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Article

Growth and Characterisation of Layered $(BA)_2CsAgBiBr_7$ Double Perovskite Single Crystals for Application in Radiation Sensing

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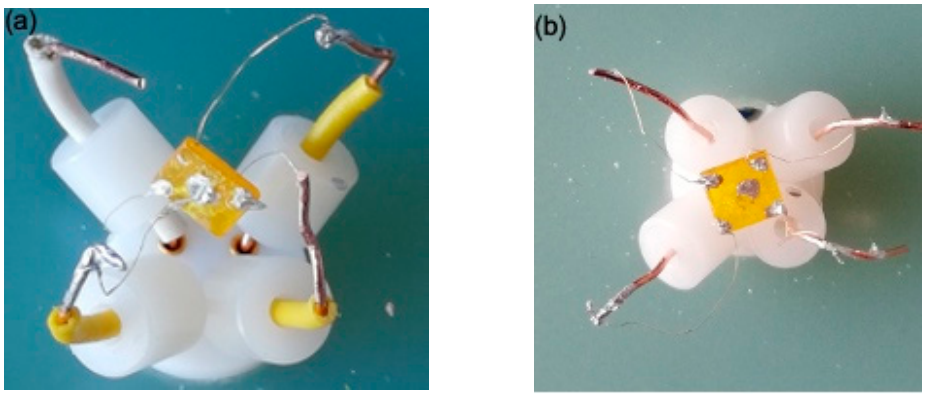
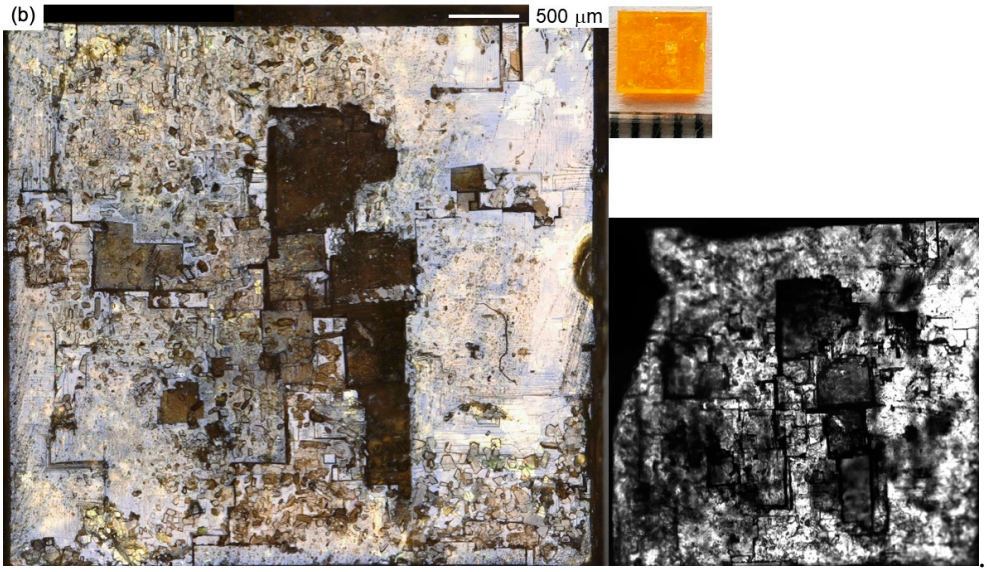


Figure S1. The *IV* measurement setup using the Keithley test fixture model 8101 4TRX and triax cables connected to the Keithley SMU 2450: Ag glue electrodes deposited on the bottom and top crystal faces of the sample $(BA)_2CsAgBiBr_7$_Exp1 and connected by 0.05 mm Au wires to two 0.5 mm copper wires inserted inside the shielded test fixture (**a**). The van der Pauw measurement setup using the shielded test fixture and triax cables connected to the SMU 2450 and 6517B: Ag electrodes deposited at equally spaced four corners of the crystal face of the $(BA)_2CsAgBiBr_7$_Exp1 (**b**) and contacted via 0.05 mm Au wires to four 0.5 mm copper wires. The test fixture was covered by Al foil to prevent photogeneration of charge carriers.


(a)
500 μm


(b)
500 μm

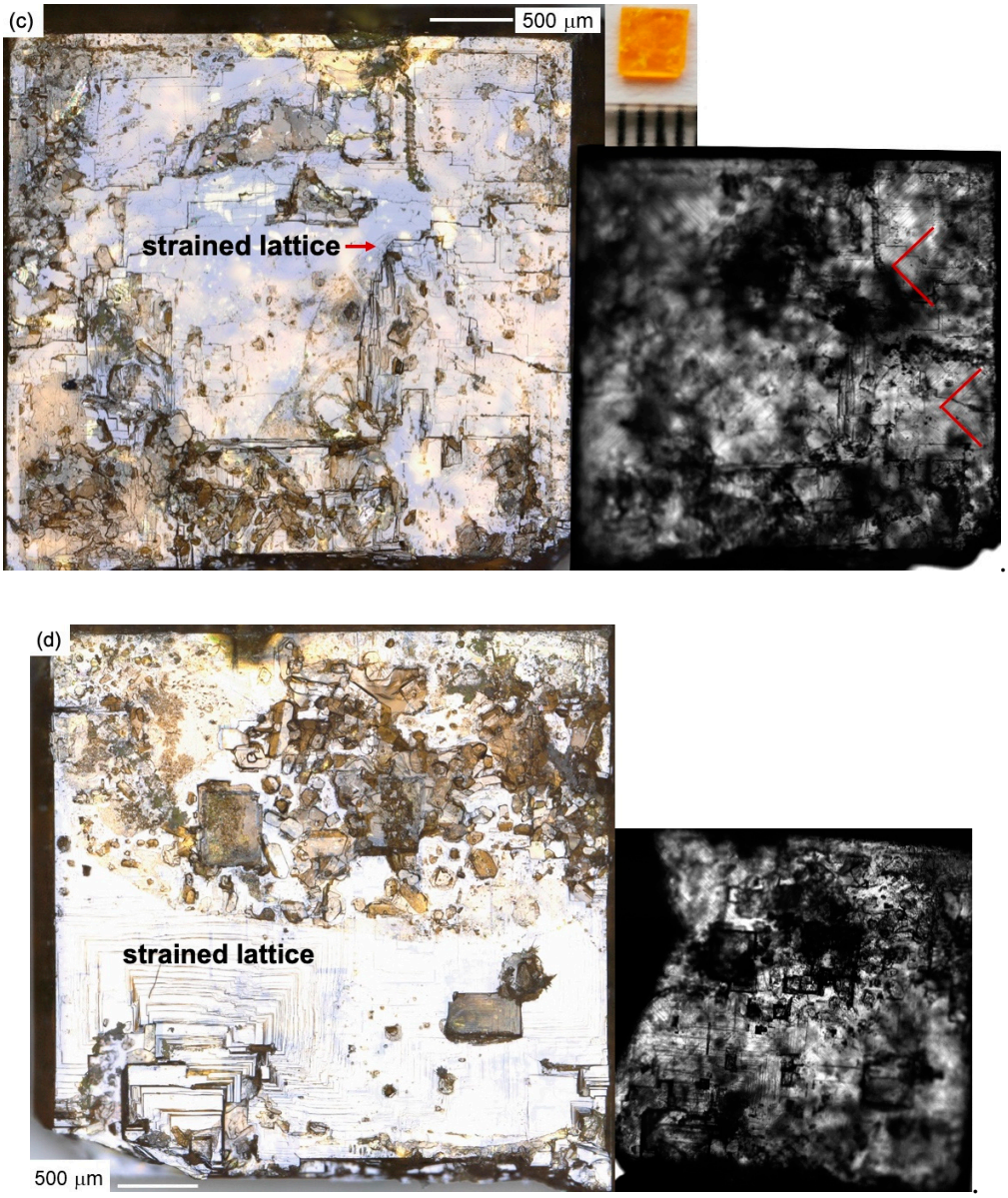


Figure S2. Sample $(BA)_2CsAgBiBr_7$_Exp2 (top right corner, 4 × 4 × 0.75 mm^3) has a top crystal surface (**a**) and bottom surface (**b**) characterised by irregular growth and dissolution features (image on the left made in reflected light and image on the right made in transmitted light). Strained lattice and defects such as twin planes characterise a top crystal face (**c**) and bottom crystal face (**d**) of sample $(BA)_2CsAgBiBr_7$_Exp3 (3.5 × 3.5 × 0.75 mm^3). The density of inclusions and precipitates is irregular and they tend to appear in clusters across the crystal faces of the two samples.

Single Crystal Structure Analysis

A single crystal structure analysis confirmed the results of Connor et al. [1]. For this purpose, a small, yellow, leaf-shaped crystal was attached to a nylon loop and measured on a Bruker Quazar/APEX II diffractometer with a charge-coupled detector. Cell refinement, data reduction, correction and integration were performed by using *SAINT*/*SADABS* (Bruker)[2,3]. Table S1 summarises the crystallographic data obtained.

Table S1. Selected crystallographic data.

Chemical composition	**$(BA)_2CsAgBiBr_7$**
Crystal system	Monoclinic
Space group (No.)	$P\ 2_1/m$ (11)
Lattice constants/Å	a = 8.0742(4) b = 8.0085(4) c = 19.8639(1) β = 101.7223(1) °
Volume of the unit cell/$Å^3$	1257.66(1)
Number of formula units	2
Density/$g \cdot cm^{-3}$	3.056
Radiation mode	Mo-K_α (λ= 0.71073 Å)
Absorption coefficient/mm^{-1}	20.305
Index range $h/k/l$	$-9 < h < 9$ $-9 < k < 9$ $-23 < l < 23$
Measured/independent data	26244/2400
N(hkl) ($I > 2\sigma(I)$)	2168
R_{int}/R_σ	0.056/0.029
Parameter	150
Goodness-of-fit on F^2	1.132
R_1/wR_2 ($I > 2\sigma(I)$)	0.038/0.104 88/0,1072
R_1/wR_2 (all data)	0.045/0.108
Residue electron density (max/min/σ)/e/Å	2.22/−2.18/0.236

References

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2. Sheldrick, G. M. *SADABS*; Institute for Inorganic Chemistry, University of Göttingen: Göttingen, Germany, 1996.
3. *SAINT*; Bruker Analytical X-ray Systems: Madison, WI, 1999.