Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting information

Trap and recombination centers study in $MAPbI_3$ perovskites

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Experimental

Fig. S1 shows a block diagram of the equipment implemented to study the influence of sample temperature, intensity of illumination and pressure inside the chamber on the photocurrent response. This equipment includes the following units:

i) Measuring chamber connected to a system of pre-vacuum ($5x10^{-3}$ mB) in whose interior is located the sample which is heated by placing it on a copper block heated through a heating resistor connected to a power supply.

ii) Photocurrent measurement system, constituted by a power supply operating at constant voltage connected to the sample and a picoammeter Keithley 485 for measuring the photocurrent generated.

iii) Electronic system implemented using virtual instrumentation with facilities to control the sample temperature through a PID algorithm and to perform functions of control, acquisition, processing and monitoring of data. The equipment also allows to realize photocurrent measurements at different pressures, which are controlled through an electronic mass flow controller connected to a cylinder with compressed air, keeping the vacuum system in operation.

The hardware used for the development of the system includes a communication module FieldPoint-1000 (FP-1000), an analog input TC - 120 module to acquire the voltage signal from the thermocouple type K used as a temperature sensor and a card NI USB-6008. The functions of control, measurement, acquisition, processing and display of data are made through a Virtual instrument (VI) developed with LabVIEW.

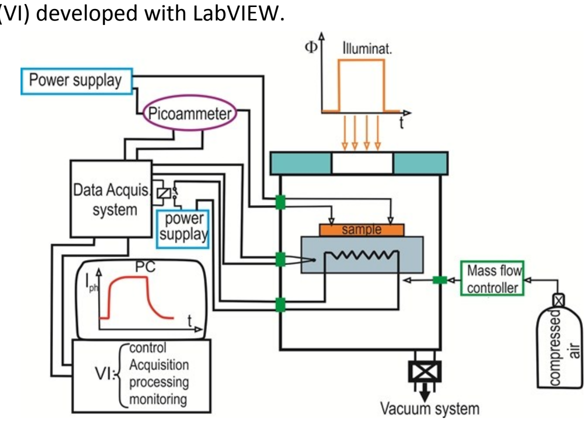

Figure S1: Block diagram of the equipment implemented for performing photocurrent measurements.

Characterizations

X-ray diffraction pattern (2θ scans) were obtained from samples of perovskite deposited on glass substrates using an X-ray diffractometer (Panalytical X'Pert Pro), using Cu-Kα radiation (λ=1.54050 Å). SEM images were performed using a VEGA3 SBU - Easy Probe SEM microscope

Fig. S2 depicts XRD spectra of a $MAPbI_3$ film annealed at temperatures ranging from 35 to 75°C. Comparison of the X-ray patterns shown in Fig, S2 indicate that the annealing to which the perovskita films were submitted does not change its crystalline structure. It is also clear from Fig. S2 that $CH_3NH_3PbI_3$ films grown on glass substrates exhibit strong preferred orientations along tetragonal (110) and (220) planes. The rest of reflections present in these three XRD spectra have been identified by other Authors in $MAPbI_3$ films grown with structure tetragonal [1].

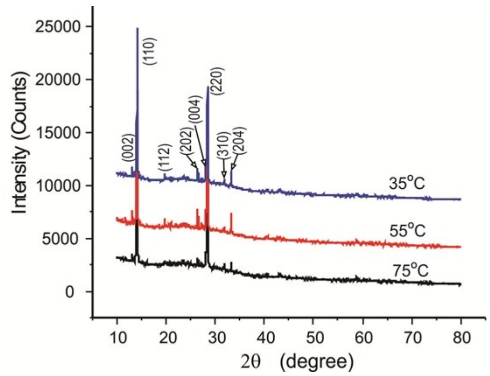

Figure S2: X-ray diffraction spectra of a typical $MAPbI_3$ film annealed at 35, 55 and 75°C respectively during 20 min.

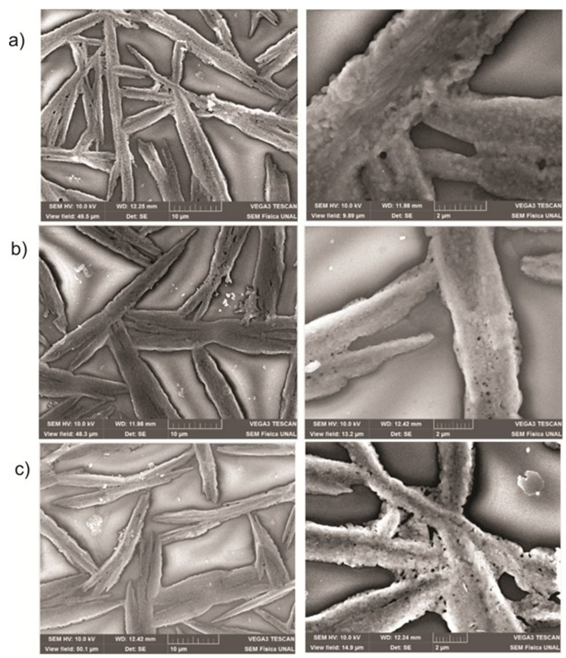

Figure S3: Top-view SEM images of a $MAPbI_3$ film annealed at **a)** 35°C, **b)** 55°C and **c)** 75°C during 20 min.

Fig. S3 shows the top-view SEM images of $CH_3NH_3PbI_3$ perovskite films annealed at temperatures ranging from 35 to 75°C. It is noted that the morphology of the sample of perovskite does not change when this is annealed at temperatures between 35 and 75°C. Similar morphology have been reported by other Authors [2] for $CH_3NH_3PbI_3$ perovskite films grown with tetragonal structure and prepared by spin-coating a solution containing equal molar ratio of CH_3NH_3I and PbI_2 in N,N-dimethylformamide (DMF) solvent .

References

[1] X. Guo, Ch. McCleese, Ch. Kolodziej, A. C. S. Samia, Y. Zhao, and Cl. Burd, Identification and Characterization of the Intermediate Phase in Hybrid Organic–Inorganic MAPbI3 Perovskite, Dalton Trans., 45, 3806-3813 (2016)

[2] Q. Wang, M. Lyu, M. Zhang, J.Ho Yun, H. Chen, and L. Wang, Transition from the Tetragonal to Cubic Phase of Organo halide Perovskite: The Role of Chlorine in Crystal Formation of $CH_3NH_3PbI_3$ on TiO_2 Substrates, J. Phys. Chem. Lett., 6 (21), 4379–4384 (2015)