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Surface and Bulk Defect Control of $CsPbBr_3$ Single Crystals for Gamma-Ray Spectroscopy

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Introduction

- $CsPbBr_3$ single crystals combine strong X/γ-ray absorption with favorable carrier transport and room-temperature operation, making them promising semiconductor spectrometers [1,2]. High-resolution γ-ray measurements require efficient charge collection and low electronic noise [2,3].
- Crystal growth and detector fabrication inevitably introduce bulk impurities and surface damage into $CsPbBr_3$ single crystals, yet their effects on carrier transport and γ-ray detection remain insufficiently understood. This work investigates bulk impurity control and surface-state engineering to address these limitations.

Surface defect control

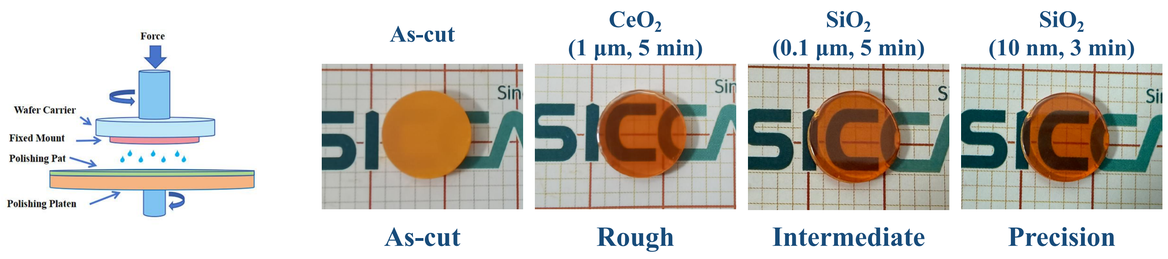


Figure 1. Polishing setup and evolution of the crystal surface

➢ Controlled polishing conditions (abrasive material and particle size, polishing time, pressure and rotation speed) yielded distinct surface states and defined the optimal processing window.

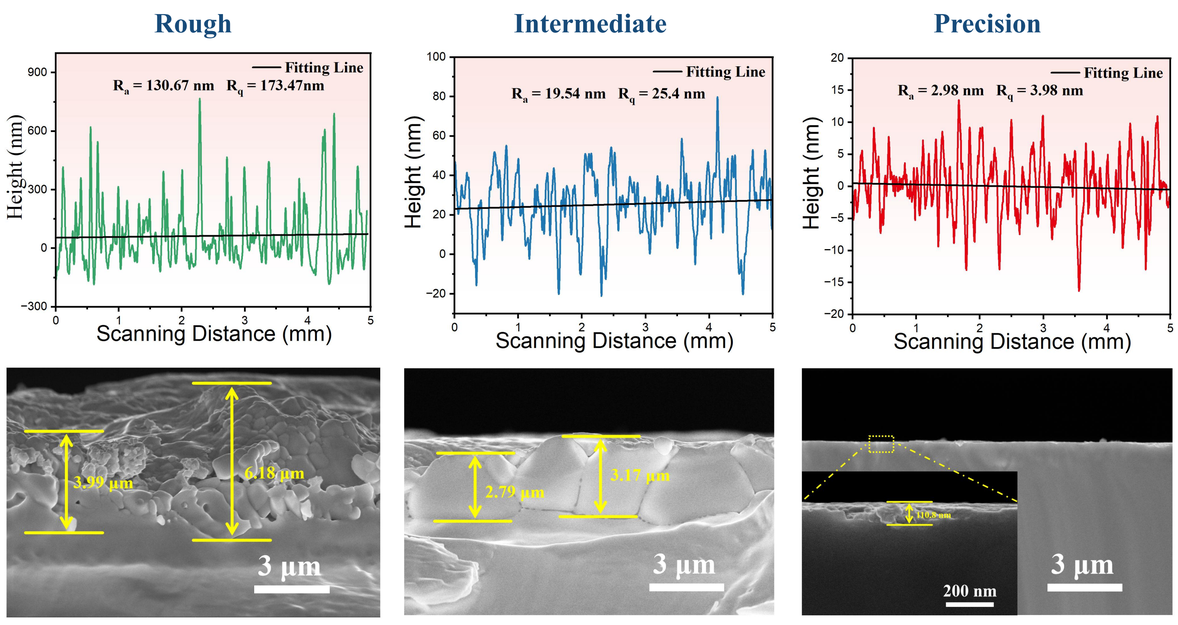


Figure 2. Surface profiles and cross-sectional damage after sequential polishing

➢ From intermediate to precision polishing, profilometric roughness decreases from 19.54 to 2.98 nm and the damage layer thins from about 3 μm to 110 nm.

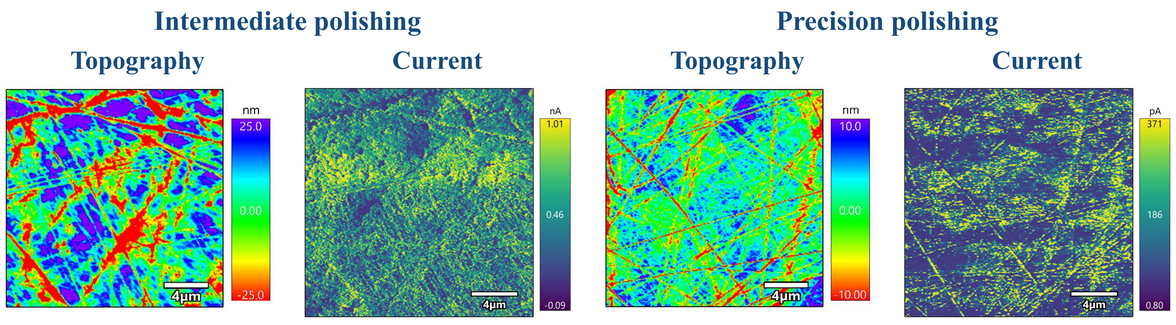


Figure 3. C-AFM topography and current maps at different surface states.

➢ Fewer scratches and local leakage paths accompany the reduced C-AFM current (from 338.1 to 141.2 pA), and the dark current decreases from 210 to 30.3 nA at 200 V.

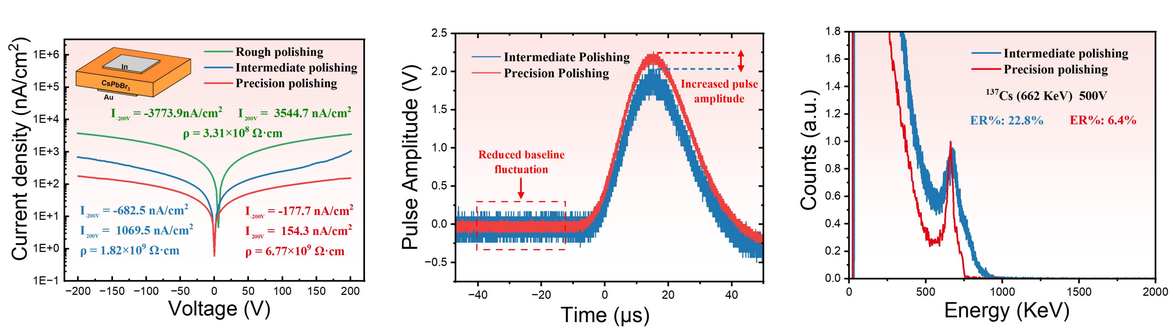


Figure 4. Comparison of current–voltage curves, pulse shapes, baseline noise and ^{137}Cs γ-ray spectra for different surface states.

➢ For the same detector under matched test conditions, energy resolution improves from 22.8% to 6.4% for ^{137}Cs 662 keV γ-rays at 500 V, consistent with higher resistivity and lower electronic noise.

Bulk impurity control

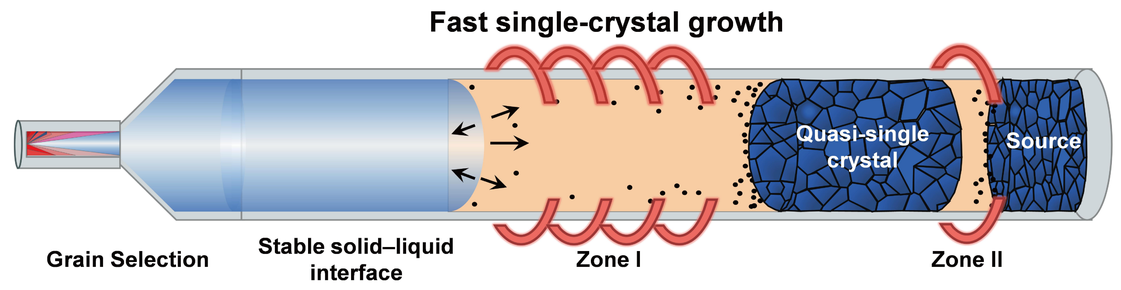


Figure 5. Dual-zone iterative refining and simultaneous crystal growth

➢ Iterative horizontal zone refining couples in situ purification with directional recrystallization to yield intact $CsPbBr_3$ single crystals at 25mm/h , a 25-fold increase over the Bridgman reference rate.

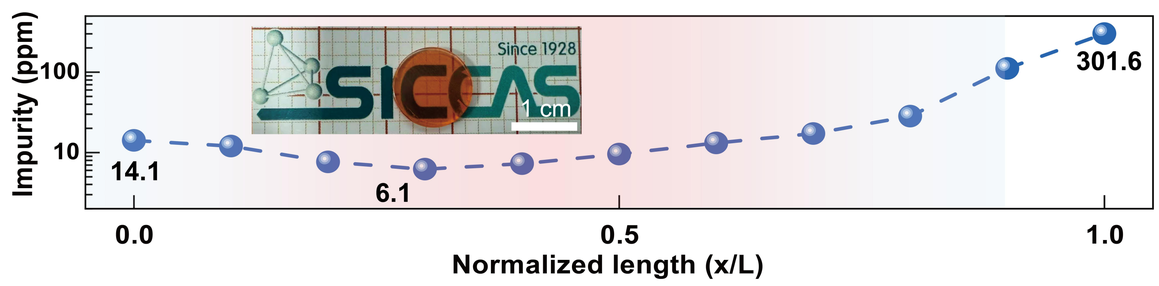


Figure 6. Axial variation in total impurity concentration

➢ Glow discharge mass spectrometry (GDMS) finds a minimum total impurity concentration of 6.1 ppm in the middle region.

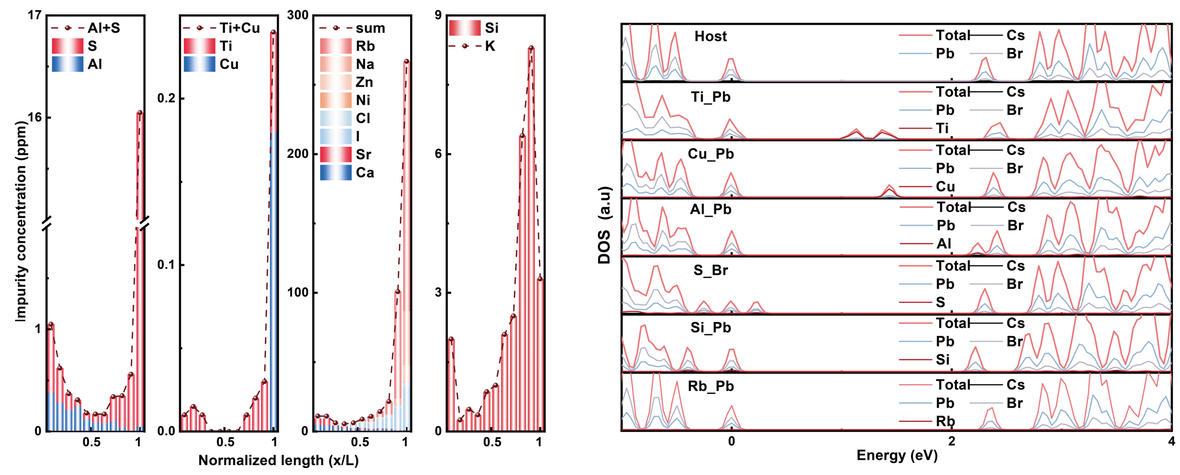
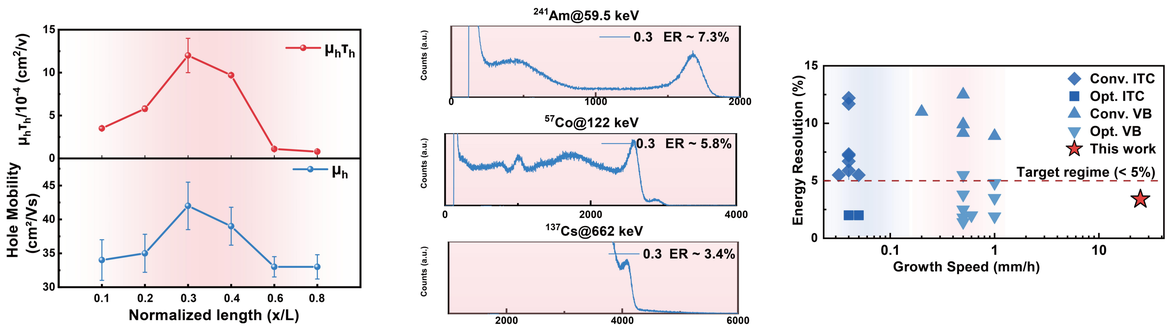


Figure 7. Axial elemental distributions and calculated densities of states

➢ GDMS analysis and DFT calculations revel that zone refining suppresses Cu- and Ti-related deep-level trapping, thereby improving charge transport.



Figures 8. Axial carrier transport, optimum γ-ray spectra, and energy resolution versus growth rate.

➢ Crystals from the middle region exhibit $\mu\tau = 1.2 \times 10^{-3}$ cm^2 V^{-1}, and the corresponding planar detectors achieve a best energy resolution of 3.4%.

Conclusions and Outlook

- **Surface optimization reduces conductive pathways and improves electrical performance, suppressing electronic noise and ultimately improving the signal-to-noise ratio and energy resolution.**
- **Iterative dynamic zone refining with synchronized dual-zone scanning directly yields high-quality $CsPbBr_3$ single crystals with low impurity concentrations.**
- **Bulk impurity control improves carrier transport, while surface damage removal suppresses leakage. Their combination could further enhance $CsPbBr_3$ γ-ray detector performance.**

References

[1] C. C. Stoumpos et al. Crystal growth of the perovskite semiconductor $CsPbBr_3$: a new material for high-energy radiation detection. *Cryst. Growth Des.* 13, 2722–2727 (2013). DOI: 10.1021/cg400645t.

[2] Y. He et al. High spectral resolution of gamma-rays at room temperature by perovskite $CsPbBr_3$ single crystals. *Nat. Commun.* 9, 1609 (2018). DOI: 10.1038/s41467-018-04073-3.

[3] Y. He et al. $CsPbBr_3$ perovskite detectors with 1.4% energy resolution for high-energy γ-rays. *Nat. Photonics* 15, 36–42 (2021). DOI: 10.1038/s41566-020-00727-1.

[4] J. Ma et al. Surface-state-dependent performance of $CsPbBr_3$ perovskite single crystals: from defect suppression to energy resolution enhancement. *J. Mater. Chem. C* (2026). DOI: 10.1039/d6tc01662f.