Achieving High Performance Consistency in $Cs_3Cu_2I_5$ Perovskite Single Crystals via Vacuum-Assisted Solvent Evaporation

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1. Introduction

In recent years, halide perovskites have drawn considerable attention for applications in LEDs, solar cells, and radiation detectors, owing to their outstanding optical and electrical properties [1-3]. Among these, the copper-based halide perovskite $Cs_3Cu_2I_5$ (CCI) has emerged as a highly promising candidate for optoelectronic applications, driven by its high photoluminescence quantum yield (PLQY) and robust environmental stability [4]. Notably, unlike conventional detector materials that rely on high-temperature melt growth techniques such as the Bridgman method, CCI can be readily synthesized using solution-based processes. However, despite its processing advantages, solution growth frequently raises concerns regarding the consistency and spatial uniformity of the resulting crystals' performance compared to their melt-grown counterparts. To address this critical issue, the present study demonstrates the optimization of a room-temperature solvent evaporation method. By systematically evaluating the physical and optoelectronic performance of the CCI single crystals grown via this approach, we confirm their exceptional quality and performance uniformity. Ultimately, this work resolves the prevailing doubts regarding the reliability of solution-grown crystals, validating this method as a robust approach for fabricating high-quality detectors.

2. Methods and Results

2.1 Growth of $Cs_3Cu_2I_5$ single crystal via vacuum assisted solvent evaporation method

High-purity precursors, cesium iodide (CsI, 99.999%) and copper iodide (CuI, 99.999%), were utilized alongside a solvent mixture of dimethyl sulfoxide (DMSO, ACS, >99.9%) and N,N-dimethylformamide (DMF, ACS, 99.8%). Formic acid (FA, ACS, ≥96%) was employed to suppress oxidation. All chemical reagents were purchased from Alfa Aesar and Sigma-Aldrich and used as received.

To synthesize the 0D perovskite, the precursor molar ratios were optimized following established inverse temperature crystallization (ITC) methodologies [5]. CsI (3.897 g) and CuI (1.905 g) were weighed in a 2:1 molar ratio and dissolved in a solvent mixture of N,N-Dimethylformamide (DMF) (3.9 mL) and Dimethyl sulfoxide (DMSO) (2.6 mL). The mixture was magnetically stirred in a crucible at 800 rpm at room temperature for approximately 6 h until fully dissolved. Subsequently, 0.6 mL of FA was added, followed by an additional 2 h of stirring to achieve complete homogenization. The solution was then filtered through a 0.45 μm syringe filter to remove any undissolved particulates.

Because the solvent evaporation rate is highly sensitive to temperature and pressure, the growth environment was strictly regulated using a laboratory oven and a vacuum desiccator. The filtered growth solution was allowed to evaporate under these constant experimental conditions for approximately two weeks, which ultimately yielded a high-quality, centimeter-scale CCI single crystal.

2.2 Characteristics of $Cs_3Cu_2I_5$ single crystal

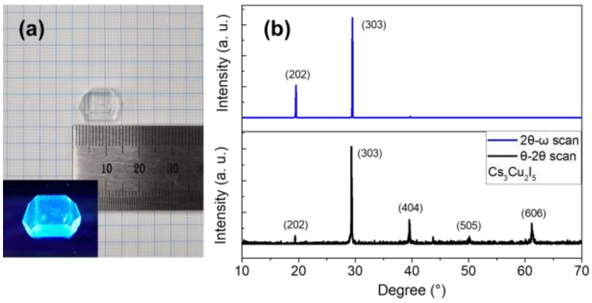

Fig. 1. (a) CCI single-crystal device. The inset shows the CCI under a 365 nm UV lamp. (b) θ-2θ, 2θ-ω XRD spectra of CCI crystal

Figure 1 shows a photograph of the CCI single crystal grown via the vacuum-assisted method. A highly transparent, crack-free crystal was successfully obtained, which exhibited bright blue emission under 365 nm UV irradiation. To evaluate its single-crystalline quality, X-ray diffraction (XRD) measurements were conducted. The resulting XRD pattern revealed no secondary phase peaks; it exclusively displayed a series of (n0n) diffraction peaks, confirming the exceptional phase purity and structural integrity of the grown crystal.

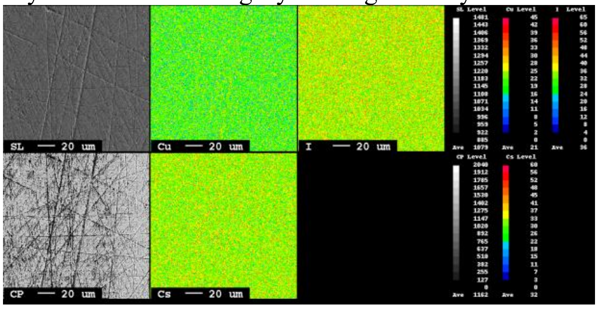

Fig. 2. EPMA elemental mapping images of the grown CCI single crystal.

Table. 1. EPMA Quantitative results of the CCI single crystal at three different regions.

	1-1	1-2	1-3	Average
Cs	29.07	28.06	28.02	28.38
Cu	21.91	22.39	21.15	21.81
I	49.02	49.55	50.83	49.80
Sum	100	100	100	100

Figure 2 illustrates the elemental distribution uniformity within the CCI device. The chemical composition was determined using an electron probe microanalyzer (EPMA), while its spatial uniformity was verified via EPMA mapping. Compositional analysis was performed at three distinct regions of the same sample. The resulting average atomic ratio of Cs:Cu:I was 28.4:21.8:49.8, which is remarkably close to the ideal stoichiometric ratio of 3:2:5. Furthermore, the elemental mapping revealed an absence of localized clusters or inclusions, confirming a highly homogeneous compositional distribution. The detailed quantitative EPMA results from the three measured points are summarized in Table 1.

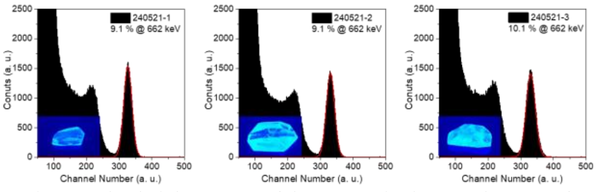

Fig. 3. Pulse-height spectra of three CCI single crystals grown from different batches under ^{137}Cs radio-isotope

To rigorously evaluate the batch-to-batch consistency of the CCI single crystals grown via the optimized method, three independent crystals were prepared from separate growth batches under identical conditions. Figure 3 presents the pulse-height spectra of these three devices used for the analysis. Their radiation detection performance was systematically compared in terms of energy resolution and relative light yield. The measured energy resolutions were 9.1%, 9.1%, and 10.1%, yielding a highly stable coefficient of variation (CV) of approximately 6.1%. More strikingly, the relative light yield indicated by the multichannel analyzer (MCA) peak channel numbers of 327, 328, and 329 (a.u.) exhibited a CV of merely 0.3%. This near-perfect reproducibility definitively confirms the outstanding performance homogeneity achievable through our room-temperature solvent evaporation approach.

3. Conclusions

In this study, we successfully demonstrated the growth of CCI single crystals using a vacuum-assisted solvent evaporation method and systematically evaluated their batch-to-batch consistency. The optimized process yielded crack-free, centimeter-scale CCI single crystals, with XRD measurements confirming their exceptional single-crystalline quality. Furthermore, EPMA quantitative result and elemental mapping verified the near-ideal stoichiometric ratio of the 0D perovskite and its highly homogeneous elemental distribution. Most importantly, pulse height spectrum evaluations revealed that three individual crystals grown from separate batches exhibited nearly identical performance. Ultimately, this work experimentally validates the outstanding consistency of the room-temperature solution growth method, effectively resolving the prevailing skepticism regarding the reliability and reproducibility of solution-grown detector materials.

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