Supporting Information

Crystallinity and Defect Reduction in $Cs_2AgBiBr_6$: Key Factors for Enhanced Optoelectronic Devices

Fahad K. Alshammari [a], Achref Jebnouni [b], Mohamed Bouzidi [a], Sana Ben Khalifa [c], Mohamed Ben Bechir [*, d, e]

[a] *Department of Physics, College of Science, University of Ha'il, P.O. Box 2440, Ha'il, Saudi Arabia*

[b] *Medical Surgical Nursing Department, College of Nursing, University of Ha'il, Ha'il, Saudi Arabia*

[c] *Department of Physics, College of Science, Qassim University, P.O. Box 6644, Buraydah Almolaydah ,51452, Saudia Arabia*

[d] *Laboratory of Spectroscopic and Optical Characterization of Materials (LaSCOM), Faculty of Sciences, University of Sfax, Tunisia.*

[e] *Department of Physics, Faculty of Sciences of Gafsa, University of Gafsa, 2112, Tunisia.*

[*] ***Corresponding author***. *E-mail address:* mohamedbenbechir@hotmail.com

Supplementary Figures

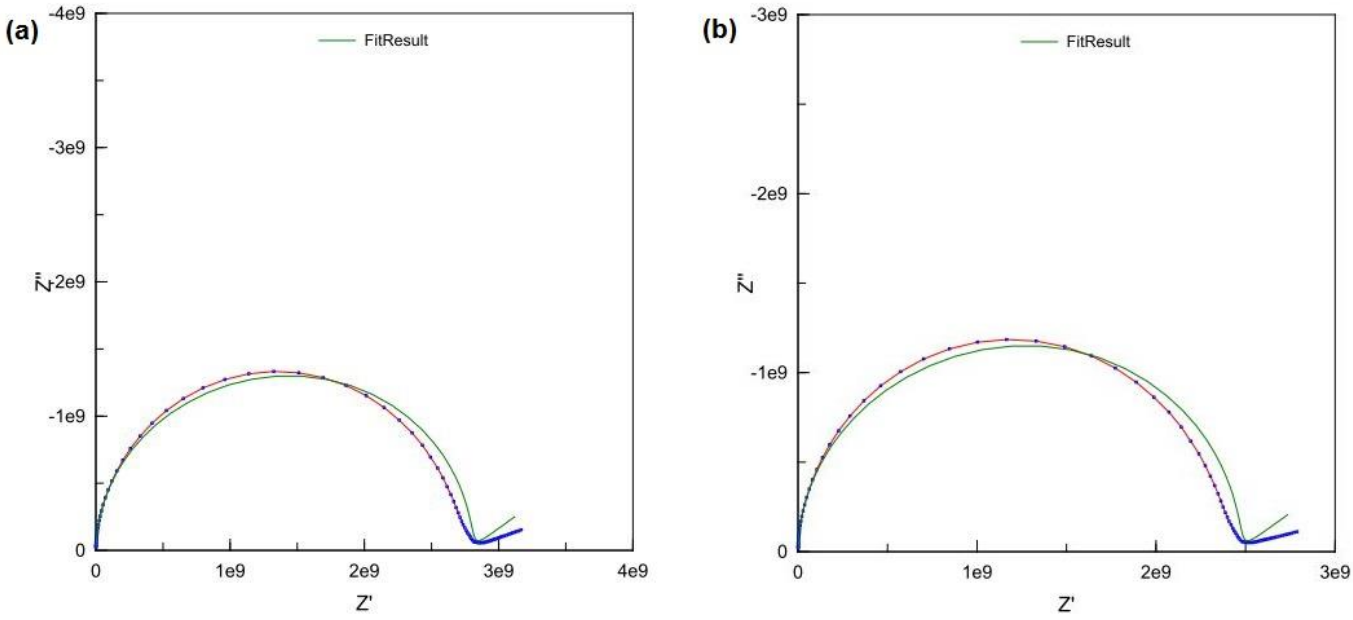

Figure. S1. Nyquist Plot Fitting Using ZView Software: (a) SCG and (b) SAG.

Supplementary Tables

Table S1. Full Width at Half Maximum (FWHM) Values for XRD Peaks of $Cs_2AgBiBr_6$ Crystals.

	FWHM (°)		L_s (%)	
Miller indices (hkl)	SCG	SAG	SCG	SAG
(111)	0.088	0.056	0.183	0.116
(222)	0.072	0.048	0.072	0.048
(333)	0.104	0.072	0.067	0.047
(444)	0.080	0.056	0.037	0.026

Table S2. Extracted Circuit Parameters from Nyquist Plots for SCG and SAG Crystals.

	SCG	SAG
R_g (Ω)	8.48×10^8	6.64×10^8
C_g (F)	1.44×10^{-14}	1.75×10^{-14}
R_{gb} (Ω)	1.93×10^9	1.78×10^9
C_{gb} (F)	1.49×10^{-14}	1.56×10^{-14}
CPE_e (F)	1.13×10^{-9}	1.36×10^{-9}
α_e	0.403	0.399

Supplementary Equations

The parameter L_s is calculated using the following expression:

$$L_s = \frac{B_s}{4 \tan \theta} \quad \text{(S1)}$$

In this context, B_s denotes the contribution of structural broadening, representing the difference in the full width at half maximum (FWHM) between the investigated sample and a reference standard. To isolate the structural broadening component, B_s is obtained through the relation :

$$B_{struct} = \sqrt{B_{obs}^2 - B_{std}^2} \quad \text{(S2)}$$

Here, B_{obs} corresponds to the observed peak broadening from the sample being examined, while B_{std} refers to the peak width measured from a standard material, which is assumed to exhibit negligible or no structural broadening effects.

The density of trap states, n_{trap}, can be determined using the following relation :

$$n_{trap} = \frac{2\varepsilon\varepsilon_0 V_{TFL}}{eL^2} \quad \text{(S3)}$$

In this expression:

- ε_0 represents the permittivity of free space, valued at 8.85×10^{-12} F/m,

- ε is the relative dielectric constant specific to $Cs_2AgBiBr_6$, with a value of 16.7,
- e denotes the elementary charge of an electron (1.6×10^{-19} C),
- L refers to the thickness of the single crystal sample, which is 1.4 mm.

The photoresponsivity (R) of the material is calculated using the following equation:

$$R = \frac{I_{ph} - I_D}{P_{irra} S} \quad \text{(S4)}$$

In this formula:

- I_{ph} refers to the photocurrent measured under illumination,
- I_D represents the current measured in the dark,
- P_{irra} is the power of the incident radiation,
- S denotes the surface area of the crystal exposed to light.

To evaluate the specific detectivity (D^*), the following relation is used:

$$D^* = \frac{R}{(2eI_D)^{1/2}} \quad \text{(S5)}$$

Here, e is the elementary charge, and I_D is the dark current. The diffusion coefficient (D), which reflects the rate of molecular diffusion, is expressed as:

$$\mathrm{D} = \mathrm{D_0 e}^{\left(-\frac{\Delta \mathrm{H}}{\mathrm{RT}}\right)} \quad \text{(S5)}$$

Where:

- D_0 is the pre-exponential diffusion constant,
- ΔH represents the activation energy required for diffusion,
- T is the absolute temperature of the system, and
- R is the universal gas constant.