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STUDY OF THE INFLUENCE OF Pb SUBSTITUTION BY Zn^{2+} IONS ON THE PROPERTIES OF $CsPbBr_{3-x}I_x$ THIN FILMS

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Abstract

This work reports results of a study on optical, morphological and structural properties of thin films of cesium lead bromide iodide mixed perovskite synthesized by sequential evaporation of precursors. Thin films of $CsPbBr_{3-x}I_x$ with a high degree of reproducibility of both the molar composition and the photovoltaic properties were achieved, using an electronic system with facilities to control the growth of the samples . Special emphasis was put in evaluating the effect that the substitution of the Pb cation by Zn^{2+} ions onto its optical, morphological and structural properties through transmittance, photoluminescence, XRD, SEM and Urbach Energy measurements.

Experimental

Thin films of $CsPbBr_{3-x}I_x$ were prepared by sequential evaporation of its precursors ($PbBr_2$, PbI_2,CsBr), using a routine that includes initial evaporation of PbI_2 followed by evaporation of $PbBr_2$ and CsBr, keeping their respective deposition rates in the range of 4-6 Å/s. The Precursors are evaporated at room temperature from Knudsen cell-type evaporation sources and after the deposition, these are annealed at normal ambient air conditions at temperatures around 250°C, for 20 minutes. Good reproducibility of both the composition and properties of samples was achieved using an equipment with facilities to control electronically the evaporation temperature and deposition rate of precursors, by means of PID and PWM algorithms. After obtaining conditions to grow thin films with composition $CsPbBr_{2.7}I_{0.3}$, a study was carried out to evaluate the influence that the partial substitution of Pb by Zn^{2+} (obtained by additional evaporation of a layer of $ZnBr_2$) produces on the optical, morphological and structural properties.

The samples prepared were characterized by means of transmittance and reflectance measurements performed using a Varian–Cary 5000 spectrophotometer, as well as by XRD measurements performed with a Philips X'Pert Pro PANalytical diffractometer, using the radiation Cu-Kα (1.540598 Å), an acceleration voltage of 40 KV and a current 40 mA, and the film thickness was determined using a Veeco Dektak 150 surface profiler. The morphological characterization was performed with an electronic scanning microscope TESCAN, model Vega 3.

Results

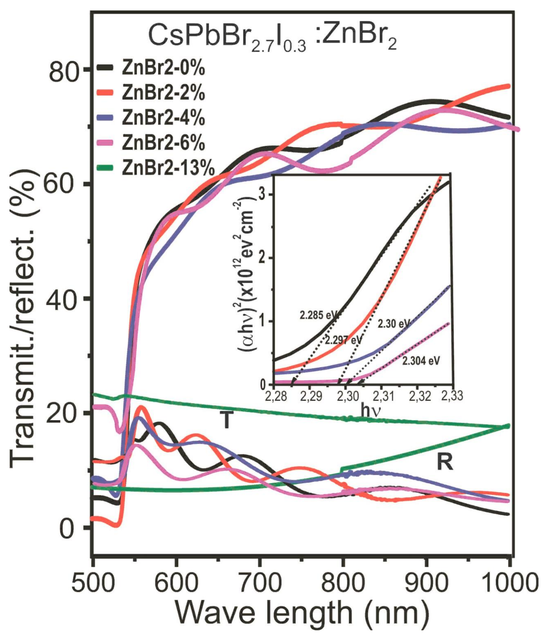

Figure 1: Transmittance, reflectance, and $(\alpha hv)^2$ vs hv curves of a reference sample with composition $CsPbBr_{2.7}I_{0.3}$, in which the Pb cation was replaced by Zn in different atomic percentages.

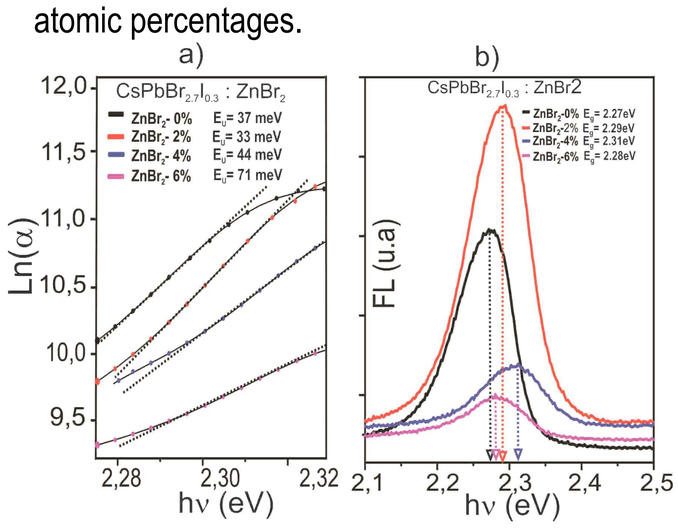

Fig. 2: a) Energy of Urbach Eu calculated from the slope of ln(α) vs hν curves and b) FL curves, obtained with $PbBr_{2.7}I_{0.3}$ films , in which Pb was replaced by Zn in a percentage that varied between 0 and 6%

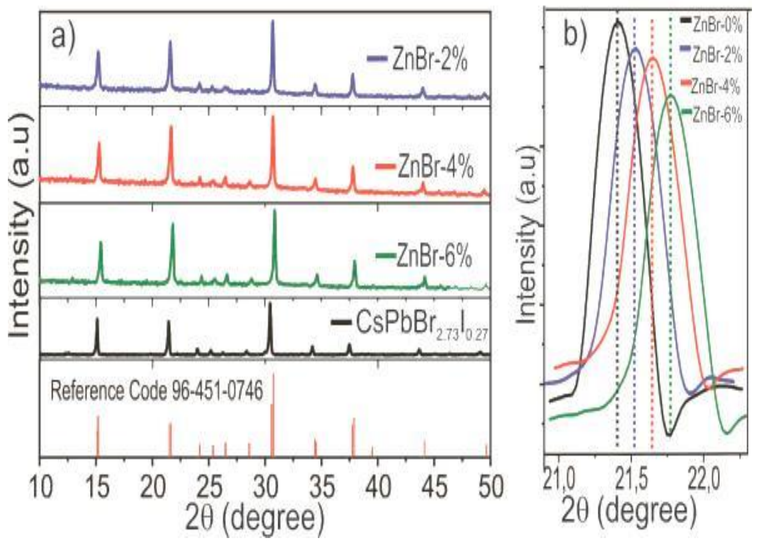

Figure 3: Effect that the substitution of Pb by Zn produces on a) the XRD pattern and b) on the shift of the characteristic peak of the phase $CsPbBr_{2.7}I_{0.3}$, observed at $2\theta = 21.5^o$.

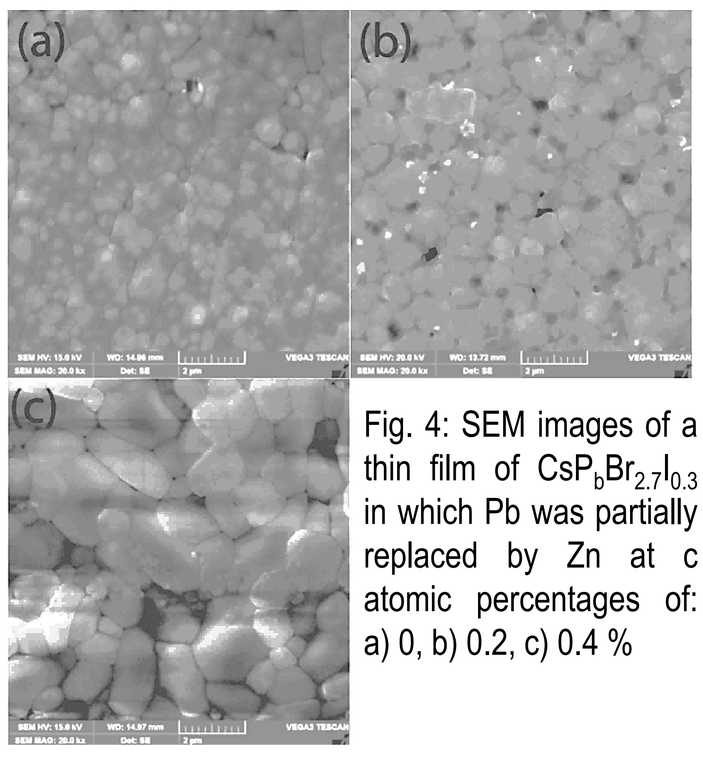

Fig. 4: SEM images of a thin film of $CsP_bBr_{2.7}I_{0.3}$ in which Pb was partially replaced by Zn at c atomic percentages of: a) 0, b) 0.2, c) 0.4 %

Conclusions

- The effect of substituting Pb cation by Zn^{2+} ions on the optical, morphological and structural properties of mixed perovskites thin films with composition $CsPbBr_{2.7}I_{0.3}$ was evaluated through, XRD, SEM, spectral transmittance, photoluminescence, and Urbach Energy measurements.
- The $CsPbBr_{2.7}I_{0.3}$ films grow in the orthorombic -phase and when Zn ions substitute the Pb cation, the crystalline structure does not change; FL measurements indicated that samples doped with Zn in atomic percentages less than 4% emit high emissions due mainly due to fundamental transitions.
- The substitution of Pb by Zn in percentages less than 6%, significantly improves the morphology which is characterized by compact grains whose size increases significantly with increasing percentage of Pb atoms substituted by Zn.