$Cs_3Cu_2I_5$ Single Crystals Grown with Oleic- and Formic-Acid-Assisted Additives: Effects on Crystal Quality and Scintillation Properties

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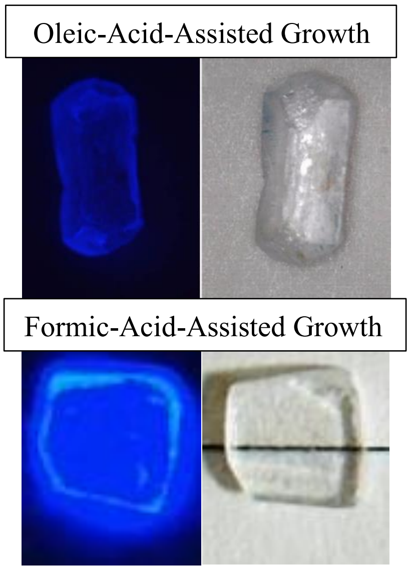
Copper-based halide perovskites such as $Cs_3Cu_2I_5$ have recently emerged as promising lead-free scintillator materials for ionizing radiation detection due to their large absorption coefficients, high light output, and low fabrication cost [1]. Solution-based growth methods, including inverse temperature crystallization and antisolvent recrystallization, have been explored for the synthesis of $Cs_3Cu_2I_5$ crystals. However, these approaches typically require stringent growth conditions, and the rapid, uncontrollable precipitation process often introduces structural defects, leading to reduced photoluminescence quantum yield [2,3]. Therefore, achieving a stable and well-controlled growth environment is essential for obtaining high-quality single crystals from solutions.



Photograph of $Cs_3Cu_2I_5$ SC under 254 nm UV lamp, and day light.

In this work, $Cs_3Cu_2I_5$ single crystals were grown at room temperature using a solvent evaporation method with two different organic acid additives: oleic acid and formic acid. The influence of these additives on crystal quality, optical properties, and scintillation performance was systematically investigated. Comprehensive structural and optical characterization was carried out using powder and single-crystal X-ray diffraction, photoluminescence emission and excitation spectroscopy, UV–visible absorption, photoluminescence decay measurements, scanning electron microscopy, and X-ray photoelectron spectroscopy. XPS analysis confirmed the absence of Cu^{2+} features in both samples, indicating that the use of organic acid additives effectively suppresses oxidation of Cu^{+} during crystal growth. Single-crystal X-ray diffraction revealed that crystals grown using formic-acid-assisted growth exhibit superior crystalline quality compared to those grown with oleic acid, as evidenced by a narrower rocking-curve full width at half maximum. Correspondingly, scintillation measurements show improved energy resolution for the formic-acid-grown crystals. These differences are attributed to the long-chain nature of oleic acid, which can lead to residual ligand incorporation and non-uniform solvent evaporation, slightly degrading optical transparency and crystallinity. In contrast, formic acid effectively regulates iodide ion availability during growth through a slow reaction with I^{3-} species at low temperature, reducing the growth rate and extending the metastable growth regime. This controlled environment favours defect-suppressed crystal formation.

1. B. Bansal, et al. NIM A 1069 (2024).
2. C. Tao, et al. Advanced Optical Materials 11, 24 (2023).
3. J. Lai, et al. CrystalEngComm 25.38 (2023).