a strength or weakness of the system. In general, transmission-based detection is more ubiquitous and faster but XRDT operates in a realm of as-of-yet not unleashed potential for providing material discrimination. While not quantitative, this table illustrates some of the tradeoffs that have typically been considered in the design of transmission and XRDT systems. Combined with the analysis described above in Sec. 2, it is clear that the cost (in terms of time, money, etc.) of measuring μ and $f(q)$ with a particular fidelity may not be equal.

Table 1: Comparison between conventional transmission-only and XRDT-only systems

	Transmission		XRDT	
	<i>Strength</i>	<i>Weakness</i>	<i>Strength</i>	<i>Weakness</i>
Speed	rapid screening			slow screening
Imaging	good spatial resolution			poor spatial resolution
Physics-based features		2-4	10-30	
Detection	high Pd	high Pfa	high Pd / low Pfa	
Price	moderate			more expensive
Deployment	widely deployed			minimally deployed

To illustrate this point, Fig. 2 shows the impact of different values of signature variability on the separability of the materials in our library. Figure 2 a1) and a4) show that XRD provides better material separation than transmission when $\alpha_\mu = \alpha_{fq}$, despite the magnitude of these variabilities. However, the off-diagonal histograms shown in Fig. 2 a2) and a3) show that unbalanced variabilities can bias the overall separability such that transmission (XRD) provides the best material discrimination when $\alpha_\mu < \alpha_{fq}$ ($\alpha_\mu > \alpha_{fq}$). This bias is quantified in Fig. 2 b), which shows the fraction of materials for which XRD is more informative than transmission as a function of variabilities in each measurement dimension. The relative value is therefore on a continuum and depends on the measurement quality. Given that a variety of factors, such as intrinsic material variability, SNR, reconstruction algorithms, etc., influence α_μ and α_{fq} and do so in different ways, it is therefore important to understand the X-ray properties of materials, X-ray scanner hardware and configurations, and data processing algorithms involved in potential scanners to create a link between the variability parameters and directly-controlled, real-world parameters.

4. METHODS

To investigate the question of how transmission and XRD can and should work together to provide accurate assessment of the composition of concealed materials, we employ two main strategies:

Figure 2: a1) - a4) histograms showing the number of material pairs with a particular value of BD_{ratio} for different variability parameters: $\alpha_{\mu} = \alpha_{fq} = 0.01$, $\alpha_{\mu} = 0.5/\alpha_{fq} = 0.01$, $\alpha_{\mu} = 0.01/\alpha_{fq} = 0.5$, $\alpha_{\mu} = \alpha_{fq} = 0.5$, respectively. b) map showing the fraction of materials for which $\text{BD}_{\text{ratio}} > 1$ (i.e. XRD provides better discrimination) for different values of α_{μ} and α_{fq} .

1. Simulation - we create virtual objects and virtual X-ray measurement systems with well-defined properties to create synthetic data for different transmission and XRD configurations and explore the available design trade space
2. Experimental investigation - we make physical measurements using testbed and commercially available equipment to improve, extend, and validate the synthetic data generated via simulation

Details of these methods are included below; together, they represent a strategy for both analyzing fundamental performance limitations and performing practical system design in an immense trade space.

4.1 Simulation

Performing design trade studies for a particular purpose (e.g., aviation or border security or medical diagnosis) requires that one create accurate virtual representations of both the target objects (e.g., bags, pallets, tumors) and the measurement systems. In addition, simulation-based studies covering a large trade space require that simulations be performed quickly in order to generate representative, statistically significant results over the many parameter permutations of interest. While a variety of tools exist for simulating transmission-based systems,^{11–13} they are often limited in the configurations or components that they can handle or are too slow. Simulating scatter, including Compton and Rayleigh scatter, is even slower and less thoroughly validated against experimental data. Relatedly, ensembles of target objects with sufficient material and shape diversity and realism are necessary but typically do not exist. We therefore use the physical simulation tool developed by Gong et al.^{14,15} to represent arbitrary transmission and scatter measurement systems and the stochastic bag generator (SBG)¹⁶ to create representative, randomly-generated virtual bags. We use these tools together to create virtual representations of existing systems (e.g. the Smiths 6040 aTiX scanner) in order to assess their performance over a controlled ensemble, to estimate the potential for performance improvements made by modifying the system, and to analyze as-of-yet unbuilt systems (using currently unavailable components). In this way, we can fully explore the hybrid space of joint transmission and XRD detection systems.

4.2 Experimental investigation

Simulation provides a wonderful method for exploring possible design scenarios; however, the models must be validated using empirical data and the conclusions derived from the models must be verified with experiment.

In this work, we use two main experimental setups: a baseline ‘real world’ and a laboratory testbed hybrid system. The ‘real world’ hybrid system consists of a Smiths 6040 aTiX scanner followed by our home-built prototype CA-XRDT scanner.¹⁷ The 6040 aTiX system is a four-view, dual energy advanced technology (AT) scanner that is certified by the TSA and currently deployed in airports throughout the world. The scientific prototype CA-XRDT scanner performs snapshot, energy-dispersive and angle-dispersive XRDT along a planar slice through the object using off-the-shelf components in a compact footprint scanner.⁵ Together, the hybrid 6040 aTiX and the scientific prototype CA-XRDT system provide a meaningful baseline of performance, in that any improvements realized in the hybrid system relative to the 6040 aTiX system alone directly translates into meaningful benefits for a next-generation system.

To complement the ‘real world’ system, we have also constructed a laboratory testbed system that enables us to make transmission and XRD measurements in nearly arbitrary configurations. The testbed system is shown in Fig. 3. It consists of an optical table with a Spellman Monoblock X-ray source (max voltage 160 kV, max current 3 mA). Collimators are mounted to the table that can be interchanged to allow for various beam configurations (cone, pencil, etc.). Currently the X-rays are collimated to a fan beam $\pm 10^\circ$ about the source focus via lead slits. The sample (30 x 30 cm cross section) is mounted on a rotation stage (whose axis of rotation perpendicular to table plane) and attached to a vertical translation stage (oriented along the rotation axis) with a range of motion exceeding 30 cm. The center of the stage is approximately 100 cm from the source.

Figure 3: Photograph of the experimental testbed system, showing the X-ray tube, source-side fan beam collimation, object stage (including translation and rotation stages), out-of-plane scatter detectors, and in-plane transmission detectors. Not shown are the detector-side optics, such as coded apertures and/or collimators, which are located between the object stage and detectors.

To measure efficiently both the transmitted and scattered X-ray signals, we employ two sets of detector arrays. Both detector arrays are currently populated with Multix ME100 detectors, wherein each individual detector module consists of a 10 cm 1-D array of pixels (0.8 mm pitch) with variable energy sampling (up to 128 energy bins) covering 20-170 keV with an energy resolution of 6-7 keV. For measuring the primary beam, we create a daisy-chained linear array of eight detectors located approximately 90 cm from the center of the sample stage and oriented along the fan beam direction. The second set of six detectors, used to record the out-of-plane scatter signal, is oriented with the pixel arrays normal to the fan beam and separated into three pairs in which the detector modules are stacked one on top of the other (spanning approximately 0.4 to 20 cm in the out-of-plane direction). These pairs of detectors are placed approximately 60 cm from the center of the sample stage and approximately 20 cm apart along the angular extent of the fan beam. The detector pairs are mounted onto a horizontal translation stage that allows them to sweep out a 2-D area above the fan beam. Finally, we place X-ray optics (e.g. collimators or coded apertures) in front of the scatter detectors to modify

the scatter signal in a known manner.

By virtue of combining the rotation and translation of the object with energy-sensitive detection, the testbed allows for emulation of a wide range of X-ray measurement configurations. For example, we can run the system in a mode that emulates multi-energy AT, hyperspectral helical CT, direct or coded aperture XRDT scanners, or a combination thereof. As such, the ‘real world’ system described above exists as a subset of the testbed measurements. The advantages of the testbed, therefore, are that it allows us to explore joint measurement strategies at the system-level that otherwise might be difficult to realize outside of a laboratory environment. In addition, the testbed provides representative experimental data for validating the simulation tools, characterizing key components (such as detectors, X-ray optics, materials, etc.), and developing data processing algorithms (e.g. reconstruction and classification).

5. RESULTS

The methods proposed above in Sec. 4 rely on a synergy between experiment and simulation. In order to demonstrate the value of each approach as well as validate the methods, we first consider the well-studied case of dual energy transmission imaging. In particular, we consider the four, dual-energy views provided by the 6040 aTiX system. Figure 4 shows false-color dual energy images of a soda can filled with soda from from different views, where the can is oriented such that the illuminating fan beam plane is normal to the axis of symmetry of the can. The colormap is defined such that the color corresponds to the effective atomic number of the material and the brightness corresponds to the overall attenuation (related to electron density). Note that the colormaps and scales are similar but not exactly the same between the different systems. The resulting images from the 6040 aTiX system, the testbed system, and the virtual (i.e. simulated) 6040 aTiX system (shown in Figs. 4 a), b), and c), respectively) show that, despite being only notionally matched (i.e., slight differences in detector response, component locations, etc. exist), the testbed and simulation give data in good agreement with the certified system.

Figure 4: Four-view, dual-energy images of a soda can generated via a) a Smiths 6040 aTiX scanner, b) our home-built testbed scanner, and c) our virtual model of the 6040 aTiX system generated via our physics simulation tool.^{14,15}

The true value in using the testbed and simulation tools, however, lies in their ability to explore the full breadth of possible transmission and scatter measurements. For example, we can use the testbed to measure the energy-dependent attenuation coefficient $\mu(E)$, rather than just a dual energy representation of the material. Figure 5 a) shows a comparison of $\mu(E)$ for TiO_2 measured in our testbed compared to that obtained in the NIST XCOM database.⁹ Similarly, Fig. 5 b) shows the normalized form factor $f(q)$ for TiO_2 measured in our testbed as compared to that obtained using a commercial diffractometer. The good agreement between the testbed measurements and the ‘ground truth’ measurements over a range of energies and momentum transfer

values illustrates the testbed's capability for investigating detection configurations that go beyond any aviation security system currently deployed today. This capability obviously also exists for the simulation tool.

Figure 5: a) Attenuation coefficient as a function of energy obtained via experimental measurement in the testbed system (blue line) and the NIST XCOM database (dashed black line), and b) XRD form factor obtained via experimental measurement in the testbed system (blue line) and a commercial diffractometer (dashed black line) for TiO_2 powder.

Returning to the initial motivation for studying hybrid systems discussed in Sec. 2, we look last at the separability between different materials based on their transmission and scatter properties (as measured in the testbed system). Figure 6 shows measurements of the attenuation coefficients (top row) and XRD form factors (bottom row) for three pairs of materials: copper and pepper, sulfur and salt, and sulfur and TiO_2 (from left to right). The values of BD_T and BD_S are shown on the figures: while transmission does a slightly better job than scatter of distinguishing copper and pepper (i.e. $\text{BD}_{ratio} < 1$), scatter better separates sulfur from salt and sulfur from TiO_2 (i.e. $\text{BD}_{ratio} > 1$). Thus, even in the presence of imperfect components and noise in the measured data, we confirm empirically the idea that scatter and transmission each provide relevant and complementary information for the task of material discrimination.

6. CONCLUSION

X-ray-based material discrimination for explosives detection is a challenging yet important task. By considering the separability of materials based on their attenuation and XRD signatures, we show that systems that rely on transmission or scatter measurements alone may face challenges in realizing sufficient performance given real-world resource constraints. A multi-modality approach that combines transmission and scatter measurements can provide significantly more material discrimination; however, designing such a system is a difficult endeavor. Our approach to this problem involves quantitatively analyzing (e.g., using information theory or other performance metrics) data generated via a combination of simulation and experimental measurement. Using this approach, we demonstrate that transmission and scatter data complement one another, but that the quality of the measurements strongly influences the relative value of the respective modalities.

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REFERENCES

- [1] Coccarelli, D., Greenberg, J. A., Thamvichai, R., Voris, J., Masoudi, A., Ashok, A., and Gehm, M., “An information theoretic approach to system optimization accounting for material variability,” *Proc. SPIE 10632, Anomaly Detection and Imaging with X-Rays (ADIX) III* **106320F** (2018).

Figure 6: a1) - c1) experimental testbed measurements of the energy-dependent X-ray attenuation coefficient and a2) - c2) the XRD form factor for copper and pepper, sulfur and salt, and sulfur and TiO_2 , respectively. The BD values in the transmission and scatter space are shown in the respective figures.

- [2] Masoudi, A., Voris, J., Coccarelli, D., Greenberg, J. A., Gehm, M., and Ashok, A., "X-ray measurement model and information-theoretic system metric incorporating material variability," *Proc. SPIE 10632, Anomaly Detection and Imaging with X-Rays (ADIX) III* **106320H** (2018). Conference presentation.
- [3] Yuan, S., Wolter, S. D., and Greenberg, J. A., "Material-identification-free detection based on material-science-informed clustering," **10187**, *Proc. SPIE* (2017).
- [4] Greenberg, J. and Iniewski, K., [*X-Ray Diffraction Imaging: Technology and Applications*], Devices, Circuits, and Systems, Taylor & Francis Group (2018).
- [5] Greenberg, J. A., Hassan, M., Regnerus, B., and Wolter, S., "Design and implementation of a fan beam coded aperture x-ray diffraction tomography system for checkpoint baggage scanning," *Proc. SPIE* **10187**, 10187 – 10187 – 7 (2017).
- [6] <http://www.donggok.co.kr/data/HS10065HDX.pdf>, "Hi-SCAN HDX 10065." online.
- [7] <https://www.morpho.com/sites/morpho/files/morpho>, "XDi." online.
- [8] Skatter, S., Fritsch, S., and Schlomka, J.-P., "Detecting liquid threats with x-ray diffraction imaging (xdi) using a hybrid approach to navigate trade-offs between photon count statistics and spatial resolution," *Proc. SPIE 9847, Anomaly Detection and Imaging with X-Rays (ADIX)* **984704** (2016).
- [9] Berger, M., Hubbell, J., Seltzer, S., Chang, J., Coursey, J., Sukumar, R., Zucker, D., and Olsen, K., "Xcom: Photon cross section database (version 1.5). [online]."
- [10] Fukunaga, K., [*Introduction to Statistical Pattern Recognition*], Computer science and scientific computing, Elsevier Science (2013).
- [11] Agostinelli, S., Allison, J., Amako, K., Apostolakis, J., Araujo, H., Arce, P., Asai, M., Axen, D., Banerjee, S., Barrand, G., Behner, F., Bellagamba, L., Boudreau, J., Broglia, L., Brunengo, A., Burkhardt, H., Chauvie, S., Chuma, J., Chytrcek, R., Cooperman, G., Cosmo, G., Degtyarenko, P., Dell'Acqua, A., Depaola, G., Dietrich, D., Enami, R., Feliciello, A., Ferguson, C., Fesefeldt, H., Folger, G., Foppiano, F., Forti, A., Garelli, S., Giani, S., Giannitrapani, R., Gibin, D., Cadenas, J. G., González, I., Abril, G. G., Greeniaus,

- G., Greiner, W., Grichine, V., Grossheim, A., Guatelli, S., Gumplinger, P., Hamatsu, R., Hashimoto, K., Hasui, H., Heikkinen, A., Howard, A., Ivanchenko, V., Johnson, A., Jones, F., Kallenbach, J., Kanaya, N., Kawabata, M., Kawabata, Y., Kawaguti, M., Kelner, S., Kent, P., Kimura, A., Kodama, T., Kokoulin, R., Kossov, M., Kurashige, H., Lamanna, E., Lampén, T., Lara, V., Lefebure, V., Lei, F., Liendl, M., Lockman, W., Longo, F., Magni, S., Maire, M., Medernach, E., Minamimoto, K., de Freitas, P. M., Morita, Y., Murakami, K., Nagamatsu, M., Nartallo, R., Nieminen, P., Nishimura, T., Ohtsubo, K., Okamura, M., O’Neale, S., Oohata, Y., Paech, K., Perl, J., Pfeiffer, A., Pia, M., Ranjard, F., Rybin, A., Sadilov, S., Salvo, E. D., Santin, G., Sasaki, T., Savvas, N., Sawada, Y., Scherer, S., Sei, S., Sirotenko, V., Smith, D., Starkov, N., Stoecker, H., Sulkimo, J., Takahata, M., Tanaka, S., Tcherniaev, E., Tehrani, E. S., Tropeano, M., Truscott, P., Uno, H., Urban, L., Urban, P., Verderi, M., Walkden, A., Wander, W., Weber, H., Wellisch, J., Wenaus, T., Williams, D., Wright, D., Yamada, T., Yoshida, H., and Zschiesche, D., “Geant4—a simulation toolkit,” *Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment* **506**(3), 250 – 303 (2003).
- [12] Kapadia, A. J., Lakshmanan, M. N., Krishnamurthy, K., Sahbaee, P., Chawla, A., Wolter, S., Maccabe, K., and David Brady, E. S., “Monte-carlo simulations of a coded-aperture x-ray scatter imaging system for molecular imaging,” *Proc. SPIE 8668, Medical Imaging 2013: Physics of Medical Imaging* (2013).
- [13] Ghammraoui, B., Tabary, J., Pouget, S., Paulus, C., Moulin, V., Verger, L., and Duvauchelle, P., “New software to model energy dispersive x-ray diffraction in polycrystalline materials,” *Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment* **664**(1), 324 – 331 (2012).
- [14] Gong, Q., Stoian, R.-I., Coccarelli, D. S., Greenberg, J. A., Vera, E., and Gehm, M. E., “Rapid simulation of x-ray transmission imaging for baggage inspection via gpu-based ray-tracing,” *Nuclear Instruments and Methods in Physics Research Section B: Beam Interactions with Materials and Atoms* **415**, 100 – 109 (2018).
- [15] Gong, Q., Greenberg, J. A., Stoian, R.-I., Coccarelli, D. S., Vera, E., and Gehm, M. E., “Rapid simulation of x-ray scatter measurements for threat detection via gpu-based ray-tracing,” *Nuclear Instruments and Methods in Physics Research Section B: Beam Interactions with Materials and Atoms* (2019).
- [16] Lin, Y., Allouche, G. G., Huang, J., Ashok, A., Gong, Q., Coccarelli, D., Stoian, R.-I., and Gehm, M. E., “Information-theoretic analysis of x-ray photoabsorption based threat detection system for check-point,” *Proc. SPIE 9847, Anomaly Detection and Imaging with X-Rays (ADIX)* **98470F** (2016).
- [17] <https://www.smithsdetection.com/products/hi-scan-6040atix/>, “HI-SCAN 6040aTiX.” online.