R4-C.2: X-Ray Diffraction Imaging

Abstract — This project investigates the development of automated explosives detection and classification in checked luggage by imaging using X-ray diffraction techniques. X-ray imaging computed tomography (CT) is the predominant modality used in luggage inspection systems for explosives detection. Conventional or dual-energy X-ray CT reconstructs the X-ray absorption characteristics of luggage contents at the different energies; however, material characterization based on absorption characteristics at these energies is often ambiguous. X-ray Diffraction Imaging (XDI) measures coherently scattered X-rays to construct diffraction profiles of materials that can provide additional molecular signature information to improve the identification of luggage. In this project, we are developing novel XDI algorithms for different architectures, which include limited angle tomography and the use of coded aperture masks. We study the potential benefits of fusion of dual-energy CT information with X-ray diffraction imaging. We illustrate the performance of different approaches using Monte Carlo propagation simulations through 3D media.

I. PARTICIPANTS

<table>
<thead>
<tr>
<th>Name</th>
<th>Title</th>
<th>Institution</th>
<th>Email</th>
</tr>
</thead>
<tbody>
<tr>
<td>David Castañón</td>
<td>PI</td>
<td>BU</td>
<td><a href="mailto:dac@bu.edu">dac@bu.edu</a></td>
</tr>
<tr>
<td>Clem Karl</td>
<td>Professor</td>
<td>BU</td>
<td><a href="mailto:wckarl@bu.edu">wckarl@bu.edu</a></td>
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<tr>
<th>Name</th>
<th>Degree Pursued</th>
<th>Institution</th>
<th>Month/Year of Graduation</th>
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<tbody>
<tr>
<td>Ke Chen</td>
<td>PhD</td>
<td>BU</td>
<td>5/2014</td>
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II. PROJECT OVERVIEW AND SIGNIFICANCE

This project investigates the development of improved automated explosives detection and classification algorithms through fusion of multiple modalities. Of particular interest are techniques that can potentially penetrate luggage and complement the information provided by dual-energy X-ray imaging. Our effort is focused on extracting additional signatures from X-ray excitation beyond the conventional density and effective atomic number, using X-ray diffraction. X-ray diffraction can provide information concerning coherent scatter distributions at different locations for different momentum transfer levels. This coherent scatter distribution is a function of the electron distribution in molecules, and provides a surrogate signature that can serve to specify the type of material in a manner that is complementary to the typical dual-energy absorption profiles.

There are major limitations in current X-ray diffraction systems. First, there is a need to localize the coherent scatter to regions so that the signatures can be associated with specific objects inside luggage. Second, the resulting scattered signals from different volumes inside the suitcase undergo complex absorption and secondary scatter on the way to detectors, which must be compensated for. Third, the measured signals are relatively weak, as the fraction of scattered photons is spread over volumetric angles in a frequency-dependent manner, so the signals collected by each detector are limited. In this project, we investigate different algorithmic and architecture approaches that can combine information from multiple frequencies and multiple scattering angles at the image formation stage, leading to improved signal to noise ratio, and subsequently
improving threat detection and classification.

Our algorithms provide the basis for coherent scatter image reconstruction for future luggage inspection systems that provide information beyond density and effective atomic number. Our architecture comparisons highlight the relative performance of alternative architectures for practical X-ray diffraction imaging systems.

III. RESEARCH ACTIVITY

A. State-of-the-art and technical approach

In our previous related work [1-4], we have developed a theory for multi-modality tomographic imaging, and successfully applied it to medical and environmental imaging modalities. We have also developed alternative approaches at fusion of diverse modalities using common structure. These approaches form the foundation for our algorithm development work.

This past year, our focus was on extension of our approaches to fusion of X-ray diffraction tomography. In X-ray diffraction [5-7], the idea is to exploit coherent scatter of X-rays to reconstruct the form factor spatial distribution of the materials being imaged, where the form factors are expressed in terms of transferred momentum that causes the deviation of photons at given wavelengths. Much of the recent interest in XDI [5-10] for security purposes stems from its ability to fingerprint materials based on molecular signature information. Originated from X-ray crystallography, XDI systems probe an object under investigation using X-ray beams and measure both straight-path transmission intensity as well as coherent scattered intensity at small angles from straight paths. The scattered intensity can be used to reconstruct diffraction profiles for material analysis. Such diffraction profiles, illustrated in Figure 1, map scattered intensity versus transferred momentum, which can be obtained from the scattered angle and the energy of the X-ray source. Location of peaks in the diffraction profile, known as the Bragg peaks, provides molecular structure information that can be used to detect the presence of specific materials of interest.

Current XDI scan systems [5,9,10] require the use of line collimators to localize scattering location, as well as polychromatic X-ray sources and photon-counting detectors to reconstruct the diffraction profile at each detector given scattering at a specified angle. As a consequence, these systems have slow scan performance and low signal-to-noise ratio (SNR) for estimating the diffraction profile, as most of the scattered photons are at angles blocked by the collimators. In an effort to gain faster scan time and better SNR, we focused our attention on X-ray Diffraction Tomography (XDT) where the off-straight path detectors are allowed to measure photons from different angles. This architecture allows the use of conventional monochromatic X-ray sources and detectors, but poses the additional challenge of localizing in space the diffraction profiles of the materials through the use of tomographic reconstruction algorithms.

Introduced in the late 1980s [11-12], XDT combines X-ray CT and XDI techniques, and thus enables visualization of physical structures in the interior of an object and component material identification. Early reconstruction algorithms for XDT [13-14] were mostly based on algebraic reconstruction technique (ART) with high computational cost. A modified three-dimensional (3D) filtered back-projection (FBP) algorithm was...
developed in [15] that resulted with two orders of magnitude faster reconstruction speed compared to ART, although at a loss in reconstructed image quality.

In our work [16,17], we developed novel tomographic inversion techniques that lead to enhanced image formation and material identification and improve on the reconstruction algorithms provided by ART, by extension of our previous work on THz diffraction tomography. We discuss the foundations of X-ray diffraction and our approach below.

The interaction of X-ray photons with matter in an energy range between 20 and 150 keV can be described by photoelectric absorption and scattering. Scattering encountered in radiology arises through coherent (Rayleigh, elastic) scattering and Compton (inelastic, incoherent) scattering. Whereas Compton scattering varies slowly with angle, coherent scatter occurs mostly in forward directions, and its angular spread has a distinct structure, characteristic of the type of material. Coherent scatter is often measured in terms of a scattering form factor $|F(q)|^2$ where $q$ is the momentum transfer, and the form factor is proportional to the scattering cross-section of the material. The momentum transfer parameter $q$ depends on the excitation wavelength $\lambda$ and the deviation angle $\Theta$ from the straight path, as:

$$q = \frac{1}{\lambda} \sin\left(\frac{\Theta}{2}\right).$$

Hence, there are different ways to vary and measure momentum transfer: knowing the X-ray excitation energy, and observing the scattered photons at different angles will vary $q$. Alternatively, knowing the angle of observation varying the excitation energy (thus wavelength), will vary $q$. The latter approach used by XDI [9-10], where the deviation of broad spectrum X-rays are measured at a single fixed deflection angle, as constrained by tube collimators, and photon-counting detectors can measure the relative photon counts for the different energy levels, corresponding to different momentum transfer levels. Such an architecture is illustrated in Figure 2, and has the advantage that the material in question is interrogated from a single direction, rather than requiring multiple directions. In addition, each detector is focused on a unique voxel, making the association between the measured scattering form factor and the physical location straightforward. However, the main limitation of the architecture is that most of the scattered photons fail to reach the detectors, and hence it takes significant time to acquire sufficient signal strength to discriminate materials reliably.

In our work, we focused on two alternative architectures that show promise for increasing signal strength by collecting scattered photons from multiple locations at each detector. This implies that localization of scattered photons must be done computationally through the solution of an inverse problem. The first architecture is an XDT architecture similar to that proposed in [12], shown in Figure 3. In this architecture, a given plane in an object is illuminated, and off-plane detectors collect scattered information from multiple locations in the plane. The illumination source rotates around the object, along with the detectors, providing multiple views of the object. In order to isolate the number of locations that contribute to scatter in each off-plane detector, vertical collimators are used to restrict the locations that contribute scattered photons to a detector to those locations in a beam aligned with the projection of the detector on the illuminated plane.

The second class of architectures we studied were coded aperture architectures, where the object of interest is not required to rotate between the source and detectors. This architecture is similar to that proposed in [19,20] and uses...
a coded aperture mask between the object of interest and the detectors, as illustrated in Figure 4. This architecture differs from the first architecture in several ways. First, it uses three fixed projections, as opposed to a rotating set of projections. Second, the system allows mixing of scatter signals from multiple beams in the plane, thereby collecting more of the scattered photons at the detectors.

The three directions of illumination are chosen to be 60 degrees in orientation to provide illumination diversity. Each direction illuminates a plane in the object, and allows the scattered photons to scatter off-plane to a set of scatter detectors. Unlike the approach in Figure 3 on the previous page, no collimators are used between columns of detectors; instead, scattered photons from the entire plane pass through a coded aperture that blocks some scatter directions on the way to detectors. Figure 4 illustrates one direction of illumination, where a plane of X-ray excitation at wavelength $\lambda$ illuminates the object under investigation. Coherent scatter radiation from the illuminated plane passes through a coded aperture before reaching a 2D detector array.

We developed mathematical models of X-ray diffraction imaging systems, and used them as the basis for developing tomographic reconstruction algorithms for X-ray diffraction images. The details of these algorithms are documented in our paper [18] and the thesis [1]. A few highlights of this work are summarized below.

One of the phantoms that we used in our analysis is a 3-dimensional block composed of a mixture of crystalline and amorphous materials: PVC, PMMA, Graphite and Aluminum. The phantom is homogeneous in the vertical dimension; since coherent scatter is measured off the plane of illumination, the vertical dimension affects the coherent scatter, with significant reduction in signal strength. This phantom is illustrated in Figure 5, along with the momentum transfer form factors and the linear attenuation coefficients for each material.

![Figure 4: X-ray Diffraction imaging.](image)

![Figure 5: Left: Experiment phantom, Middle: momentum transfer form factors, and Right: linear attenuation coefficients for each material in the phantom.](image)

A main result of our analysis is determination of whether fusion with dual-energy CT information is required to perform X-ray diffraction tomography. Dual-energy CT can provide information regarding the wavelength-dependent linear attenuation coefficient of the object of interest; this information is useful to compensate for photon losses along the incoming and scattered paths. Without this information, one must make approximations regarding these losses as part of the reconstruction algorithms. We performed reconstructions using both accurate linear attenuation coefficients as well as the approximations developed when one did not have this side information, using multienergy excitation from 60 to 72 keV, and using photon counting detectors with 4 keV resolution, with the X-ray Diffraction architecture of Figure 3. The results are summarized in Figure 6. The results highlight that, for this architecture, the use of the approximate model provides reconstructions that are only slightly degraded relative to the reconstructions obtained using the side information. This suggests that the architecture of Figure 3 can form images without fusion from dual-energy CT.
We performed a similar analysis using the coded aperture architecture of Figure 4 on the previous page, with 3 illumination directions. To simplify the reconstruction, we use monochromatic illumination, and we remove measurement noise in our simulated experiments. The results are shown in Figure 7 on the next page. The results indicate that, for this coded aperture architecture, it is essential to use fusion information regarding linear attenuation coefficients in order to compensate for photon path loss in the reconstruction algorithms.

Additional analysis and performance comparisons can be found in [1, 18]. The main conclusions are that X-ray diffraction imaging using tomographic architectures is feasible using reconstruction algorithms that exploit compressive sensing principles, and these architectures provide stronger signals than previous X-ray imaging architectures, thereby establishing the potential for real-time imaging. Another important conclusion is that there are significant advantages to architectures that fuse X-ray diffraction imaging with conventional CT imaging, and to architectures that use low-resolution photon counting detectors versus total energy detectors.
Figure 7: Images of coherent scatter form factors at 0.86, 1.30, 1.66 and 2.14 nm\(^{-1}\) using the coded aperture imaging architecture of Figure 4.

B. Major contributions

- Provided a systematic analysis of alternative X-ray diffraction architectures and established performance limitations, as well as requirements for fusion.
- Developed prototype algorithms for tomographic reconstruction of X-ray diffraction images and characterized their relative performance.
- Developed results that establish the feasibility of tomographic X-ray diffraction architectures that have greater efficiency in collecting coherent scatter signals when compared with current commercial models.

C. Future plans

- Explore new types of reconstruction algorithms using adaptive basis representation.
- Validate results with more complex simulations, including additional materials and classes.
- Explore algorithms with reduced computation requirements or parallel implementation.
- Perform information theoretic analysis of performance for potential classification of materials.
- Explore performance for materials of interest including liquids and homemade explosives.

IV. RELEVANCE AND TRANSITION

A. Anticipated end-user technology transfer

Prototype systems are currently under investigation by many companies, including Morpho, Analogic, L-3, Reveal and others.
V. PROJECT DOCUMENTATION AND DELIVERABLES

A. Peer reviewed conference proceedings

B. Other presentations

C. Student theses or dissertations

VI. REFERENCES


