Deep Learning for Elemental Mass Quantification using Spectral X-Ray Radiography

November 5, 2019

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PNNL is operated by Battelle for the U.S. Department of Energy

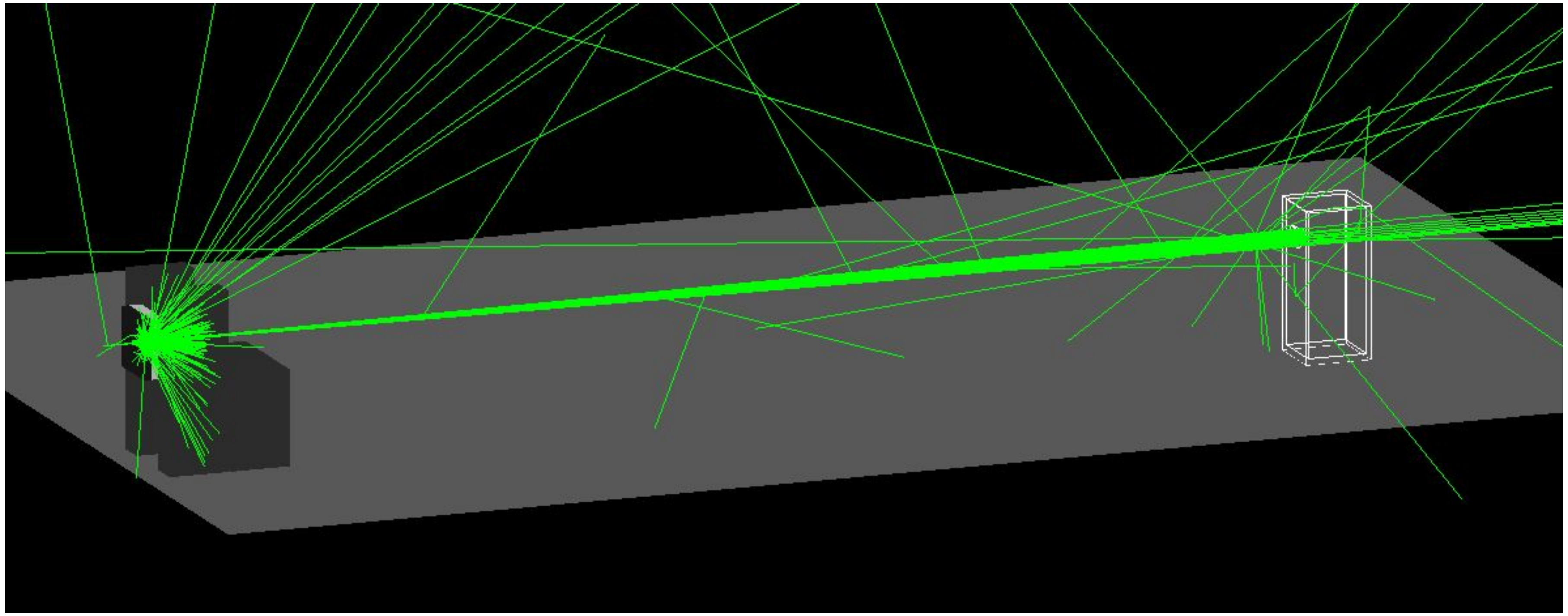
Overview

1. Introduction
2. Spectral X-Ray Radiography
3. Convolutional Neural Networks
4. Dataset Synthesis
5. Results and Conclusion

[1] “The Invisible” (1896)

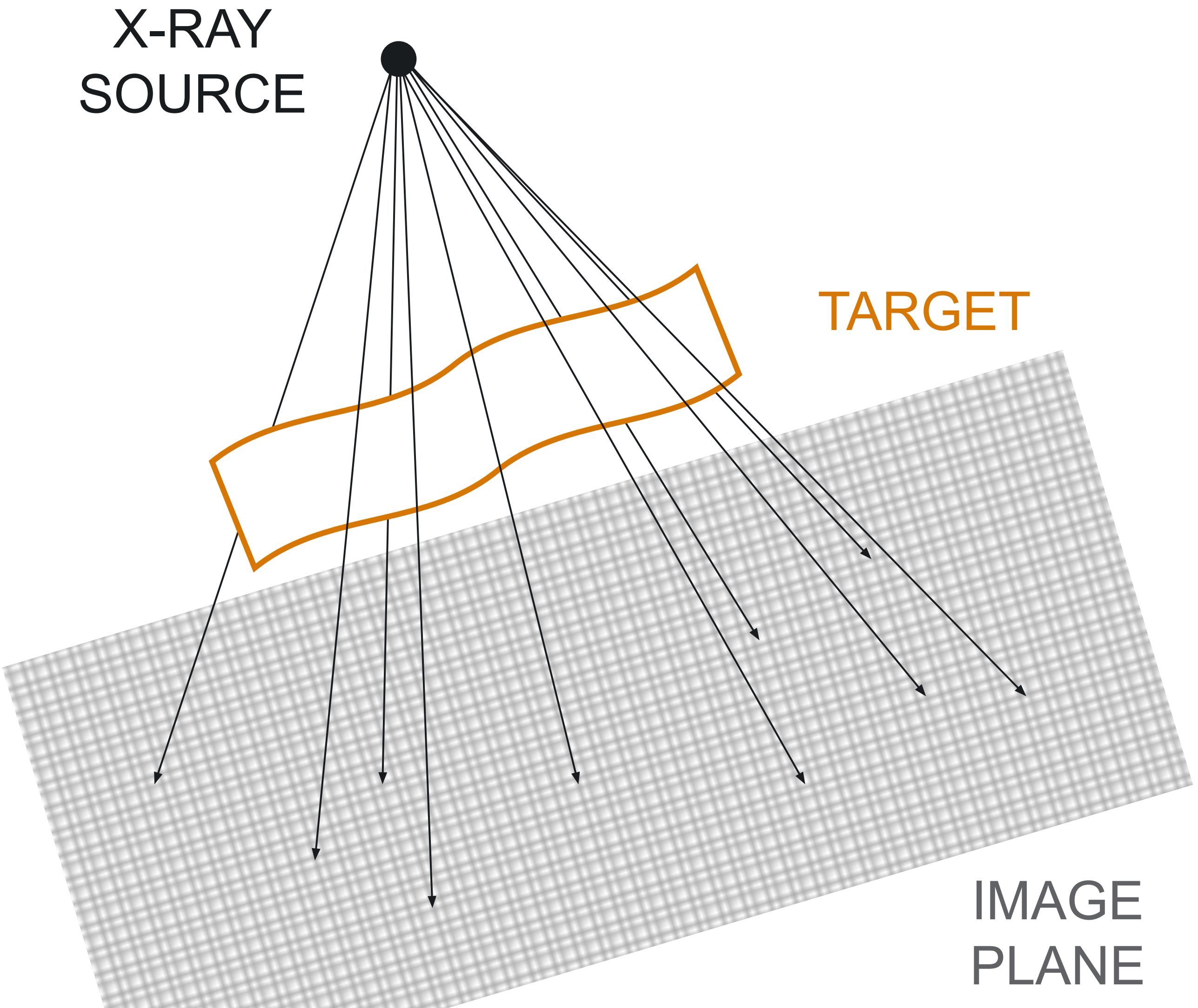
Objective of this work

- Use deep learning to predict mass of each element present in a sample from spectral radiograph within 1% relative error
  - Test Case: Bi_2O_3 powder

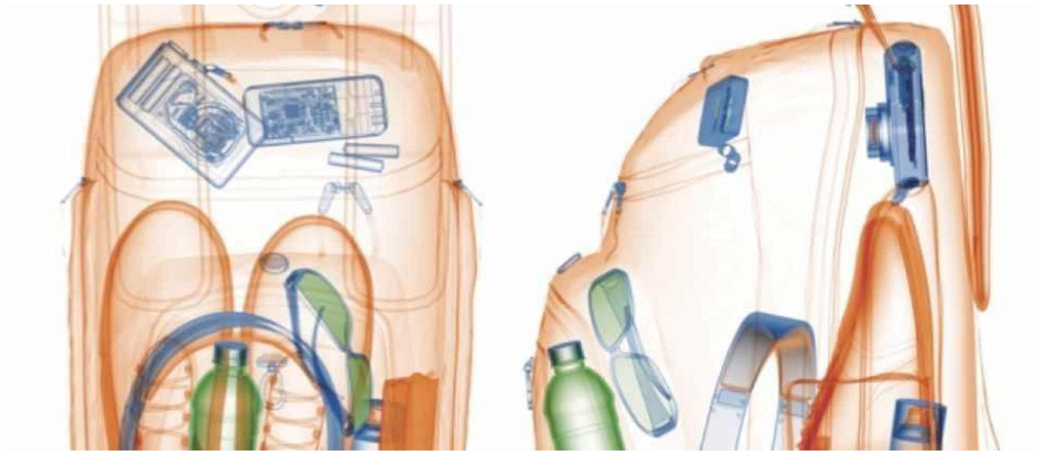


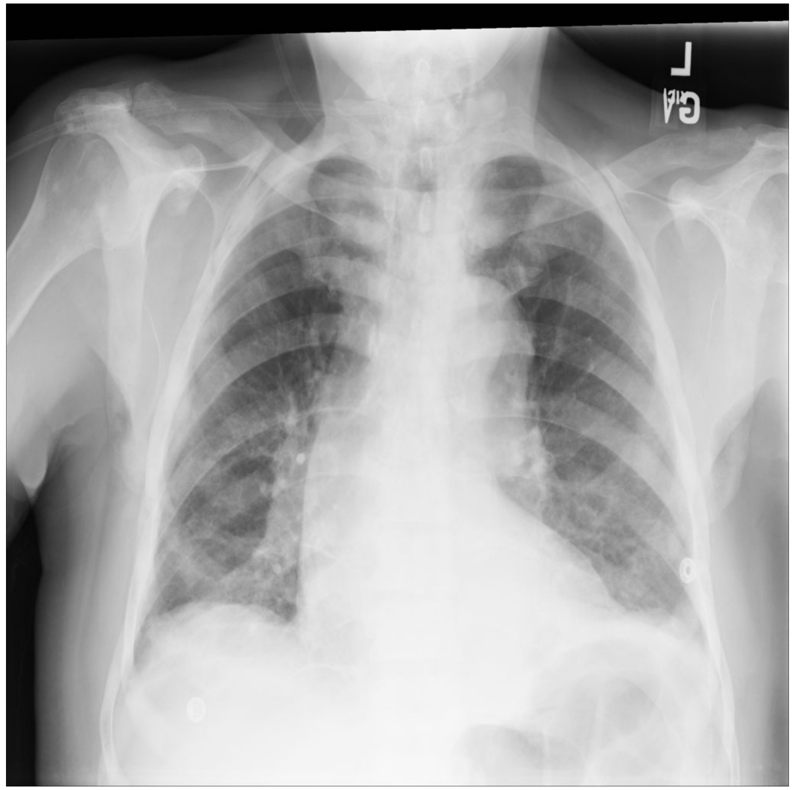
X-Ray Radiography

Typical Planar Configuration:



[2] “How does an airport scanner work?”





[3] Wang et al. (2017)

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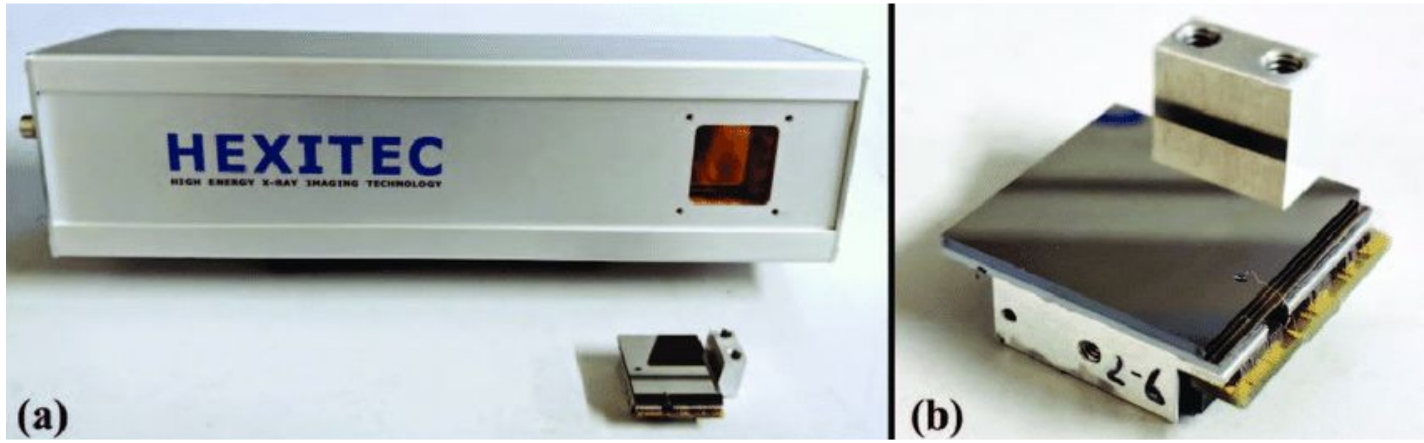
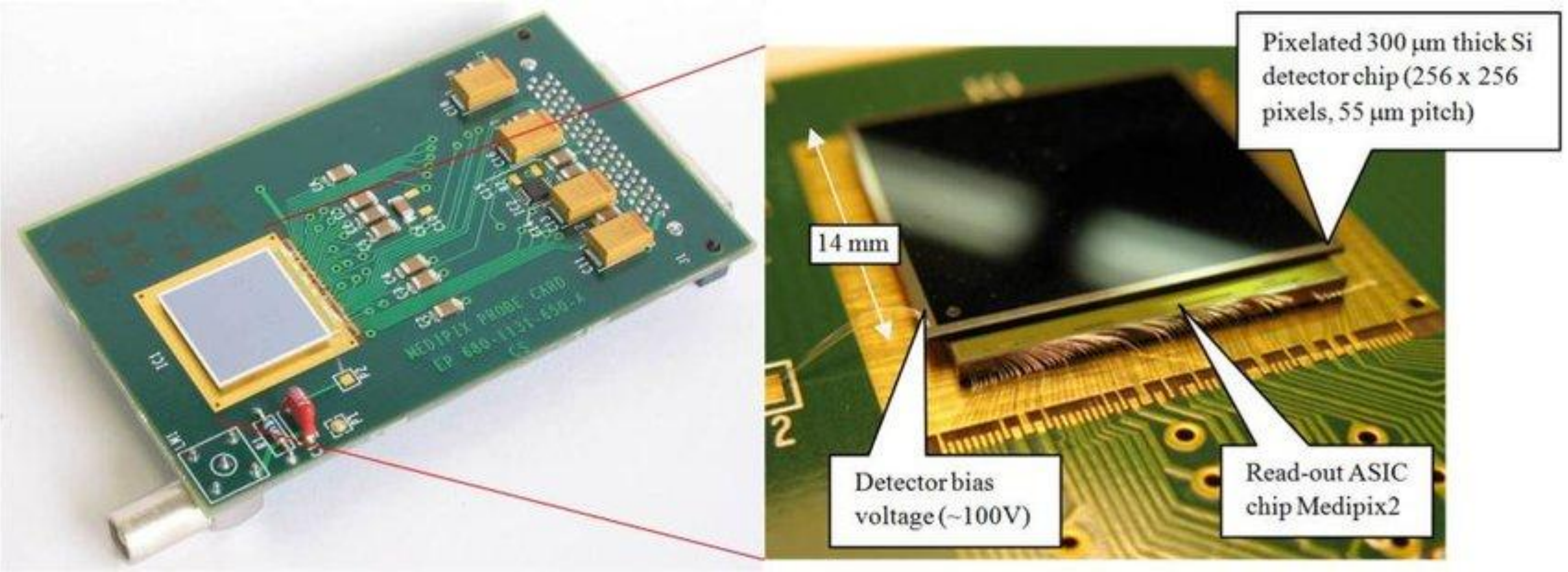
Energy-Sensitive, Pixelated Detectors

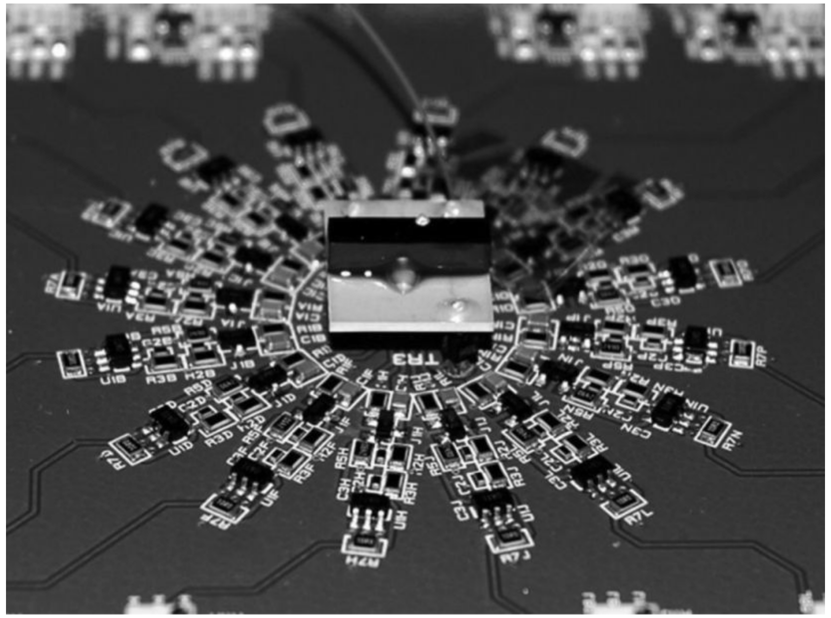


HEXITEC [4]



Medipix2 array detector [5]

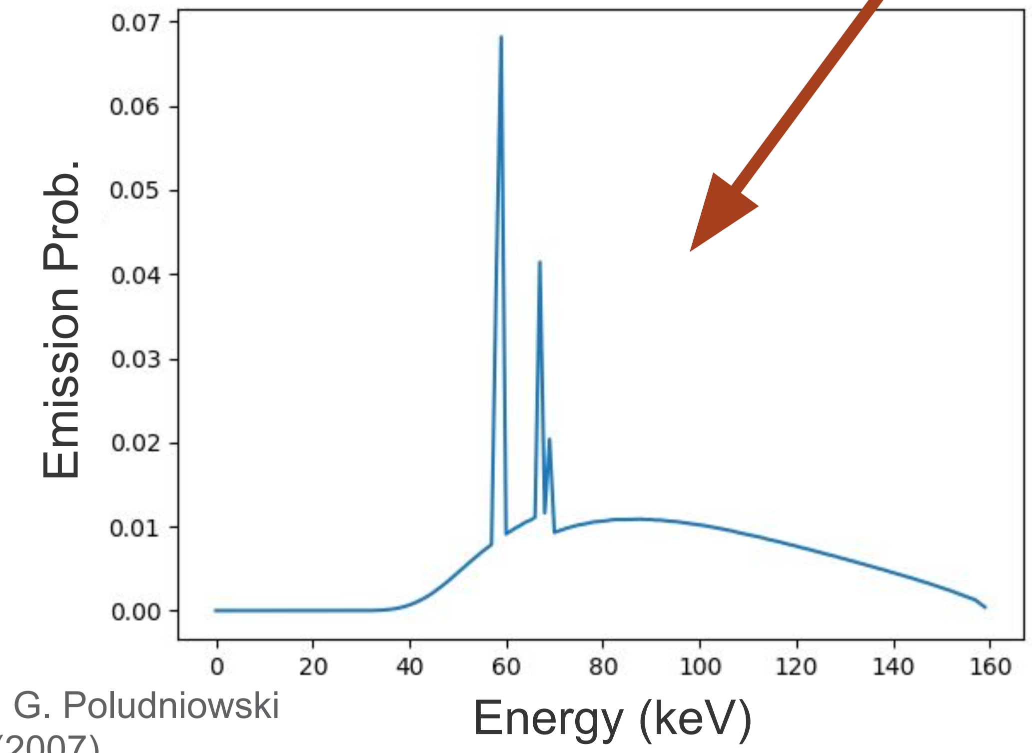
Readout board for LETI linear CdTe detector [6]



Spectral X-Ray Radiography

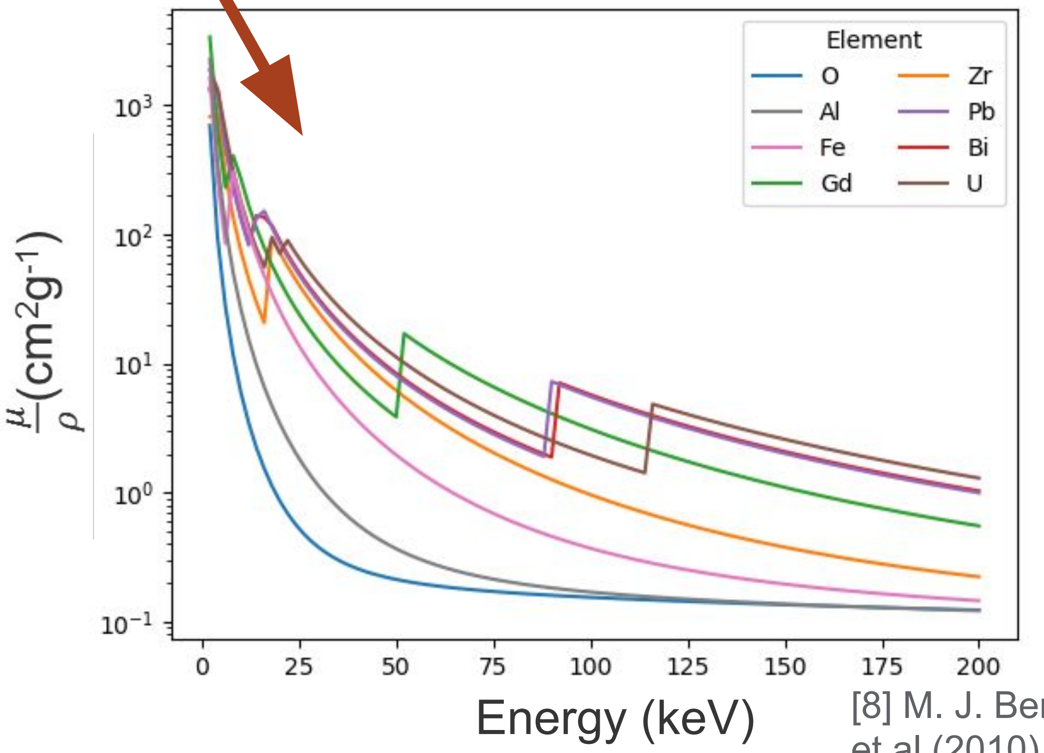
$$\Phi(E) = \boxed{\Phi_0(E)} e^{-\sum_k \boxed{\mu_k(E)} x_k} + \Phi_{scatt}$$

Initial Spectrum



[7] G. G. Poludniowski et al (2007)

Attenuation Coefficients



[8] M. J. Berger et al (2010)

Solve for x_k

- Presence: Material Discrimination
- Amount: Mass Quantification

Numerical Approaches

$$\Phi(E) = \Phi_0(E) e^{-\sum_k \left(\frac{\mu}{\rho}\right)_k (\rho_A)_k}$$

$$T(E) = \frac{\Phi(E)}{\Phi_0(E)}$$

$$-\ln T(E) = \sum_k \left(\frac{\mu}{\rho}\right)_k (\rho_A)_k$$

$$r_i = \int_{E_i} -\ln T(E)\, dE$$

$$\vec{r} = A\vec{\rho}_A$$

$$\vec{\rho}_A = (A^T A)^{-1} A^T \vec{r}$$

[5] M. Firsching et al (2008)
[6] J. Rinkel et al (2011)
[9] "Medipix2…" (2002)
[10] G. Beldjoudi et al (2010)

Sandia for explosives detection

- Apply Simplex Method by approximating energy dependence with Legendre polynomials
- Performed CT reconstruction

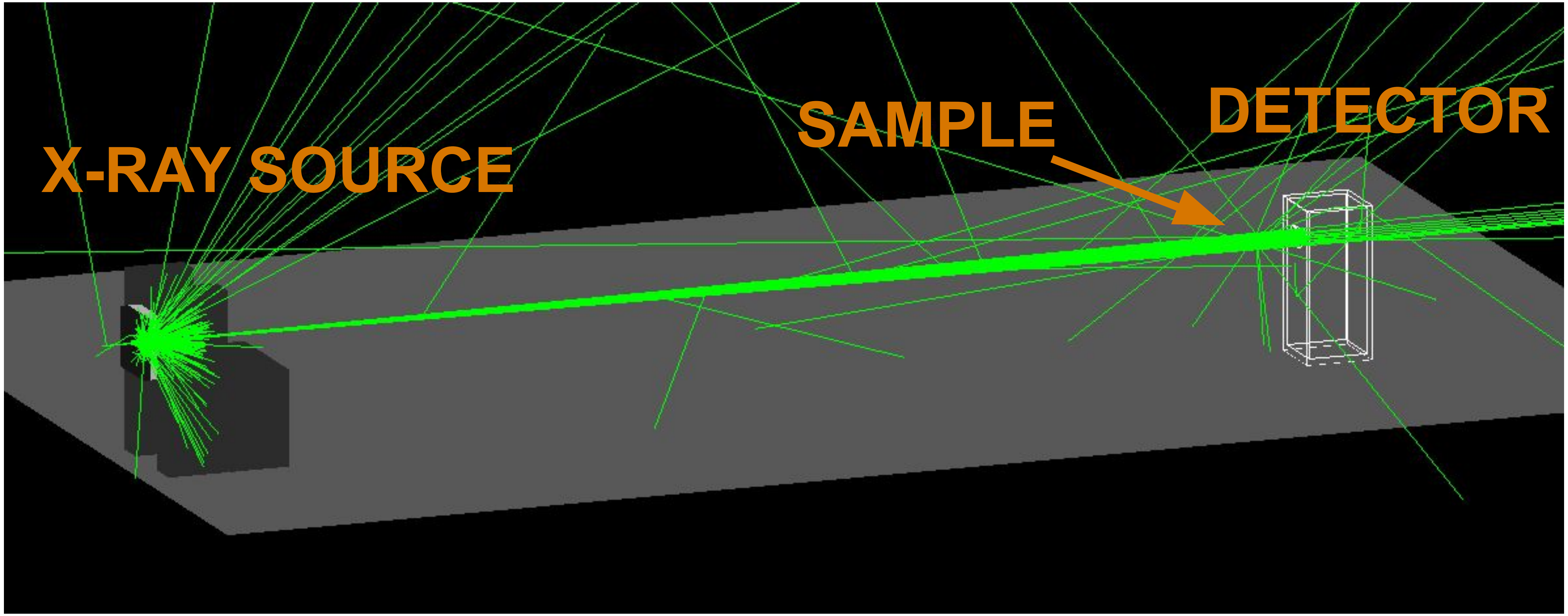
[11, 12] E. S. Jimenez et al (2014)
[13] N. Collins et al (2017)
[14] E. S. Jimenez et al (2016)

PNNL for Safeguards

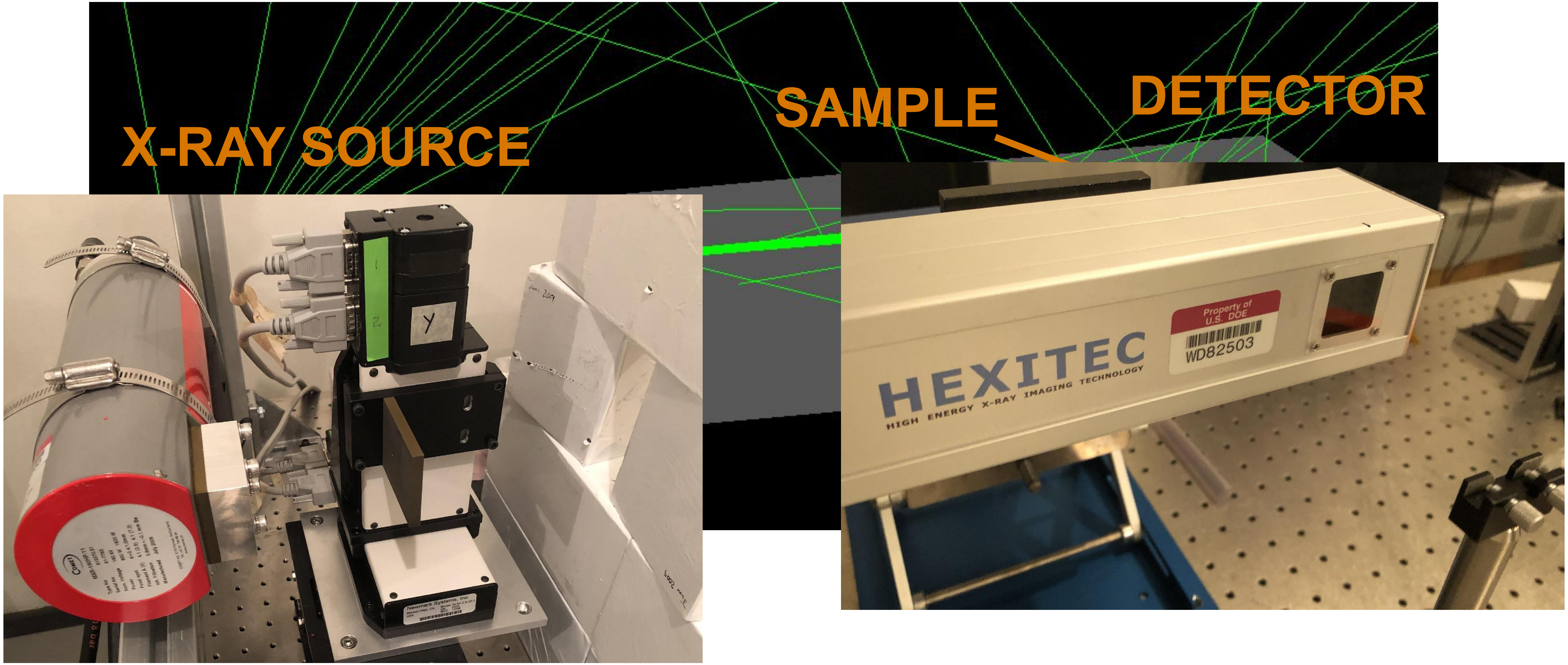
- Apply Quadratic Method: Non-linear least-squares
- Used non-negativity constrained Gauss-Newton method with reduced Hessian

[15, 16, 17] A. J Gilbert et al (2014, 2016, 2017)

Experimental Setup

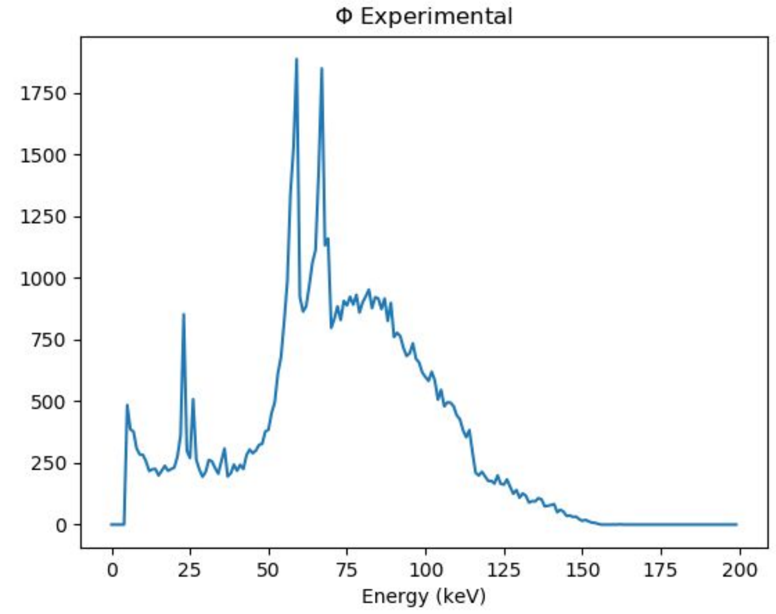


Experimental Setup

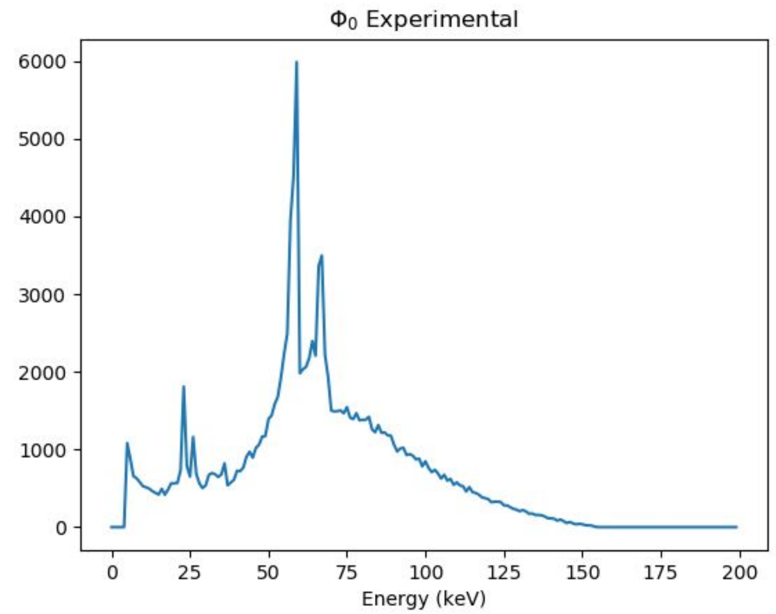


Experimental Spectral Radiographic Data

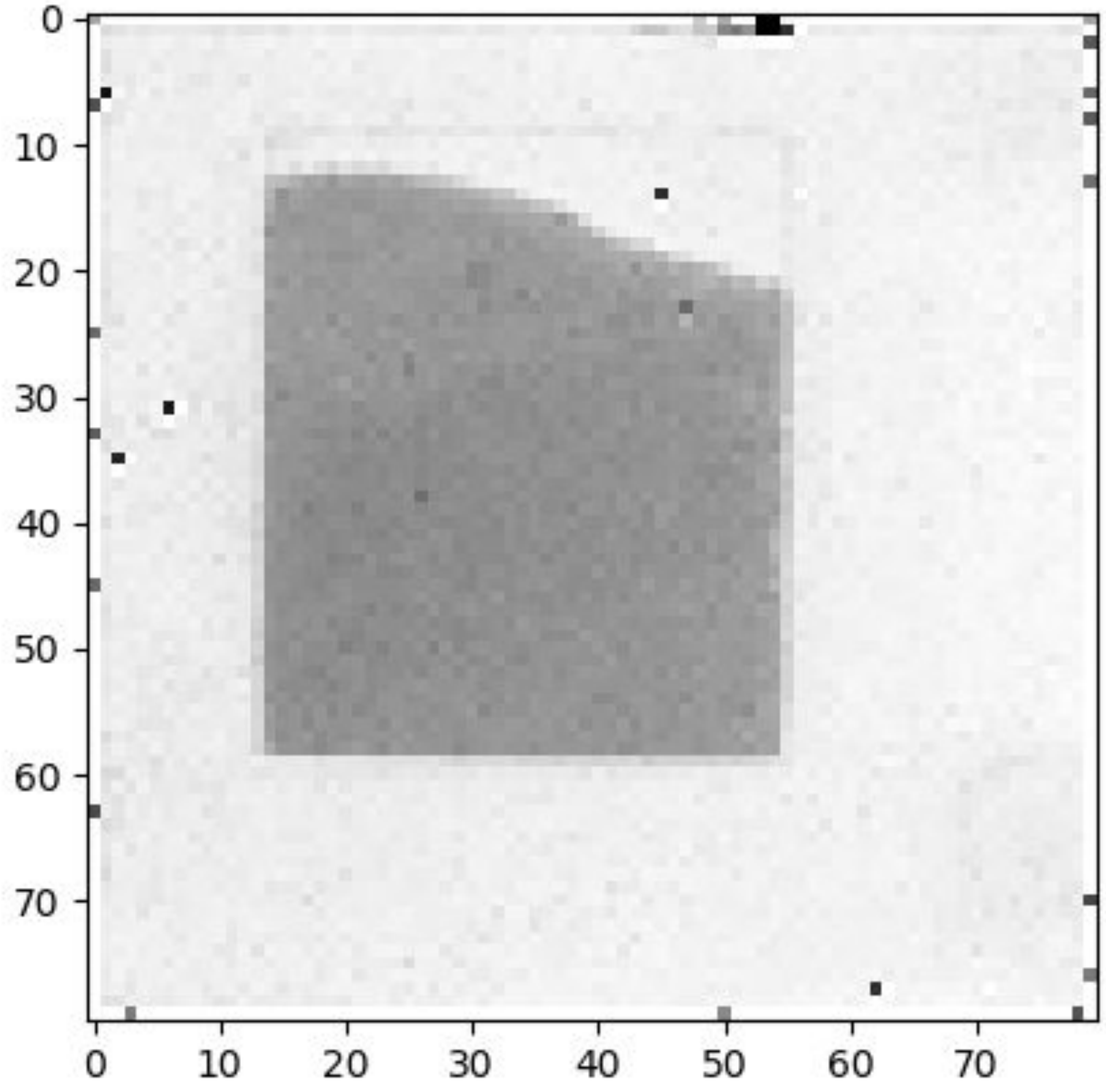
Attenuated Beam



Unattenuated Beam

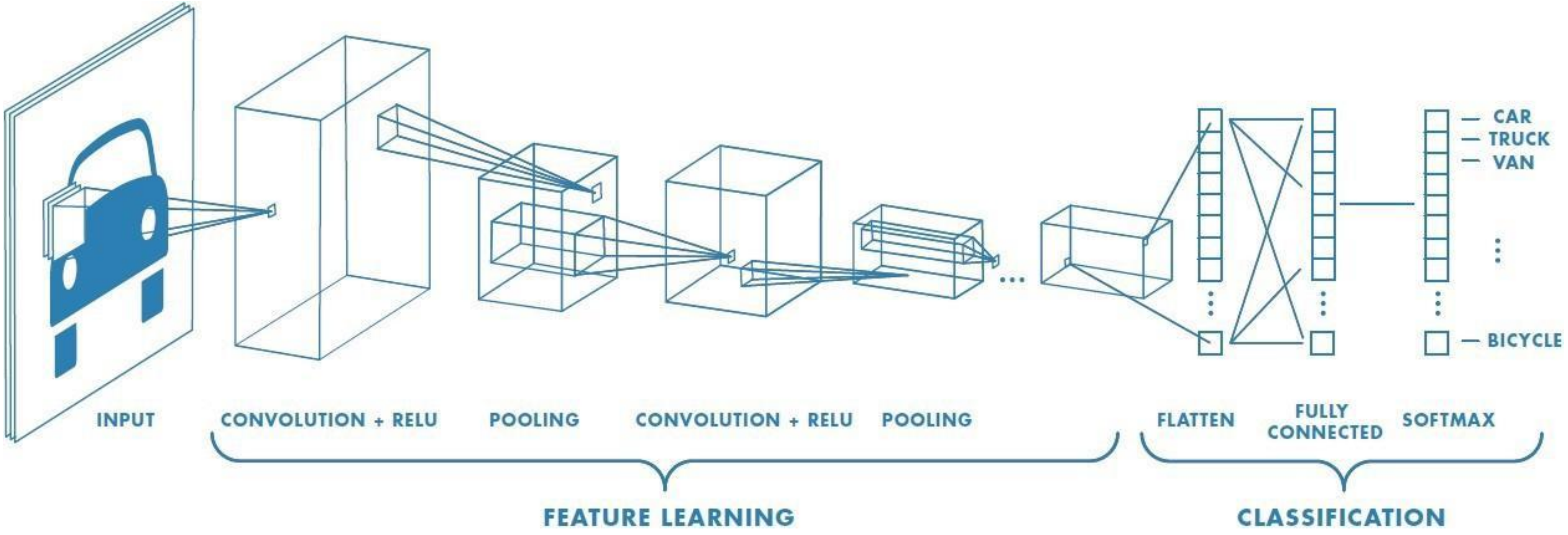


Energy-Integrated Image



Propose Convolutional Neural Networks

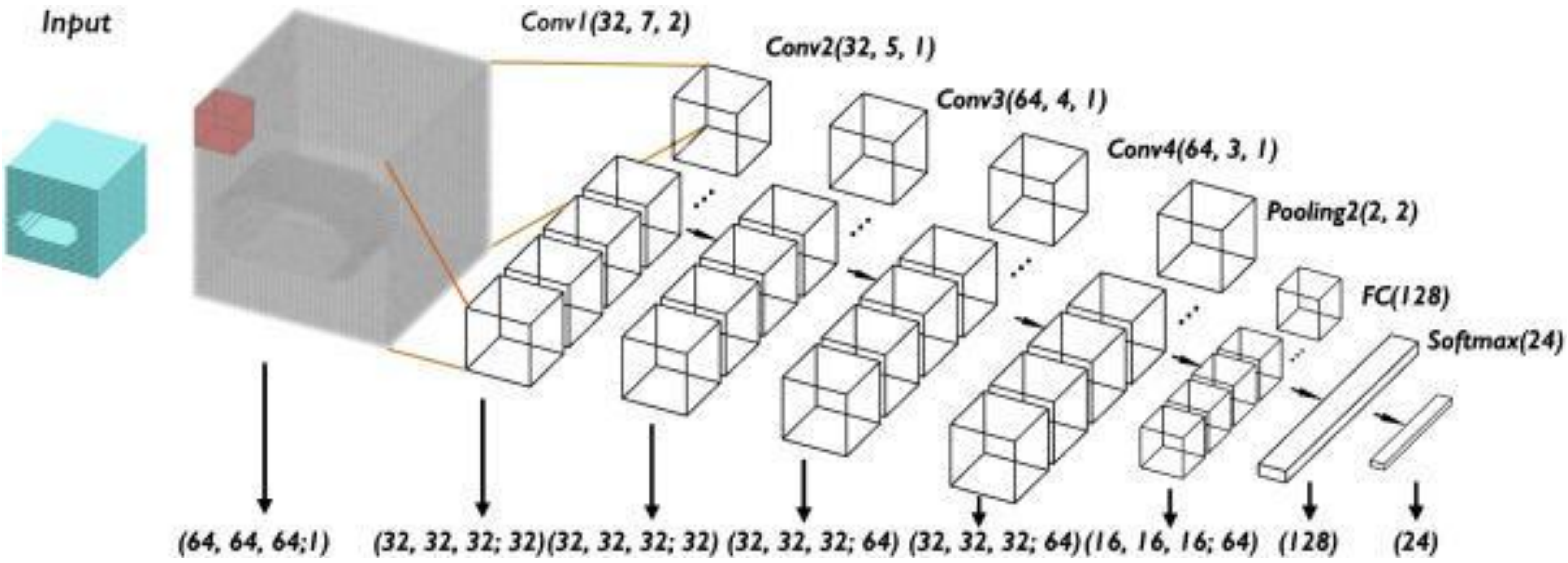
- First shown to thrive in image classification
- Uses notion of “filter” instead of normal connections
- Extracts “spatially” relevant features/patterns in data
- Not just limited to space. Now used for temporal, etc.



[18] S. Saha (2018)

3D CNNs

- Spectral radiograph has 2 spatial, 1 energy dimension
- ResNet-34



[19] Z. Zhang et al (2018)

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What about the data?

- Deep learning needs thousands or millions of training examples

Experimental Data

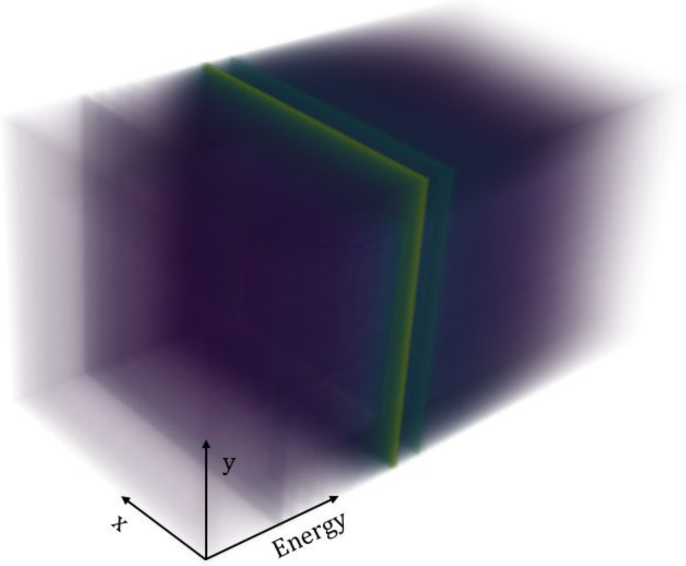
Pros:	Cons:
• Training set is representative of what it is trying to learn • No required post-processing (though may be useful)	• How well is the mass really understood? • Time consuming • Need diversity of examples

Simulated Data

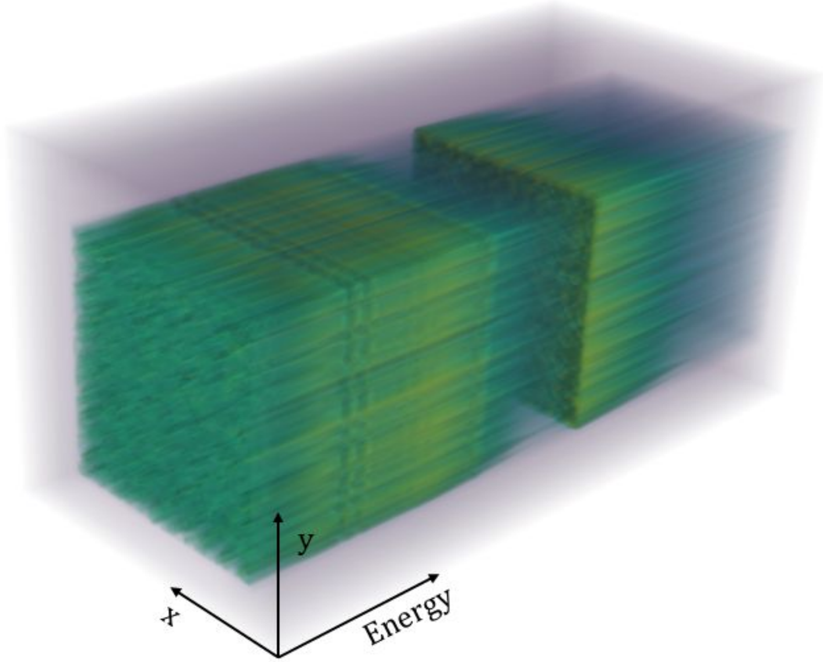
Pros:	Cons:
• Inexpensive • Know mass perfectly • Ability to add variation and expand dataset	• Not necessarily reflective of reality

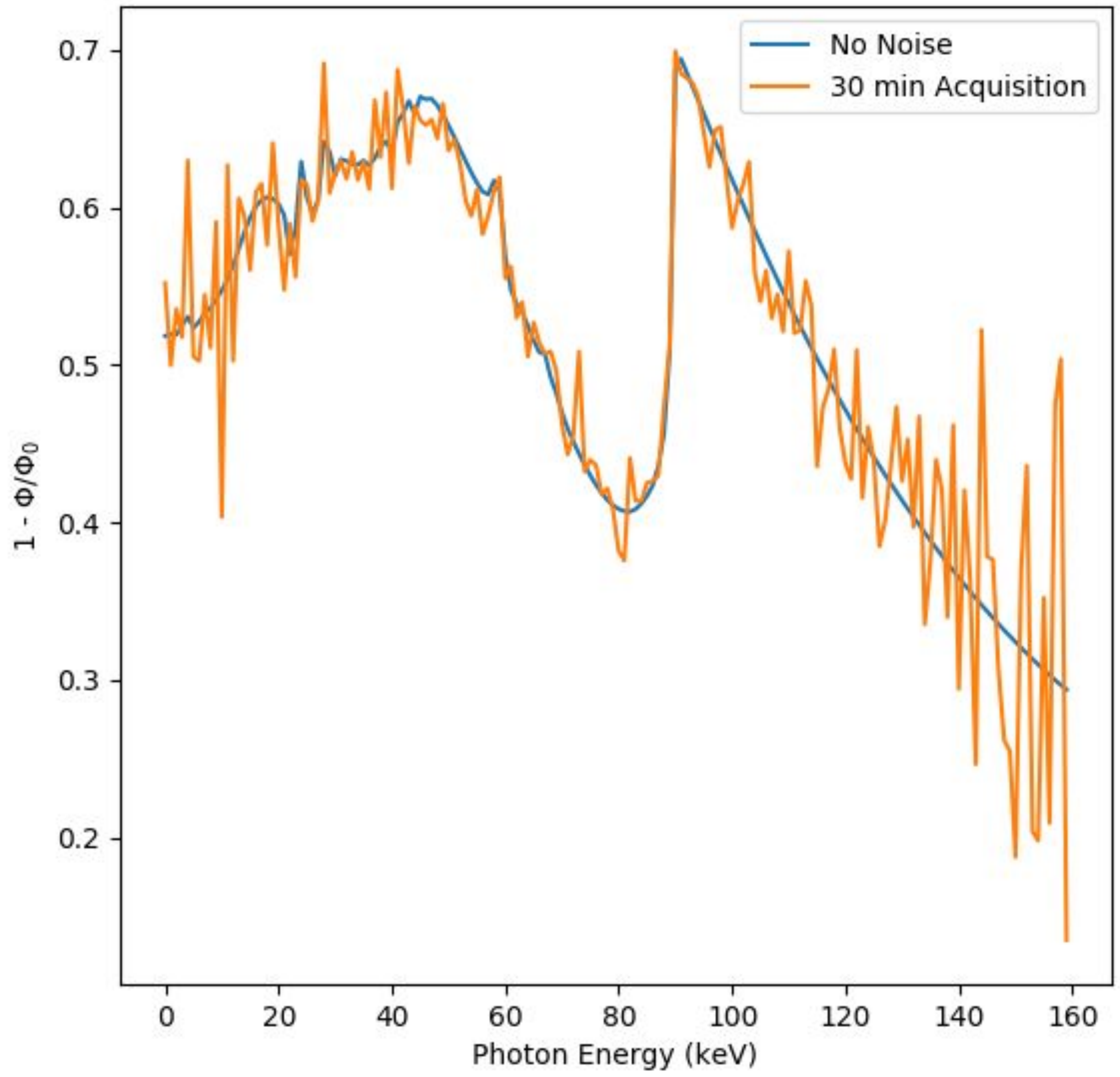
Examples of dataset

$\Phi(E)$

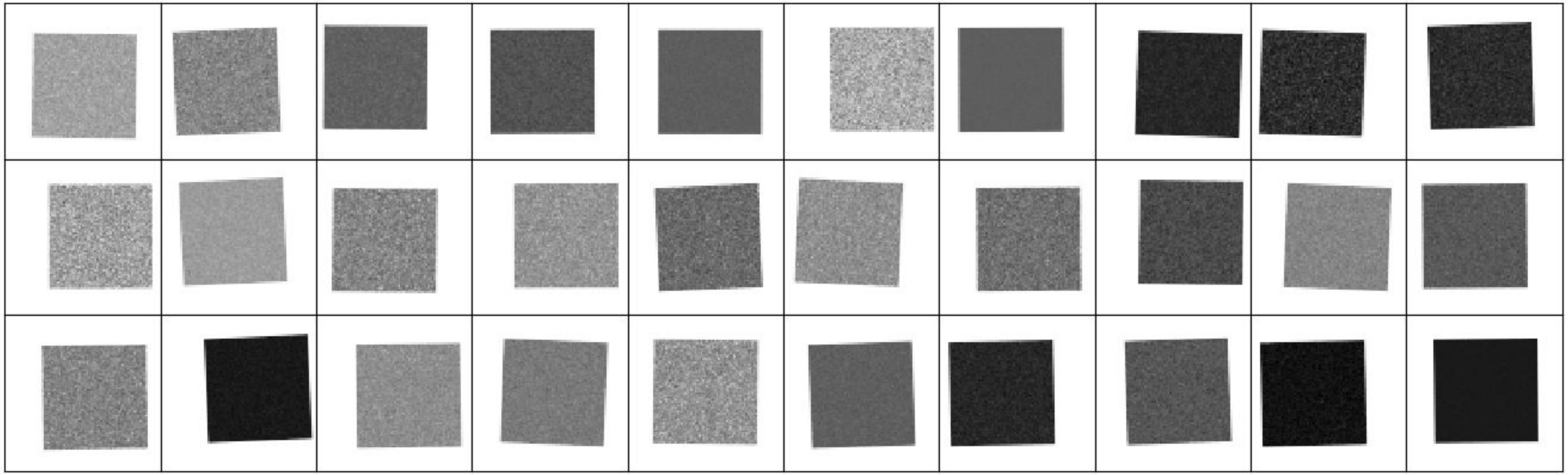


$$1 - \frac{\Phi(E)}{\Phi_0(E)}$$





Examples of dataset



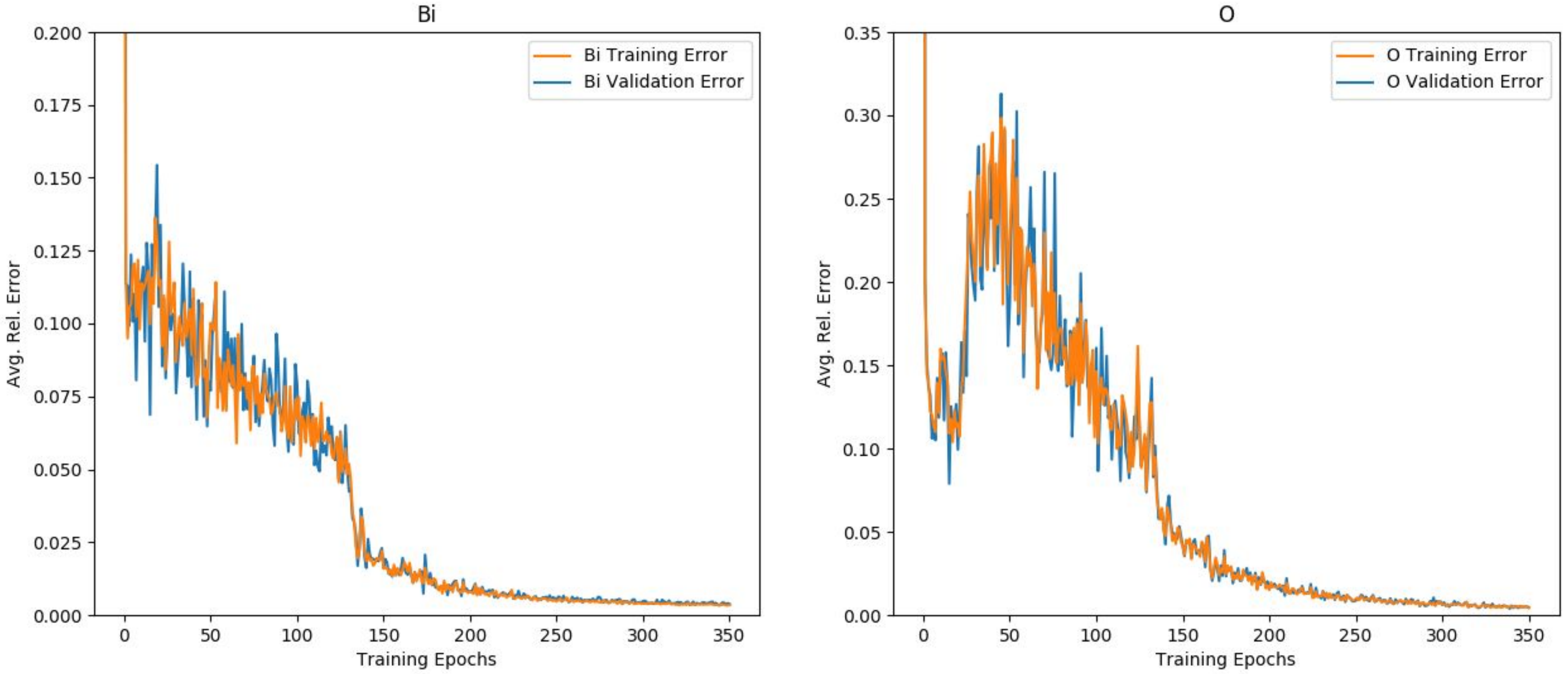
[20] S. Agostinelli et al (2003)
[21] J. Allison et al (2006)

Training and Validation Results: 1800 s

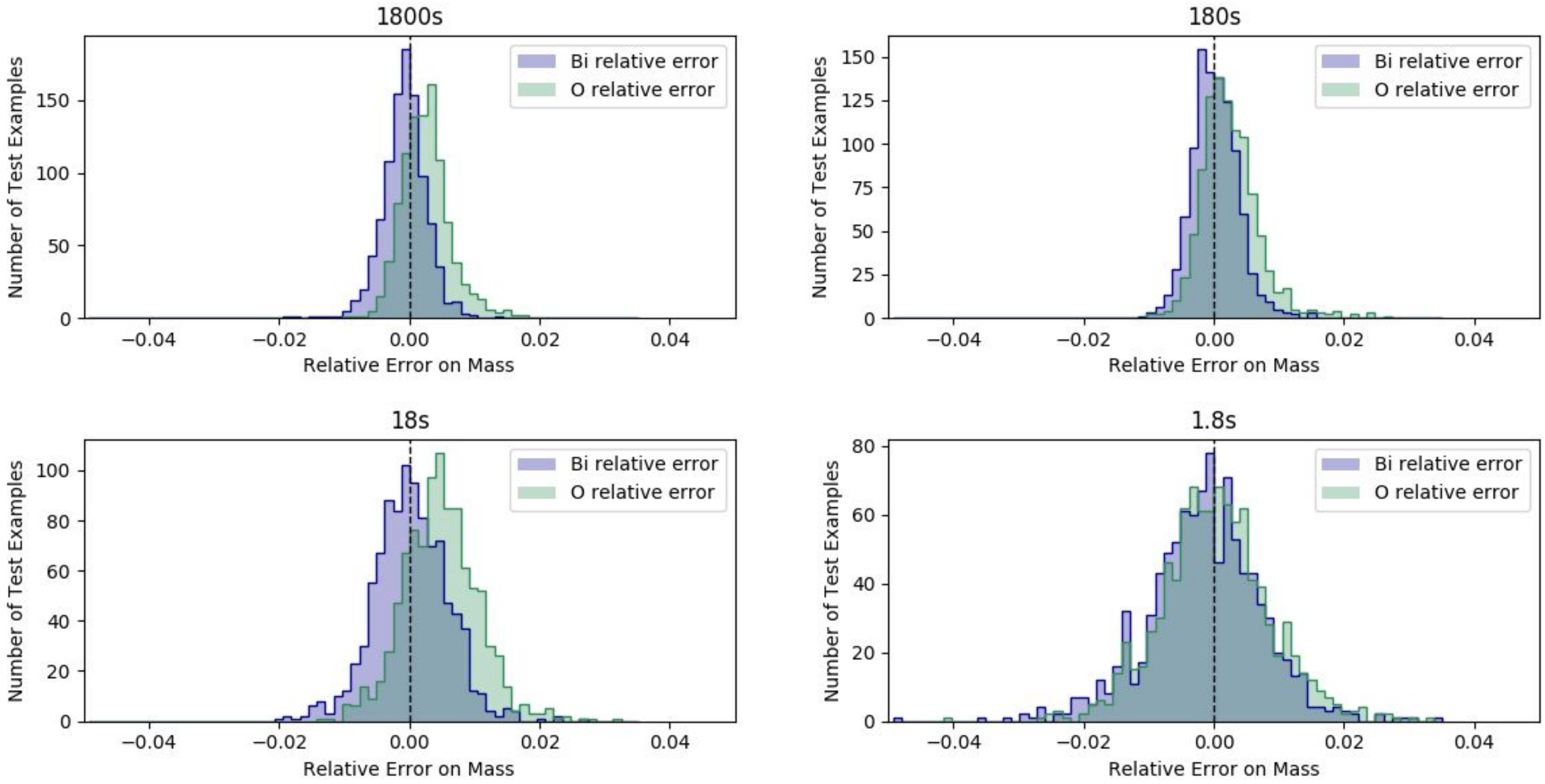
$$Rel.Error = \frac{\hat{y} - y}{y}$$

$\hat{y}$: calculated from network

y: ground truth



Relative Error Distribution on Test Dataset



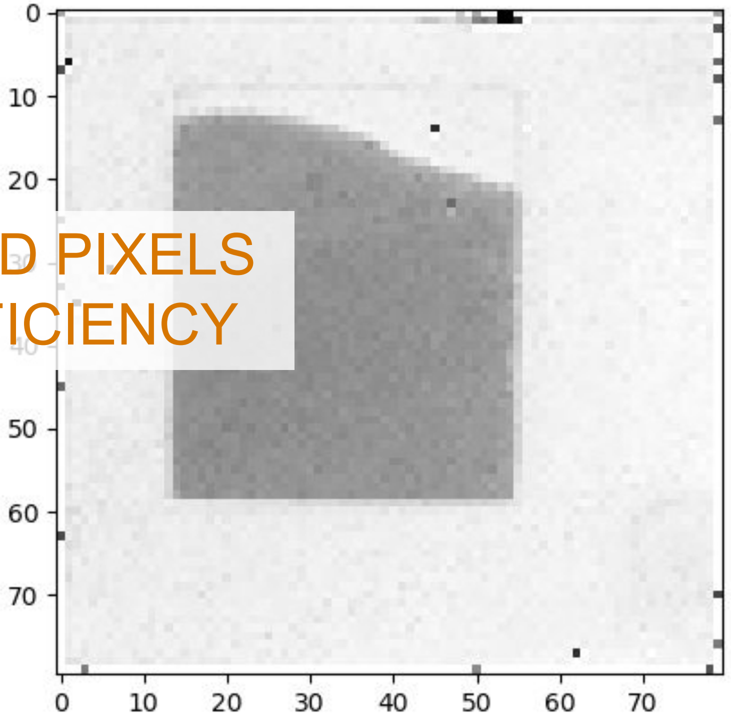
Conclusion

- Presented DL approach to mass quantification
  - Synthesized dataset using Monte Carlo
  - Transformed simulations via augmentation, DRF, noise
  - Applied 3D ResNet-34 CNN to predict mass
  - Tested on 4 acquisition durations

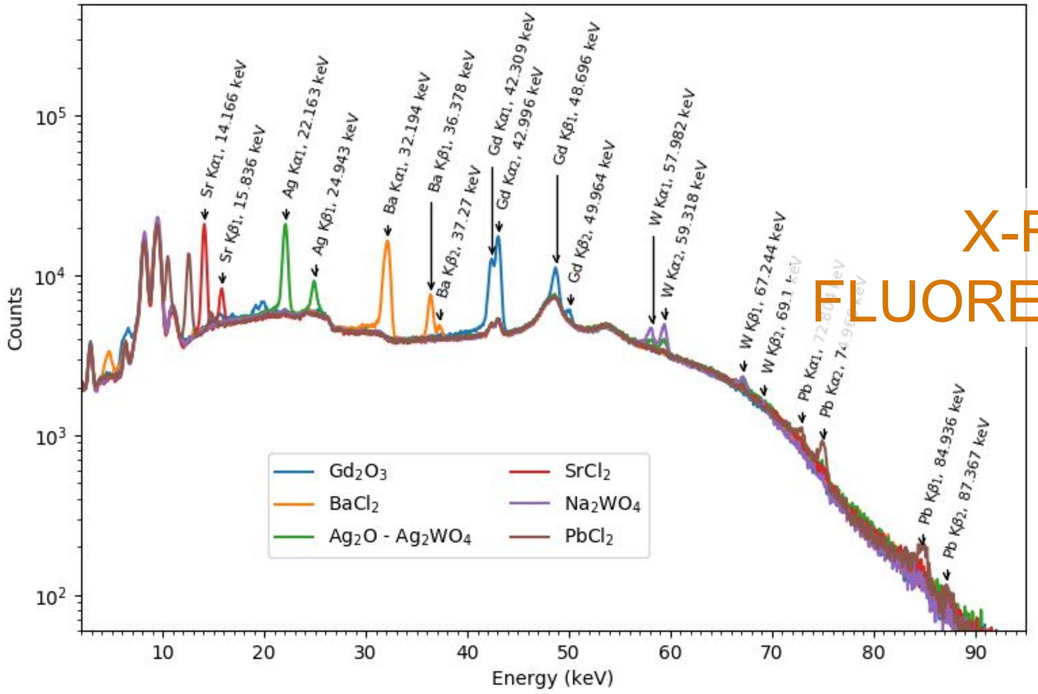
- Capable of average performance < 1% test error
  - Longer acquisitions gave had tighter distributions

Future Work

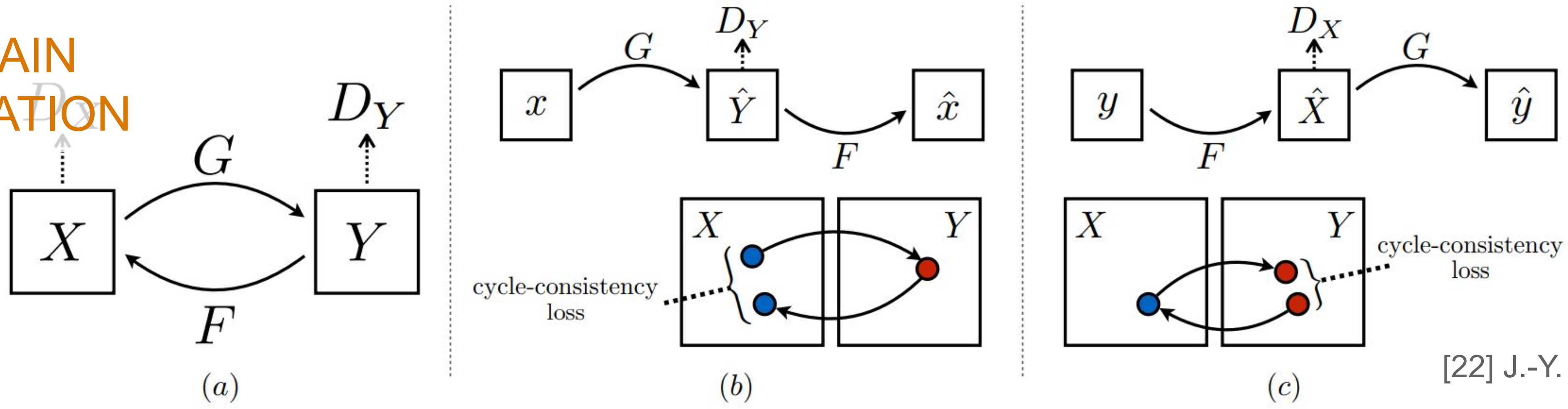
DEAD PIXELS
EFFICIENCY



X-RAY
FLUORESCENCE



DOMAIN
ADAPTATION



[22] J.-Y. Zhu et al (2017)

Acknowledgements

- Advisor: Anna Erickson, GT
- PNNL: Karl Pazdernik, Andy Gilbert, Ben McDonald, Deb Fagan, Rick Wittman, Alex Hagen, Becky Jones
- PNNL ASF Internship Program
- Nuclear Nonproliferation International Safeguards Graduate Fellowship:

  This research was performed under appointment to the Nuclear Nonproliferation International Safeguards Fellowship Program sponsored by the National Nuclear Security Administration's Office of International Nuclear Safeguards (NA-241).

- And all the PNNL staff that have been so helpful and patient

References

1. Roentgen, W. 1896 “The Invisible.” Published in New York Times article by Nicholas Bakalar, 2009.: https://www.nytimes.com/2009/06/16/health/16firs.html
2. “How does an airport scanner work?” in article by Richard Hodson. *Science Focus*. BBC Studios. https://www.sciencefocus.com/future-technology/how-does-an-airport-scanner-work/
3. Wang X, Peng Y, Lu L, Lu Z, Bagheri M, Summers RM. ChestX-ray8: Hospital-scale Chest X-ray Database and Benchmarks on Weakly-Supervised Classification and Localization of Common Thorax Diseases. IEEE CVPR 2017, http://openaccess.thecvf.com/content_cvpr_2017/papers/Wang_ChestX-ray8_Hospital-Scale_Chest_CVPR_2017_paper.pdf
4. Veale, Matthew & Seller, P & Wilson, Matthew & Liotti, Enzo. (2018). HEXITEC: A High-Energy X-ray Spectroscopic Imaging Detector for Synchrotron Applications. Synchrotron Radiation News. 31. 28-32. 10.1080/08940886.2018.1528431.
5. M. Firsching, P. T. Talla, T. Michel, and G. Anton, “Material resolving x-ray imaging using spectrum reconstruction with medipix2,” Nuclear Instruments and Methods in Physics Research A, vol. 591, no. 1, pp. 19–23, 6 2008.
6. J. Rinkel, G. Beldjoudi, V. Rebuffel, C. Boudou, P. Ouvrier-Buffet, G. Gonon, L. Verger, and A. Brambilla, “Experimental evaluation of material identification methods with cdte x-ray spectrometric detector,” IEEE Transactions on Nuclear Science, vol. 58, no. 5, pp. 2371–2377, 10 2011.
7. G. G. Poludniowski and P. M. Evans, “Calculation of x-ray spectra emerging from an x-ray tube. part i. electron penetration characteristics in x-ray targets,” Medical Physics, vol. 34, no. 6 Part1, pp. 2164–2174. [Online]. Available: https://aapm.onlinelibrary.wiley.com/doi/abs/10.1118/1.2734725
8. Berger, M.J., Hubbell, J.H., Seltzer, S.M., Chang, J., Coursey, J.S., Sukumar, R., Zucker, D.S., and Olsen, K. (2010), XCOM: Photon Cross Section Database (version 1.5). [Online] Available: http://physics.nist.gov/xcom [2019, April 26]. National Institute of Standards and Technology, Gaithersburg, MD.
9. “Medipix2: a 64-k pixel readout chip with 55-um square elements working in single photon counting mode,” IEEE Transactions on Nuclear Science, vol. 49, no. 5, pp. 2279–2283, 12 2002.
10. G. Beldjoudi, V. Rebuffel, V. Kaftandjian, and J. Rinkel, “Multidimensional data processing methods for material discrimination using an ideal x-ray spectrometric photon counting system,” IEEE Nuclear Science Symposium and Medical Imaging Conference, pp. 3808–3815, 10 2010.
11. E. S. Jimenez, L. J. Orr, M. L. Morgan, and K. R. Thompson, “Exploring mediated reality to approximate x-ray attenuation coefficients from radiographs,” vol. 9215, 8 2014.
12. E. S. Jimenez, L. J. Orr, and K. R. Thompson, “Object composition identification via mediated-reality supplemented radiographs,” IEEE Nuclear Science Symposium and Medical Imaging Conference (NSS/MIC), 11 2014.
13. N. Collins, E. S. Jimenez, and K. R. Thompson, “Material identification with multichannel radiographs,” AIP Conference Proceedings, vol. 1806, no. 1, p. 130004, 2017.

References

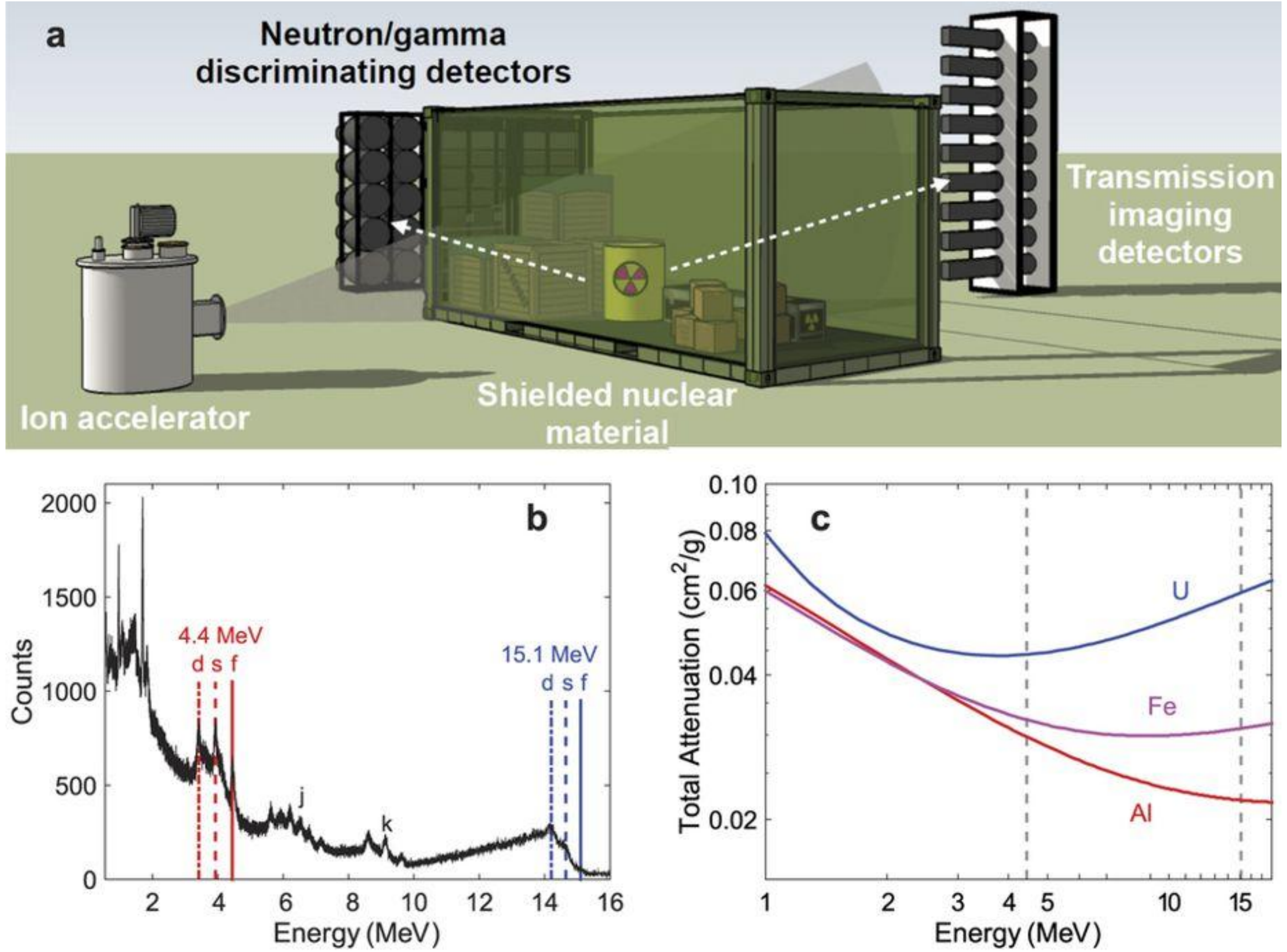
14. E. S. Jimenez, N. M. Collins, E. A. Holswade, M. L. Devonshire, and K. R. Thompson, “Developing imaging capabilities of multi-channel detectors comparable to trditional x-ray detector technology for industrial and security applications,” SPIE Optical Engineering + Applications, p. 99690A, 10 2016.
15. A. J. Gilbert, B. S. McDonald, S. M. Robinson, K. D. Jarman, T. A. White, and M. R. Deinert, “Non-invasive material discrimination using spectral x-ray radiography,” Journal of Applied Physics, vol. 115, p. 154901, 4 2014.
16. A. J. Gilbert, B. S. McDonald, and M. R. Deinert, “Advanced algorithms for radiographic material discrimination and inspection system design,” Nuclear Instruments and Methods in Physics Research, vol. 385, pp. 51–58, 2016.
17. A. J. Gilbert, B. S. McDonald, and L. E. Smith, “Spectral x-ray radiography for safeguards at nuclear fuel fabrication facilities: A feasibility study,” 2017 International Conference on Mathematics and Computational Methods Applied to Nuclear Science and Engineering, 2017.
18. S. Saha. “A Comprehensive Guide to Convolutional Neural Networks – the ELI5 Way.” (2018) Article in *Towards Data* Science. https://towardsdatascience.com/a-comprehensive-guide-to-convolutional-neural-networks-the-eli5-way-3bd2b1164a53
19. Zhibo Zhang, Prakhar Jaiswal, Rahul Rai, FeatureNet: Machining feature recognition based on 3D Convolution Neural Network, Computer-Aided Design, Volume 101, 2018, Pages 12-22, ISSN 0010-4485, https://doi.org/10.1016/j.cad.2018.03.006. (http://www.sciencedirect.com/science/article/pii/S0010448518301349)
20. S. Agostinelli et al., “Geant4—a simulation toolkit,” Nuclear Instruments and Methods in Physics Research, vol. 506, p. 250–303, 2003.
21. e. a. J. Allison, “Geant4 developments and applications,” IEEE Transactions on Nuclear Science, vol. 53, pp. 270–278, 2006.
22. J.-Y. Zhu, T. Park, P. Isola, and A. A. Efros. “Unpaired image-to-image translation using cycle-consistent adversarial networks.” *arXiv preprint arXiv:1703.10593, 2017.*
23. P. B. Rose, A. S. Erickson, M. Mayer, J. Nattress, and I. Javanovic, “Uncovering special nuclear material by low-energy nuclear reaction imaging,” Scientific Reports, vol. 6, p. 24388, 4 2016.14
24. He, Kaiming; Zhang, Xiangyu; Ren, Shaoqing; Sun, Jian (2015-12-10). "Deep Residual Learning for Image Recognition". *arXiv:1512.03385.* https://arxiv.org/pdf/1512.03385.pdf

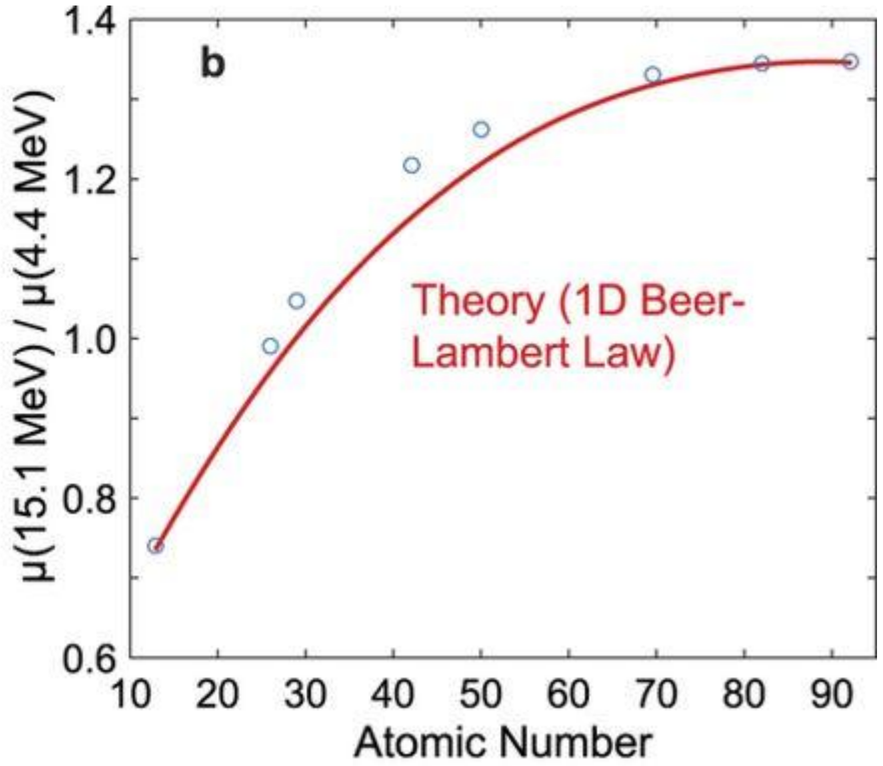
Thank you

Numerical Approaches: Transmittance Logarithm

Georgia Tech and Penn State

$$\frac{\ln T(E_1)}{\ln T(E_2)} = \frac{\mu(E_1)}{\mu(E_2)}$$





[23] P. B. Rose et al (2016)

ResNet-34

- Skip Connections:
  - Help with vanishing gradient problem
- Adapted to 3D convolutions
- Implemented in TensorFlow
- Input: Spectral Radiograph
- Output: Elemental Mass

[24] K. He et al. (2015)