Abstract— This project investigates the development of automated explosives detection and classification algorithms for increased throughput by using combinations of sensors in an active, adaptive testing scheme. Multi-modal sensors can help find and distinguish the features of existing threats, and even discover and classify new ones. The significance of this project lies in the potential to use multiple modalities fused together to detect the presence of explosives, for both portal and stand-off systems, and then to classify their natures as specifically and sensitively as possible. In our recent work, we have developed new theories for increasing the signal/noise ratio in diffraction tomography using sensors that collect measurements at multiple frequencies, by adapting techniques previously exploited for multi-modal imaging in medical applications. For X-ray systems, this includes investigating the use of multi-energy X-ray techniques and X-ray diffraction tomography. This past year, we have continued our work on fusion of X-ray diffraction tomography along with conventional X-ray computed tomography, in order to extract information from coherent scatter of materials to fuse with the conventional CT absorption images. The focus has been on exploring architectures that provide stronger signals, included coded aperture imaging, and consider the full spectral characteristics of X-ray sources and detectors.

I. PARTICIPANTS

<table>
<thead>
<tr>
<th>Faculty/Staff</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Name</strong></td>
</tr>
<tr>
<td>David Castañón</td>
</tr>
<tr>
<td>W. Clem Karl</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Students</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Name</strong></td>
</tr>
<tr>
<td>Ke Chen</td>
</tr>
</tbody>
</table>

II. PROJECT OVERVIEW AND SIGNIFICANCE

This project investigates the development of improved automated explosives detection and classification algorithms through fusion of multiple modalities. Consider a suite of diverse sensors collecting bulk and trace detection data associated with a single scene, e.g., X-ray imagers, terahertz (THz) spectroscopy, microwave, infrared (IR), and hyperspectral imaging in a standoff configuration. Each sensor provides vectors of features associated with individual areas in the scene. Detection and classification exploit partially independent information from each modality in fusing these features, first to arrive at a threat/no-threat decision, and second, in the event of a threat, to classify its nature, e.g., type and amount of explosives, etc.
Of particular interest are techniques that can potentially penetrate luggage and complement the information provided by dual-energy X-ray imaging. Our early work focused on THz diffraction tomography as a complement to X-ray Computed Tomography. However, the penetration strength of THz excitation in luggage limits the received signal strength of THz, and prevents accurate resolution and imaging of material properties inside the luggage. For the past two years, we have refocused our effort on exploiting information from modalities that can penetrate luggage, such as X-ray excitation. Our recent focus has been 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.

III. RESEARCH AND EDUCATION ACTIVITY

A. State-of-the-Art and Technical Approach

In our previous related work [1-3], 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. Our goal is to extend this signal fusion theory, along with matched filtering to generate joint multi-modal imagery from dual energy X-ray, THz, and other modalities.

Our past work focused on multi-frequency THz imaging techniques based on diffraction tomography. Our colleagues at RPI pioneered the use of diffraction tomography for imaging with THz excitation [4,5]. They produce relatively broad spectrum THz pulses and measure excitation at the back of the object of the diffracted field. Although the excitation is broadband, the diffraction properties of the object are frequency dependent, and thus the approach pursued in [4,5] is to segregate the contributions of the measured fields for each frequency, and reconstruct an image at each frequency of interest, which limits the signal-to-noise ratio used for each image. In our work [6], we developed novel techniques that combine information from all frequencies to form improved images at each frequency and demonstrated enhanced resolution and increases in effective signal-to-noise ratios that improved materials discrimination performance.

Last year, our focus was on extension of our approaches to fusion of X-ray diffraction tomography. In X-ray diffraction [7-9], 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 X-ray diffraction imaging (XDI) [7-12] for security purpose 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 Fig. 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 [7,11,12] require the use of line collimators to localize scattering location, as well as multichromatic 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 [13-14], 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 or XDT [15-16] 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 [17] that resulted with two orders of magnitude faster reconstruction speed compared to ART, although at a loss in reconstructed image quality.

In our current (Year 5) work [18], 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 150keV 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, 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 [11-12], 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 on the following page, and has the advantage that the material in question is interro-
gated 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 order to increase the signal strength, one can use a different architecture, such as that proposed in Figure 3. In this architecture, sheet collimators are used instead of tube collimators, so that coherent scatter from an excited voxel in the object is collected by a vertical line of scatter detectors, thus receiving scatter at multiple angles from the same voxel. Thus, each detector collects scattered photons from a line of voxels, mixing the scatter from multiple locations. This requires tomographic principles, with illumination from different angles, in order to determine the form factors for each scattering location. In our work last year [12], we assumed monochromatic x-ray sources that interact with the material on a slice plane, with the scattering measured on a plane perpendicular to the illuminated slice, as shown in Figure 3. The illumination is rotated around the object to collect enough information to allow for tomographic reconstruction of the scattering form factors.

The relevant equations are summarized in [16,17]. The observation is basically the ratio of the scattered intensity measured by each off-plane detector to the transmitted intensity measured by the direct path. This depends on the form factor $|F(t,s,h)|^2$ for scattering the ray at in-plane offset $t$ from the source to an off-plane height of $h$ after traversing through material to a voxel distance $s$ away from the source, where the detector plane is located at distance $G$.

$$P_\phi(t, h) = \frac{I_\phi(t, h)}{I_{trans}(\phi, t)} = \int_0^G |F(t, s, h)|^2 \xi(t, s, h) ds$$

where the geometric factor shows the change in effective area for a detector on a plane as:

$$\xi(t, s, h) = \frac{G^2(G - s)}{(h^2 + (G - s)^2)^{3/2}}$$

For our investigations, we implemented three algorithms: an algebraic reconstruction algorithm, a filtered backprojection algorithm and our own algorithm: iterative reconstruction with edge preserving regularization (IREP). The details of these algorithms are included in [18]. The IREP algorithm is an extension of our prior work in [1-3,6] that uses regularization with object constraints across the different form factor images, so that edges between objects are made consistent across the different form factor levels.

To evaluate our algorithms we used a Monte Carlo simulation for photon propagation in a phantom. The phantom consists of Lucite, kapton and water, and is around 100 mm in diameter, with air as background, as shown in Figure 4. We as...
sume the use of parallel beam X-ray at 60keV, and a detector array of 30 rows and 151 columns perpendicular to the object plane. The detector array is 30 mm in height and 151 mm in width, covering scattering angle between 0 and approximately 8 degrees, corresponding to a transferred momentum range between 0 and 2nm⁻¹ of interest. The source-detector distance is 1135 mm, and the distance from the source to the center of the rotation amounts to 760 mm. The detectors rotate around the phantom, taking projections at every 5 degrees over a full rotation.

Figure 5 shows the q-images reconstructed with the 3D filtered back-projection method FBP, the ART algebraic reconstruction technique, and the iterative feature-preserving reconstruction method IREP for three selected momentum transfer levels. The FBP method suffers from having a limited number of viewing angles and uncertainties in measurement, which degrades the quality of backprojection reconstruction. ART brings in computational burden without significant quality improvement. Our IREP method achieves improved edges by combining structural features indicated at all q values and estimating a shared boundary field. This results in more accurate reconstruction of not only edges and piece-wise smooth image, but also smooth diffraction profiles across transferred momentum.

Figure 6 on the following page shows the form factor reconstructions comparing the different tomographic methods with a comparable reconstruction using direct imaging, when the number of photons is kept constant across both methods. Each graph shows the reconstructions obtained for three voxels of each of the main material types. The tomographic methods provide smoother reconstructions which are much closer to the true form factors displayed in Fig. 4 because of the improved number of photons collected. In contrast, the direct imaging method provides much noisier reconstruction, due to the limited number of photons which reach the detector.

During the past year, we focused on exploring alternative architectures that would increase the number of photons reaching detectors. One such architecture, CAXSI [19-21], was proposed by David Brady at Duke, using coded apertures to break the symmetry of the scatter measurements collected by each detector. In simple experiments using two isolated voxels of homogeneous, crystalline materials, they were able to demonstrate reconstruction of coherent scatter form factors for these two voxels. This suggested that the approach could be generalized appropriately to fan-beam and parallel-beam coherent scatter configurations, which we investigated.
The basic configuration for coded aperture x-ray coherent scatter imaging is shown in Figure 7. A plane of x-ray excitation illuminates the material of interest. Coherent scatter radiation from the illuminated plane passes through a coded aperture before reaching a sheet of detectors. The coded aperture blocks selected paths from voxels in the material to specific detectors, providing a spatially varying sum of scattered photons on each detector. The detectors are assumed to be intensity detectors, typical of what is available in medical imaging CT scanners. The coded aperture blocks roughly 50% of the scattered photons from reaching the detector, which allows many more photons to reach the detectors than either the direct imaging architecture of Figure 2 or the tomographic imaging architecture of Figure 3. In the papers [19-21], the suggestion is that the form factors of the voxels in the illuminated plane can be reconstructed from a single view. This is a challenging task, because the resulting reconstruction would be a 3-dimensional image (two spatial coordinates plus a spectral coordinate for momentum transfer), whereas one is only collecting a single two-dimensional set of measurements from the array of detectors.

To perform the reconstruction, we extended our previous algorithms using compressive sensing techniques that exploit several types of ‘sparsity’: First, we assume some spatial regularity in the composition of the objects of interest, so that the object being imaged is composed of several regions, each of which is of a homogeneous material with similar form factor. Second, we assume that the form factors of interest are composed of relatively few sharp peaks (from Bragg peaks) and smoother sections for more amorphous materials. Using these assumptions, we developed extensions of our previous tomographic IREP algorithms to do coded aperture form factor reconstructions using different configurations.

Our results are summarized below. We constructed a spatial phantom using 4 materials: graphite, alumi-
num, PMMA and PVC. The coherent scatter form factors for these materials is shown in Figure 8. Aluminum and Graphite are crystalline materials that exhibit sharp Bragg peaks, whereas PMMA and PVC are amorphous materials with relatively smooth coherent scatter form factors. The spatial layout of the materials is shown in Figure 9, using the same color coding as Figure 8. We simulated this phantom using a coded aperture composed of parallel lines, as in [17], and simulated the phantom as illuminated by monochromatic x-ray radiation at 72 keV. We simulated the detector intensities collected from four different views, by moving the x-ray source from -60 degrees to 60 degrees around the object, using three different configurations: First, we looked at the imaging configuration without a coded aperture, with the expectation that the angular diversity could provide enough information for an accurate reconstruction. Second, we collected the information using sheet collimators as in the architecture of Fig. 3, to see whether limited-angle tomography reconstructions would be sufficient. Third, we collected the information from a single view using coded aperture imaging, and from the four views using coded aperture imaging.

We posed the reconstruction problem for each of the architectures as an inverse problem, and analyzed the spectral characteristics of the resulting algebraic operator that maps the unknown material characteristics (voxel locations and form factors) into the measured intensities. Each of these operators can be analyzed in terms of its singular values to identify how much information the measurements provide for reconstruction, versus how much information must be inferred from other sources of knowledge beyond the measured data. We have already suggested that reconstructing a 3-dimensional object from a single 2-dimensional measurement is ill-posed.

Figure 10 shows the singular values of the operators for 3 different conditions: The measurements without coded aperture, the measurements with sheet collimators, and the measurements with coded aperture.
measurements with a coded aperture. The first observation is that the singular values of the operator without the coded aperture fall quickly to 0, as the vertical scale is logarithmic. This indicates that there is significant redundancy in the measurements, and limits the unambiguous information that can be extracted from such measurements. A surprising result to us was that the operator with limited angle tomography exhibited much better conditioning for the first 9000 elements, but then dropped off, indicating that 4 views with limited angle may not provide enough information diversity. The coded aperture singular values provided a much better set of linearly independent measurements.

Figure 11 shows the reconstructions of the form factors achieved using two of our compressive sensing algorithms comparing the configuration without a coded aperture to that using a coded aperture. The results show that, without a coded aperture, the presence of crystalline materials can alias form factors reconstructed for the amorphous materials, so that even the crystalline form factors cannot be recognized. The added linear independence of measurements provided by the coded aperture serves to separate the form factors appropriately. The results highlight the potential of coded aperture imaging to provide accurate reconstruction of form factors from very limited viewing angles.

B. Major Contributions

The new tomographic algorithms for X-ray diffraction show that using shared object structure across different momentum transfer levels can enhance the reconstruction quality and lead to improved recognition in low signal to noise environments. The new algorithms also show promise for implementation using a different architecture from the current generation of X-ray diffraction instruments that can generate higher signal-to-noise ratios in the resulting images, leading to enhanced recognition performance as well as faster processing times.

IV. FUTURE PLANS

In spite of the promising results above, the experiments to date have only used 2-dimensional simulations. Therefore, the coherent scatter photons scatter only once, and do not interact with objects on the way to detectors. It is critical to analyze the result of full 3-dimensional spatial geometries, and develop novel algorithms specially tailored for these environments. In particular, one must also address the computational issues associated with generating accurate coded aperture images in real-time. Currently, this is a difficult problem even for the 2-dimensional geometries we are testing.
In addition, one must also extend the results to address multi-energy excitation that is typical of commercial X-ray sources such as tungsten sources. The use of single energy excitation simplifies the modeling, and avoids considerations of beam-hardening that are typical when different energy levels have different absorption and scattering characteristics. We are currently working to address these issues, developing algorithms that integrate the multi-energy characteristics of the sources, and working to develop techniques to compensate for beam hardening. One of the key approaches here may be the fusion of multi-energy CT imaging with coherent scatter imaging.

Another direction is to develop algorithms that avoid streaking, a phenomenon that is typical of CT imaging in the presence of metallic objects. The large difference in absorption characteristics between metallic objects and their neighbors leads to aliasing of the imaging. For coherent scatter, we see similar aliasing taking place between crystalline scattering materials with sharp Bragg peaks and amorphous materials.

An element that is ignored in our analysis but which may have significant impact in fielded systems is the presence of multiple scatter. In particular, the removal of collimators in front of the detectors allows for multiple-scattered photons (either Compton or Rayleigh) to reach the detectors, increasing significantly the noise floor. A proper study of this would require the use of particle scattering simulators such as GEANT4.

Finally, our architectures used only intensity detectors. The use of photon-counting detectors can lead to improvements both in the ability to do beam hardening corrections as well as in the accuracy of the reconstruction, and should be investigated.

VII. DOCUMENTATION

A. Seminars, Workshops and Short Courses


VIII. REFERENCES


