Contract No:

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Disclaimer:

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$FA_3Bi_2I_9$: An emerging Lead-Free Perovskite for Radiation Detection

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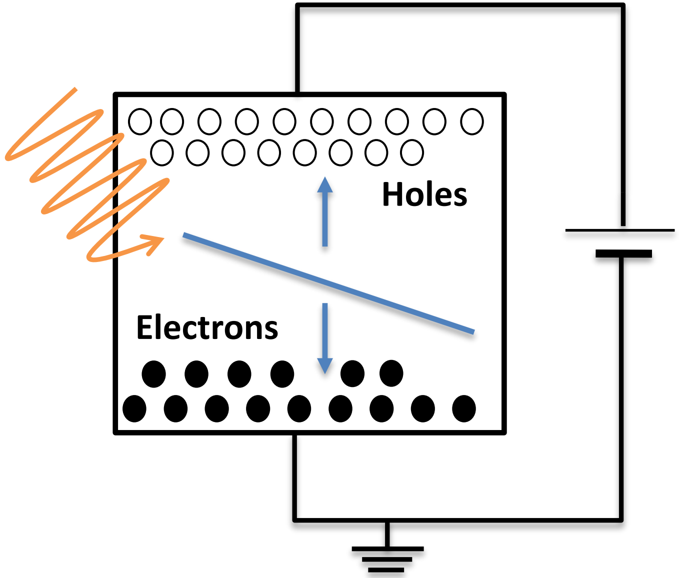
Outline

- Background and Motivation
- Study Approach
  - Crystal Growth
  - General Properties
  - Electrical Characteristics
  - X-ray Response
  - Mechanical Properties
- Conclusion and Future Study

Background and Motivation (1/3)

Ionizing radiation detector R&D --- driven by applications

- Homeland security
- Medical diagnosis
- Industrial nondestructive inspection, etc.



Semiconductor Detector (Direct detection)

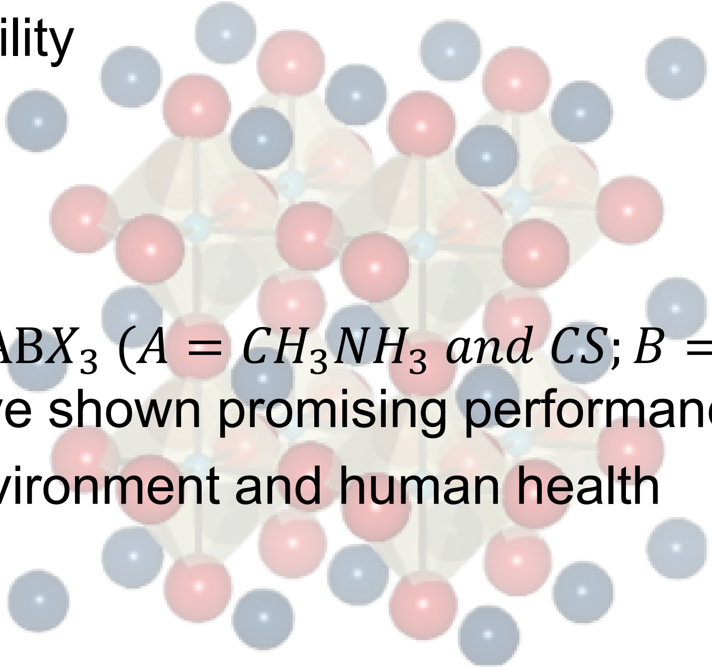
- High detection efficiency
- Tunable bandgap
- Excellent charge transport properties

➡ **Compared to indirect detection systems such as scintillators, semiconductor radiation detectors can offer much higher energy resolution**

Background and Motivation (2/3)

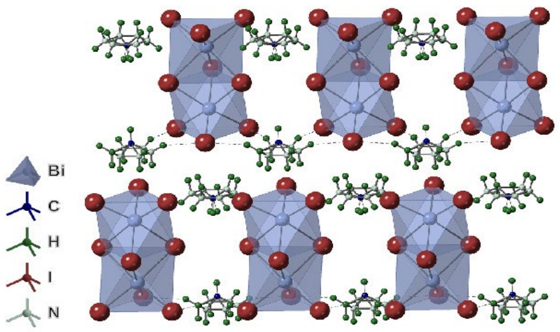
- **Perovskite: a new class of radiation detector material**
  - High stopping power & absorption coefficient
  - Long carrier lifetime & High carrier mobility
  - Cost-effective manufacturing process

- **Lead (Pb)-based Perovskites**
  - Lead (Pb)-based perovskites, such as $\mathrm{AB}X_3$ $(A = CH_3NH_3\ and\ CS; B = Pb\ and\ Sn; X = I, Br, and\ Cl)$ family, have shown promising performance.
  - However, the toxicity of lead to both environment and human health poses realistic concerns.



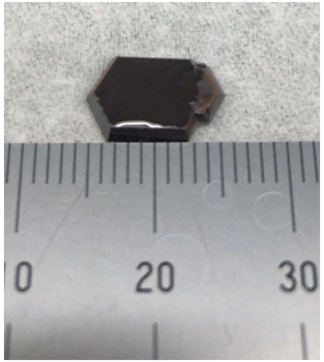
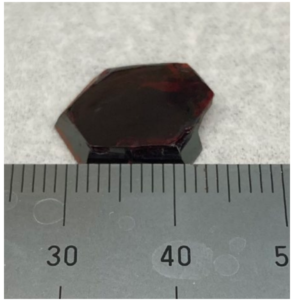
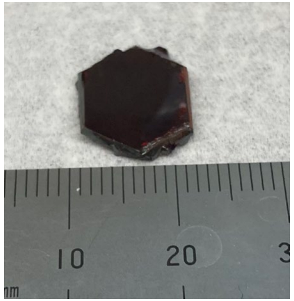
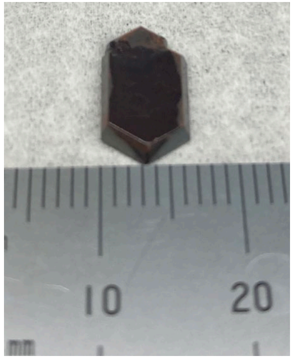
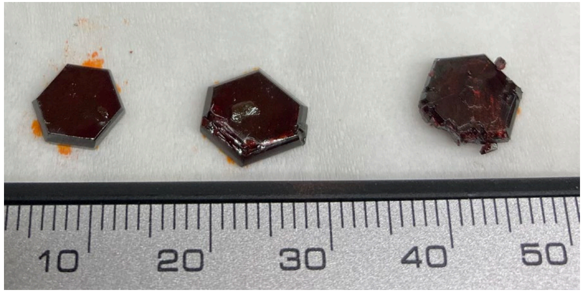
Background and Motivation (3/3)

- $FA_3Bi_2I_9$: **Lead-free formamidinium bismuth iodide perovskite** $(FA = CH(NH_2)_2)$
  - One of the $A_3Bi_2I_9$ $[A = Cs, MA\ (= CH_3NH_3)]$ perovskites family
  - Bismuth (Bi)-based perovskite: Non-toxic
  - Reasonable bandgap: ~2.1 eV
  - Material availability with high resistivity
  - Controllable growth and fabrication processes
  - $\mathrm{FA_3Bi_2I_9}$ thin films were first explored by Lan et al. for solar cells in 2019
  - Potential X-ray detection was proposed by Li et al. in 2021



W. Li, D. Xin, S. Tie, J. Ren, S. Dong, L. Lei and W. H. Zhang, Zero-Dimensional Lead-Free FA3Bi2I9 Single Crystals for High-Performance X-ray Detection, J. Phys. Chem. Lett., 2021, 12(7), 1778–1785.

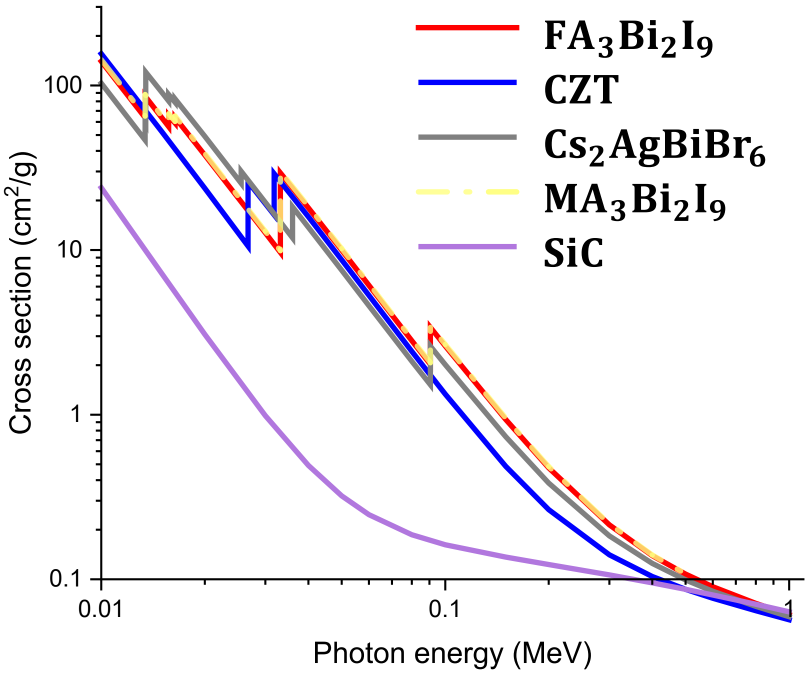
We successfully grew large $FA_3Bi_2I_9$ Crystals

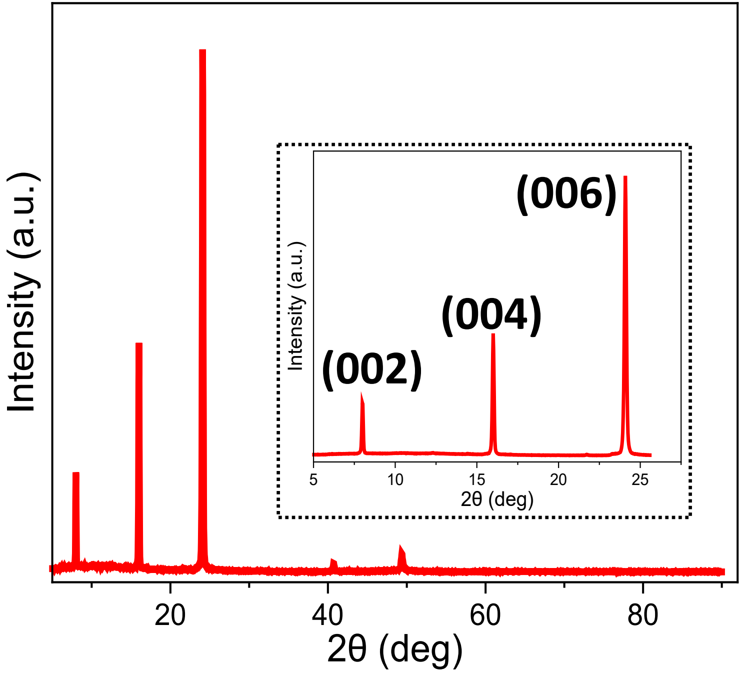
- Color: Dark-red
- Shape: hexagonal
- Size:
  - Area: up to $1.5 \times 1.5\ cm^2$
  - Thickness: up to $3\ mm$

General Properties of as-grown $FA_3Bi_2I_9$ Crystals

- Cross-section Data from XCOM

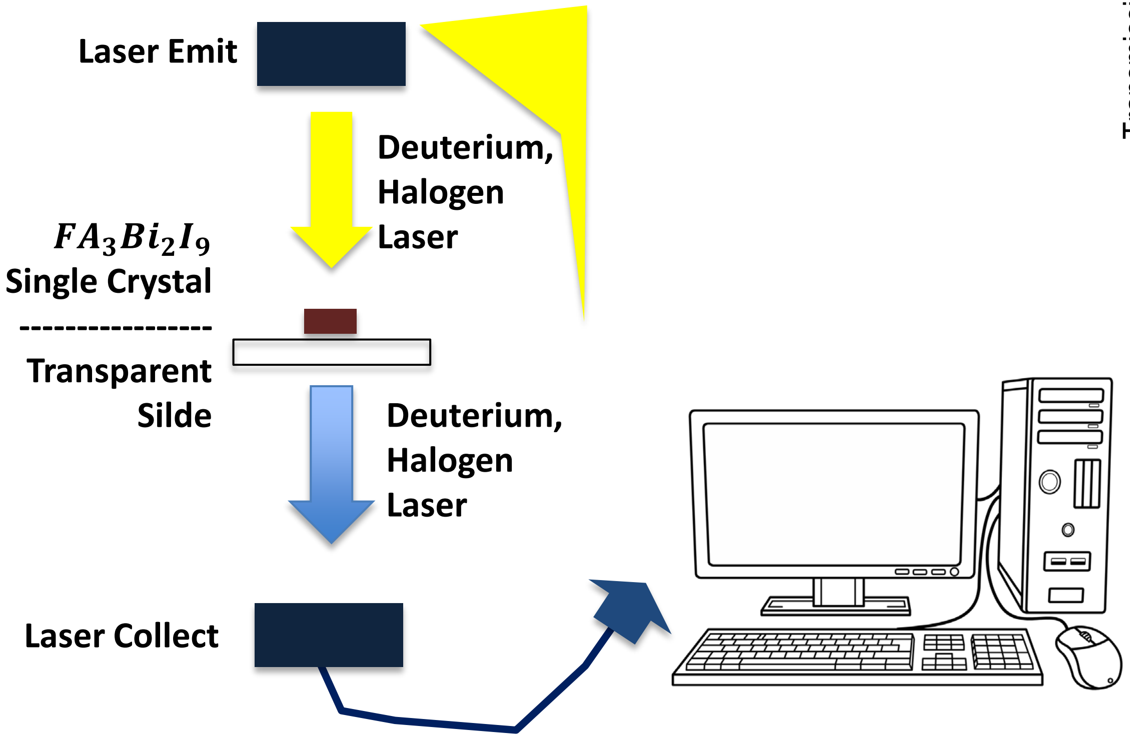


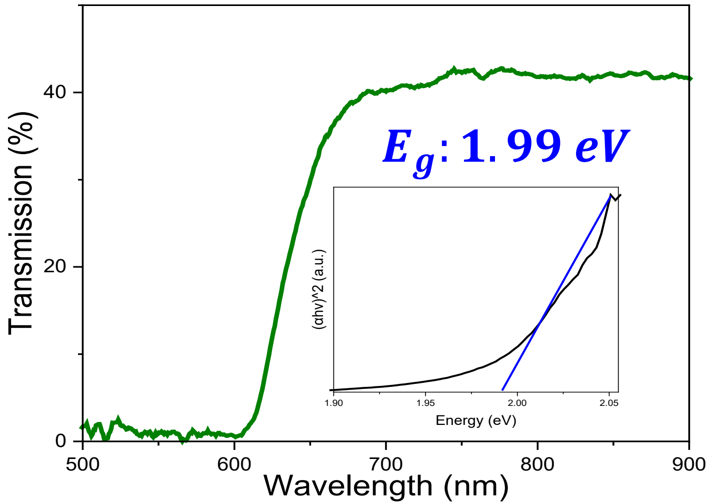
- Single Crystal XRD Results



General Properties (2/2)

- UV-vis measurement for bandgap





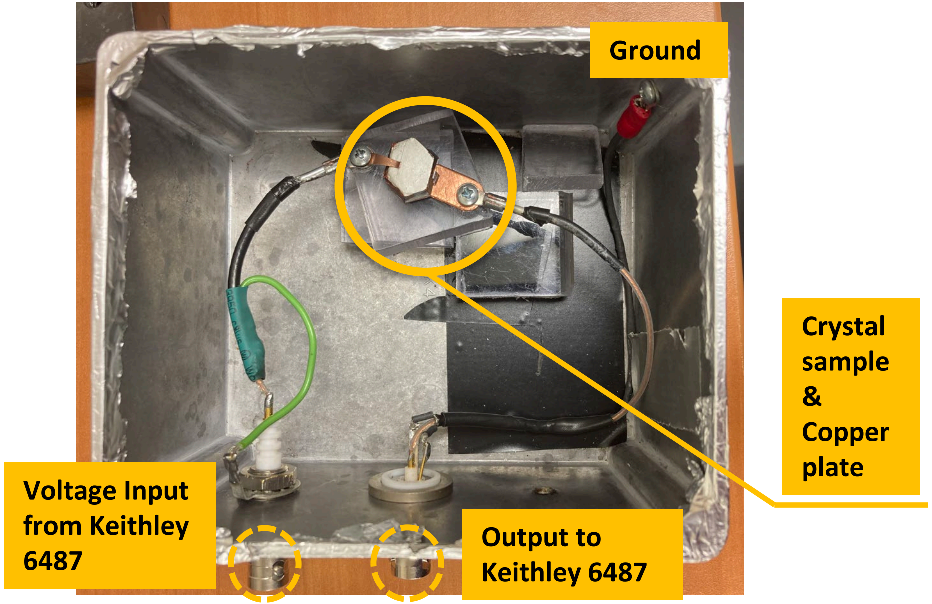
Tauc Equation

$$(\alpha \cdot hv)^{1/\gamma} = B(hv - E_g)$$

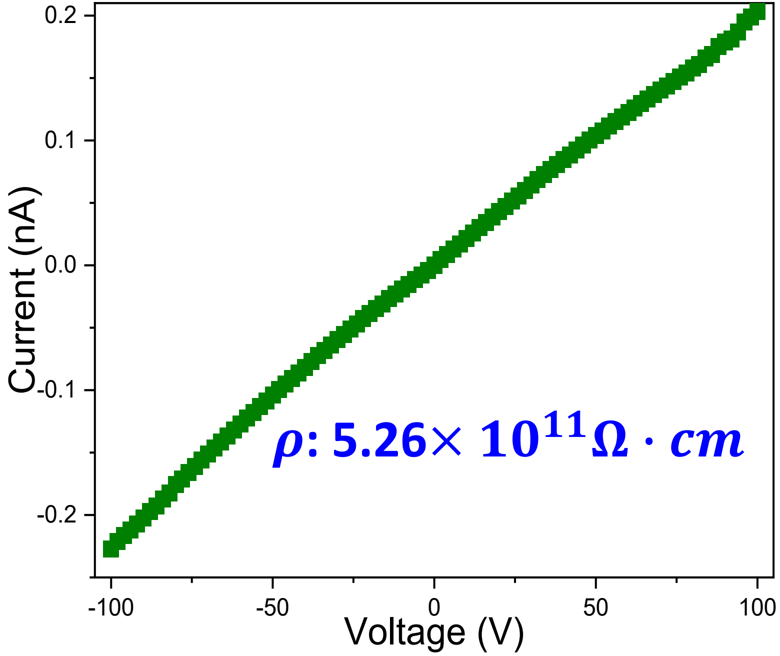
- α: absorption index
- γ: ½ for direct bandgap,
  2 for indirect bandgap

Electrical Properties (1/2)

- Fabrication of Ag/$FA_3Bi_2I_9$/Ag Detector Device
- Test Box

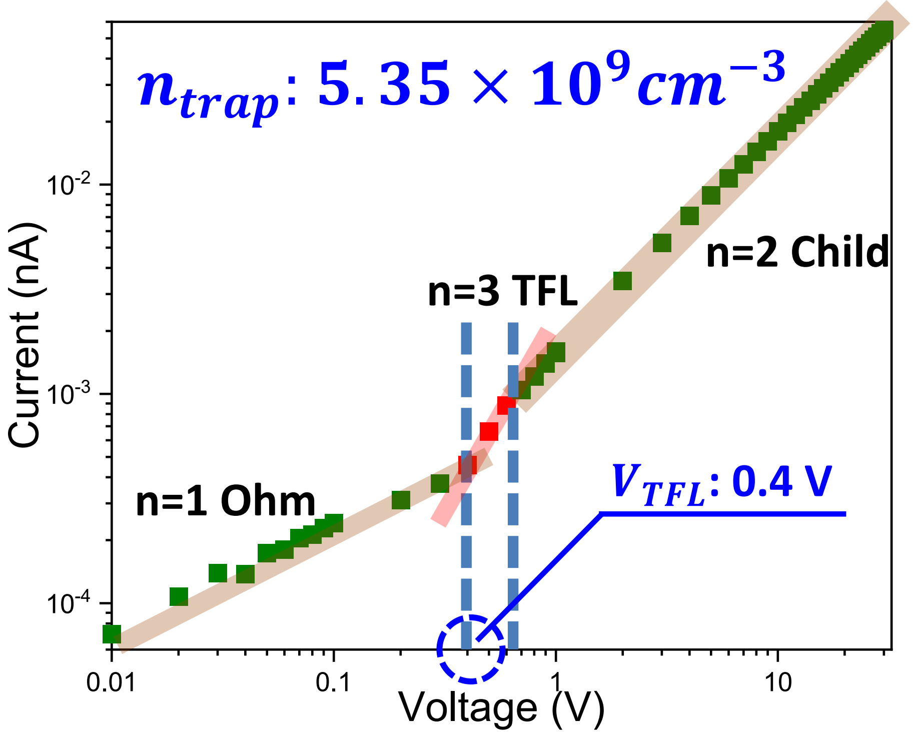


- Resistivity



Electrical Properties (2/2)

- **Space-charge-limited current (SCLC)**

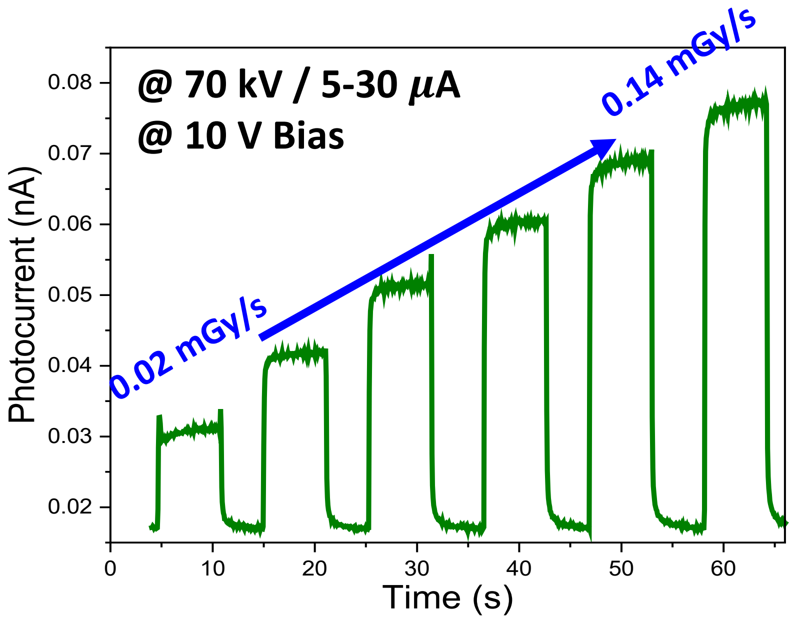


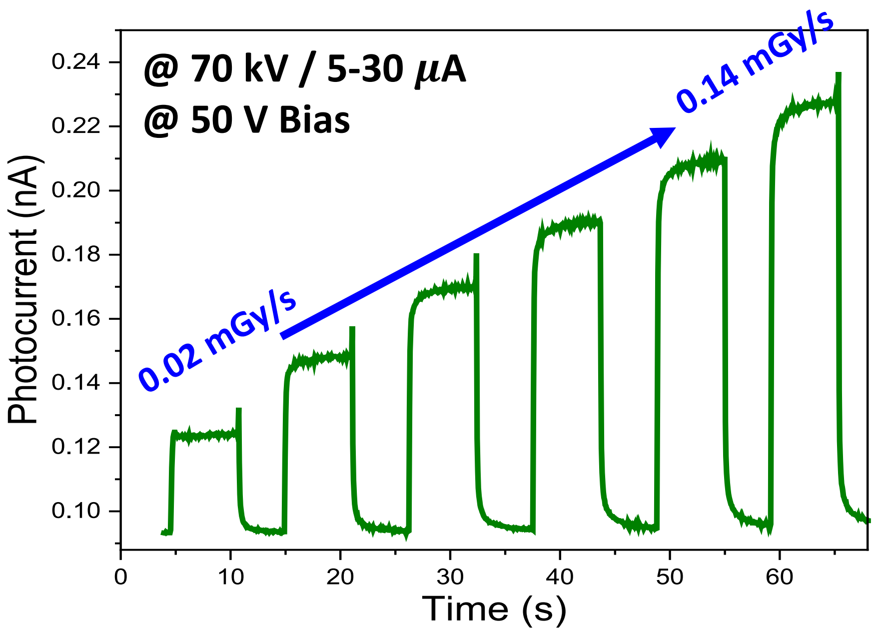
$$V_{TFL} = \frac{q n_{trap} L^2}{\varepsilon_0 \varepsilon_r}$$

- n_{trap}: Trap density
- L: Sample thickness
- V_{TFL}: Trap-filled limit voltage
- ε_0: Vacuum dielectric constant
- ε_r: Relative dielectric constant

X-ray Response

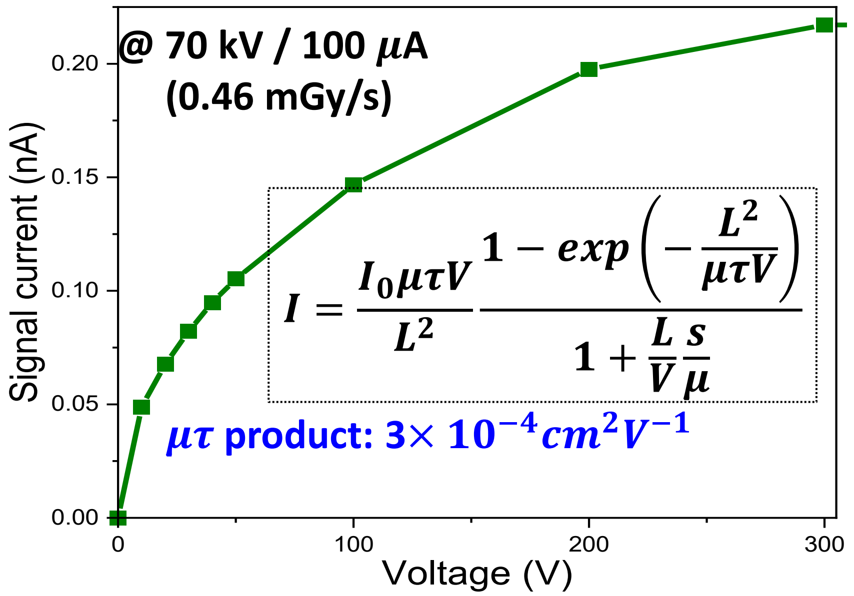
- X-ray Response Linearity





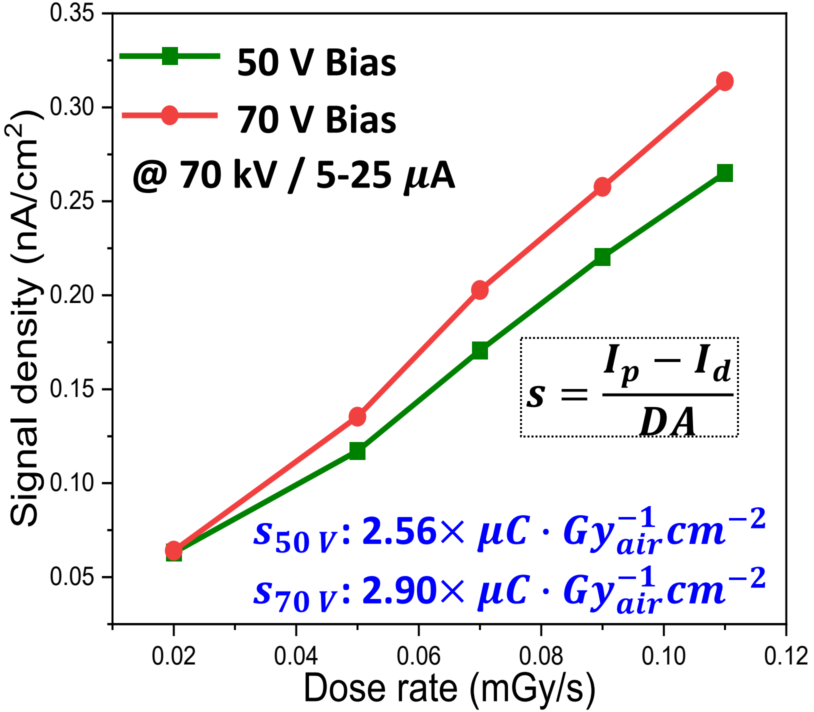
X-ray Response

- $\mu\tau$ product



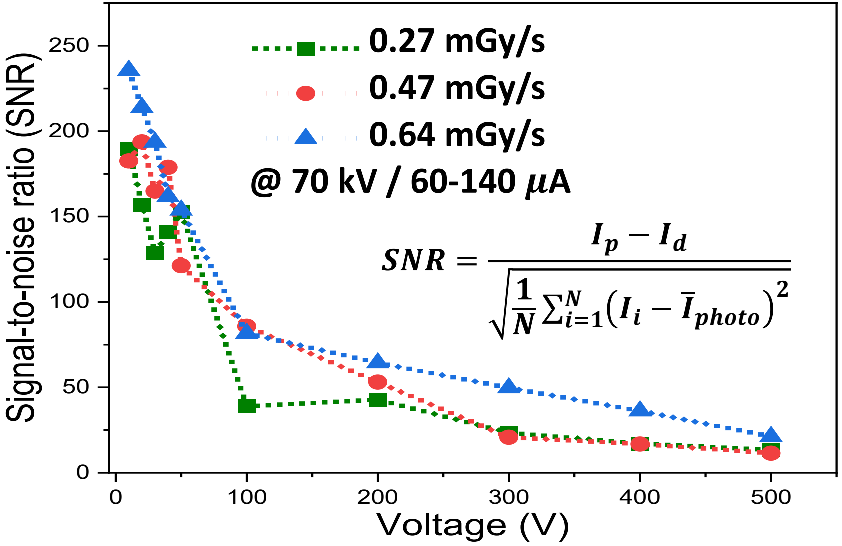
Saturated current (I_0) at around 300 bias voltage

- Sensitivity



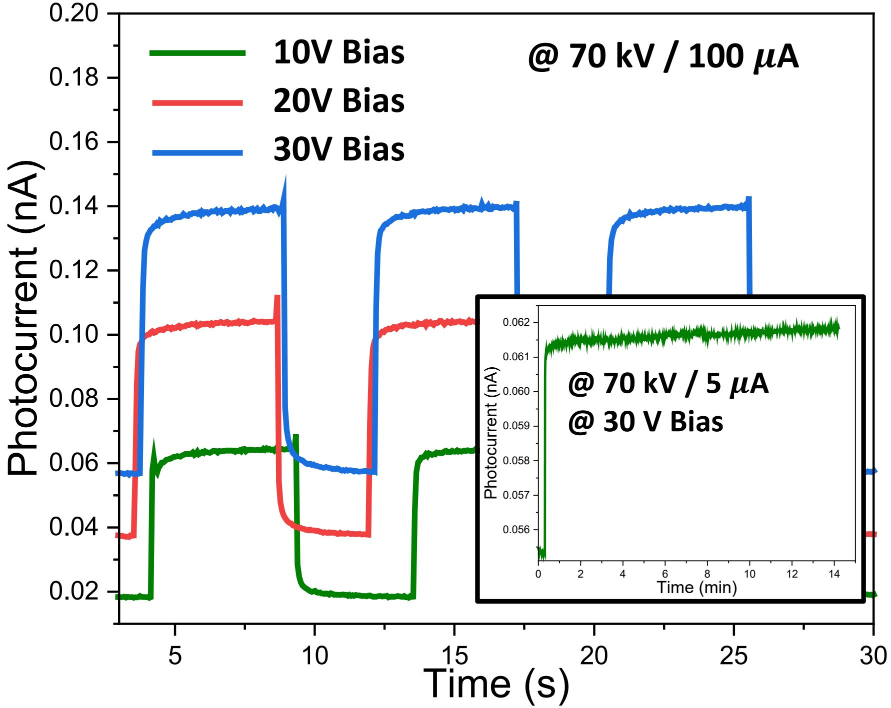
X-ray Response

- Signal-Noise Ratio (SNR) of current



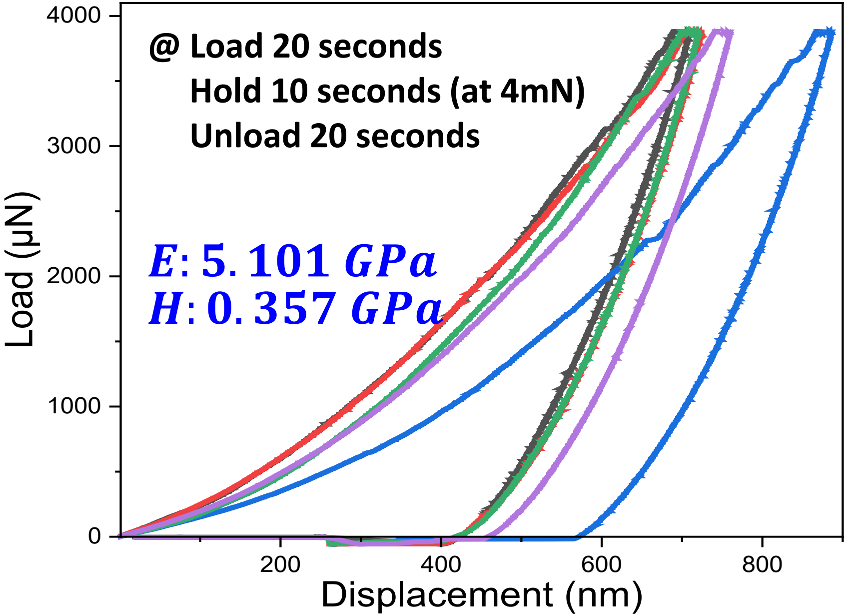
SNRs decreased until around 100 V bias. After 100 V bias, less change occurs.

- Bias Dependence and Stability



Mechanical Properties

- **Nanoindentation**



The {001} plane was selected for nanoindentation according to XRD results

Nanoindentation Results

- **Mean contact depth: 644.643 nm**
- **Std. dev of contact depth: 142.232 nm**

- **Mean hardness (H): 0.357 GPa**
- **Std. dev of hardness (H): 0.036 GPa**

- **Mean Young's modulus (E): 5.101 GPa**
- **Std. dev of Young's modulus (E): 0.42 GPa**

The values of hardness (H) and Young's modulus (E) are highly reliable with low standard deviation.

Conclusion

- **Conclusion**
  - Large $FA_3Bi_2I_9$ single crystals have been successfully grown.
  - Appropriate bandgap energy and high resistivity for radiation detector applications
  - High X-ray linearity and On/Off ratio, high $\mu\tau$ product, low trap density
  - Stability to long exposure of X-rays

  ➡ **$FA_3Bi_2I_9$ single crystals is a promising material for radiation detection**

- **On-going work**
  - Cathodoluminescence (CL) and photoluminescence (PL) measurements
  - Gamma-ray and alpha particle spectroscopy measurements
  - Stability measurements to different environment (humidity, temperature, etc.)

Thank you for your attention!