The Effect of Zinc Compounds on Toxicity and Stability of Organo-Metal Halide Perovskite Materials

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Introduction

What is Perovskite?

- The active layer material of a new generation solar cell .
- Coming from Russian mineralogist Lev PEROVSKI.
- Similar crystal structure $\rightarrow ABX_3$ $\rightarrow$Organo metal halide
- This work is about Methylammonium lead Iodide ($MAPbI_3$)

Why Perovskites?

- Efficient absorption in the visible range.
- Simple and cheap synthesis method.
- High diffusion lengths (up to 1 μm).

Some of their Issues:

- Presence of Toxic element i.e. Pb.
- Unstable against moisture and air etc.

Method

- **Selection of materials:**

MAI (CH_3NH_3I), PbI_2, ZnI_2, $ZnCl_2$, GBL (γ-butyrolactone)

- **Synthesis:**

$MAPbI_3$ $\rightarrow$ The equimolar ratio (1:1) of readily synthesized MAI and PbI_2 were dissolved in GBL and kept at 60°C for overnight with stirring.

ZnI_2-$MAPbI_3$ and $ZnCl_2$-$MAPbI_3$ were synthesized in same way by decreasing the 20% of PbI_2 concentration and adding 20% of ZnI_2 and $ZnCl_2$.

Deposition:

the naked perovskite films were prepared on glass slides by spinning for 30 seconds at 2000 rpm on the spin coater. The slides were heated on a hot plate for 10 min at 50°C.

References

[1] N. Soleimanioun, M. Rani, S. Sharma, A. Kumar, S.K. Tripathi; "Binary metal zinc-lead perovskite built-in air ambient: Towards lead-less and stable perovskite materials"; *Sol. Energy Mater. Sol. Cells.* **191** (2019) 339–344.

[2] N. Soleimanioun, M. Rani, B. Singh, G.S.S. Saini, S.K. Tripathi; "Potential replacement to lead: Alkali metal potassium and transition metal zinc in organo-metal halide perovskite materials"; *Journal of Alloys and Compounds* **861** (2021) 158207.

Characterization of Materials

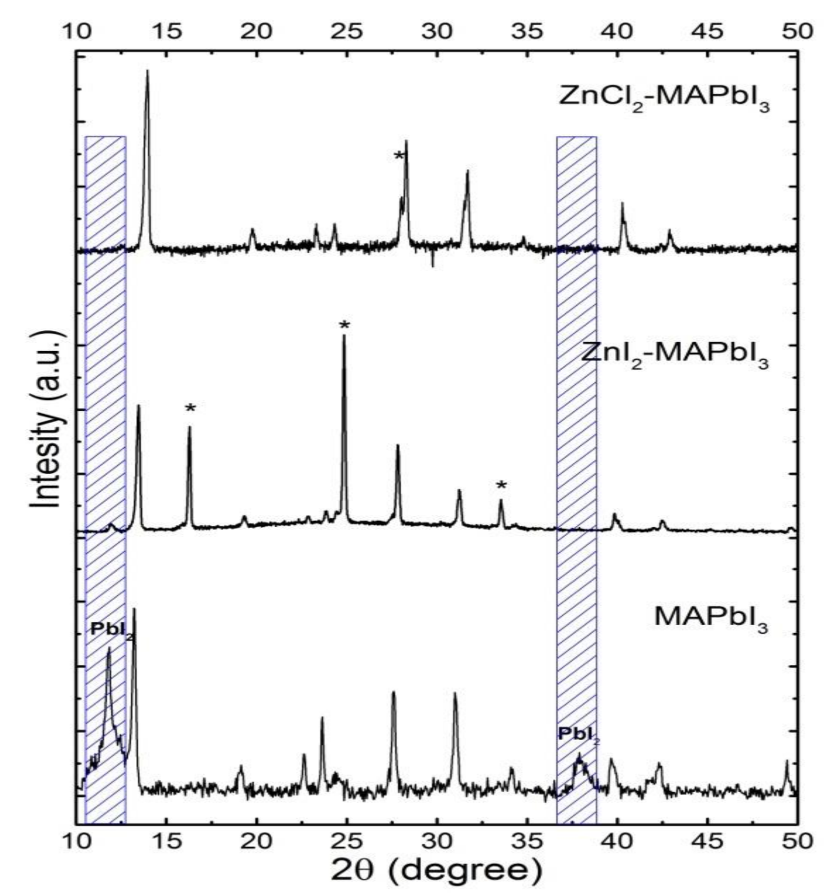

Fig 1. XRPD of fresh samples.

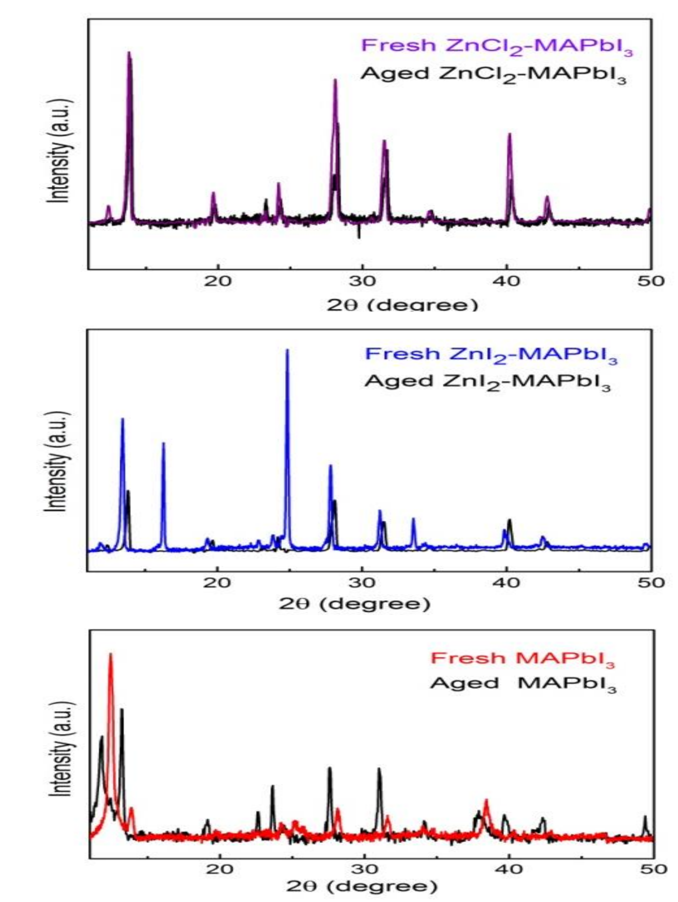

Fig 2. XRPD of aged samples.

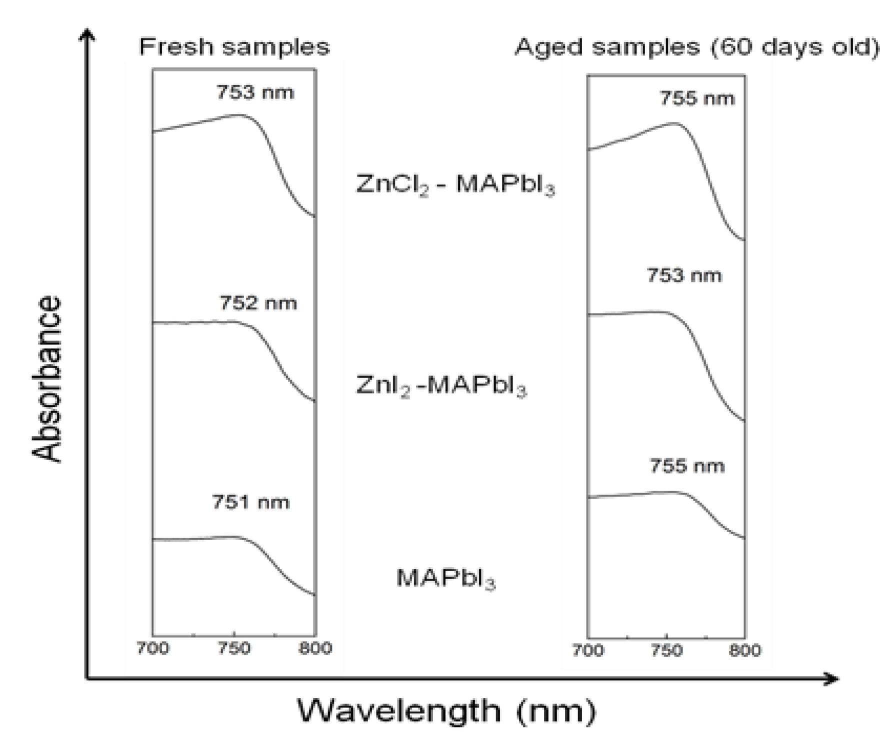

Fig 3. UV-Vis of fresh & aged samples.

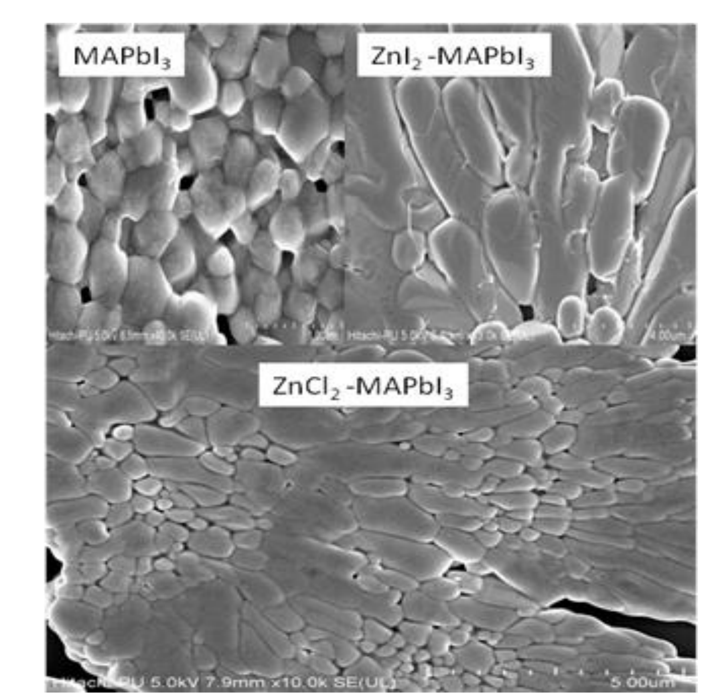

Fig 4. surface morphology of films.

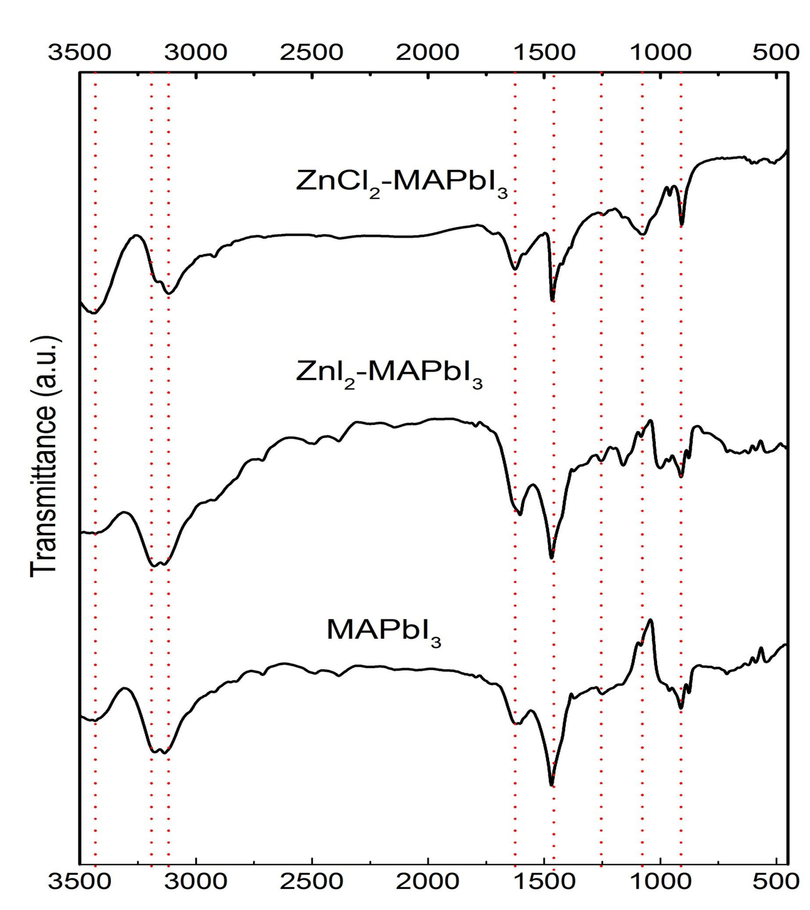

Fig 5. FTIR results of fresh samples.

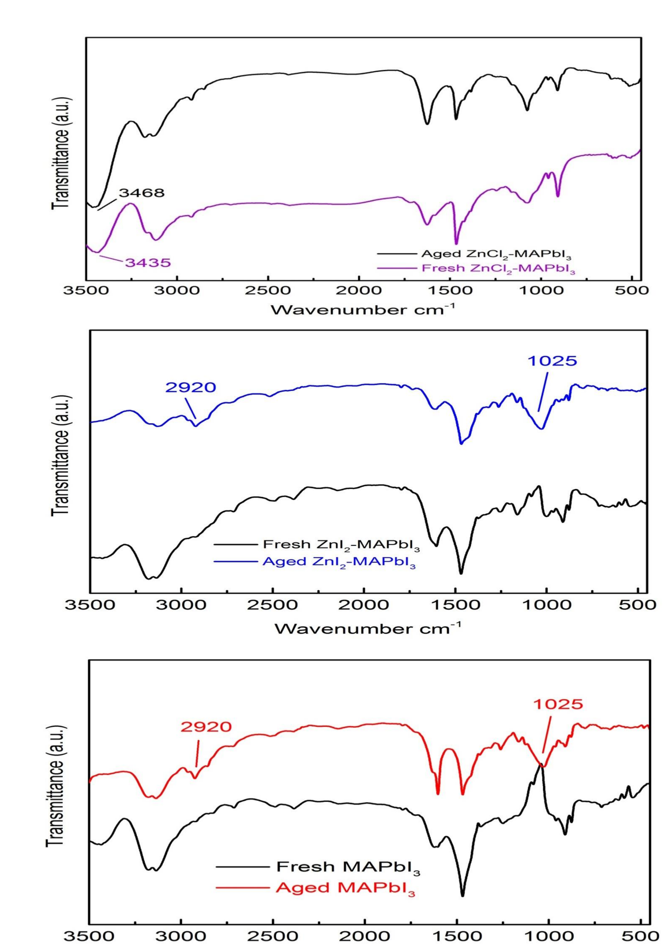

Fig 6. FTIR results of aged samples.

Results and Discussion

XRPD:

✓Deduction of peaks related to PbI_2.

✓Presence of new peaks shown by * related to new perovskite compounds.

✓Shifts towards higher angles which can be due to the smaller ionic radii of Zn^{2+} in comparison to Pb^{2+} and reported to improve the crystallinity.

✓For aged samples the lesser changes in structural characteristics are observed after adding Zn especially $ZnCl_2$.

UV-Vis spectroscopy:

✓For fresh samples a slight redshift is observed which shows the particle size is increasing by adding Zn. The band gaps also is decreased.

✓For aged samples a considerable redshift in pristine sample can indicate the faster degradation as compared with Zn ones.

FESEM images:

✓The change of grain shapes from cuboids to fibers are observed after adding Zn.

✓Grain size: $MAPbI_3$≈0.3-0.5 μm, ZnI_2-$MAPbI_3$≈ 0.5-2.5 μm & $ZnCl_2$-$MAPbI_3$≈>5 μm

FTIR:

✓It is observed that the change in the molecular parameters of the NH_3 group in perovskite molecules takes place on alloying with Zn.

✓In aged samples a minor effect of moisture is observed.

Photoconductivity: $\sigma_{Ph}=I_{ph}\, t/\, VLd\ (Sm^{-1})$

$MAPbI_3$≈ $51*10^{-9}(Sm^{-1})$, ZnI_2-$MAPbI_3$≈ $53*10^{-9}(Sm^{-1})$ & $ZnCl_2$-$MAPbI_3$≈ $200*10^{-9}(Sm^{-1})$

Conclusions

- Replacing Pb with Zn upto 20% was done successfully and the new compounds showed better characteristics than pristine sample.
- Zn can be introduced as an essential element to increase the stability of $MAPbI_3$.
- $ZnCl_2$-$MAPbI_3$ behaved more conductive and stable than ZnI_2-$MAPbI_3$ also.

26th Annual IASBS Meeting on
Condensed Matter Physics

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