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# An ion beam surface sputtering characteristics of magnesium substitutes in lead-based perovskite compound using SRIM-2013

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## ABSTRACT

The organic-inorganic lead halide perovskite are materials used for the production of low-cost and effective solar photovoltaic with a base made up of Electron Transport Layer (ETL) and the utmost effective of these organic-inorganic perovskite solar cells are made of Methylammonium Lead Iodide (MALI), $CH_3NH_3PbI_3$ but the presence of lead has made it toxic. However, Magnesium metal cation could possibly replace lead in MALI since it is less-toxic We report another approach to study the behavior of perovskites without lead conducting a Monte Carlo (MC) sputtering calculation of of Methylammonium Lead Iodide (MAMI), lead and tin perovskites. The sputtering characteristics these materials were compared. The outcomes indicated a momentous display of comparable sputtering attributes with a greatest sputtering yield at 78 ° ion incidences. The outcomes likewise demonstrated a relationship between the sputter values of MALI and MAMI.

**Key words:** IBSS, Sputter Yield, Magnesium Perovskite, Perovskite Solar Cell,

## 1. INTRODUCTION

The use of Perovskite solar cells (PSC) with an absorber material made of metal halide perovskites is associated to major encouraging PV devices for future of solar PVs. A notable increase in the conversion efficiency (PCE) from 3.8% [1-5] to over 22% within few years [6-8] confirmed this. This excellent piece is due to the special characteristics of metal halide perovskites displaying great high absorption coefficients, charge densities, direct tunable band gaps, hole transport and a balanced electron, [9], and long carrier diffusion lengths [10-12]. Other significant improvement is that they can be prepared via a variety of ways (13-21). A replacement of lead with non-toxic and naturally benign elements becoming lead-free perovskites can be obviously gotten by way of homovalent replacement of Pb with isovalent metallic cations like group-14 elements, transitions metals (Mn, Cu) and alkaline-earth metals (Mg, Ca). Quite a number of elements with constant oxidation state of $^{+}2$ are in more appropriate for replacement of Pb which has the same valence, in the perovskite structure. Group 2 metals in the periodic table as magnesium (Mg) and barium (Ba) can be possible alternatives because of suitable ionic radii, abundant, harmless and similar oxidation state to $Pb^{2+}$ [22&23]. On the other hand, alkaline earth metal perovskites exist stable perovskite structure [3, 23, and 24]. Magnessium has been reportedly used to substitute lead (Pb) in methylammonium lead iodide perovskite structure leading to methylammonium magnesium iodide, but with lower effective masses, direct tunable band gaps and good absorption coefficients [25, 26]. The bandgaps of AMgI3 perovskites was projected to not to be fixed when different A-site cations are used with theoretical gaps of 1.5 eV ($CH_3NH_3MgI_3$), 0.9 eV for ($CH(NH_2)_2MgI_3$) and 1.7 eV ($CsMgI_3$) [26]. Regardless of the smaller ionic radius of $Mg^{2+}$ of 72 pm, magnesium halide perovskites was predicted theoretically to be stable [26, 27]. Amongst the alkaline-earth metals, $Mg^{2+}$ has the best structural and optical data for photovoltaic applications, with more stability and a crystal system of tetragonal space group.

With the goal of reducing the toxicity of lead in perovskite applications, magnesium was used to replace lead in the pseudo-cubic phase $CH_3NH_3PbI_3$ structure

To study the sputtering characteristics of materials, new method was proposed by Oyewande & Akinpelu, 2018, by conducting ion beam surface sputtering using SRIM. Sputtering is the removal of atoms from particular target when bombarded by fast moving ion. There is ejection of atoms from the target material by energy transfer from an attacking particle, usually a gaseous ion. Benefit of sputtering is that materials with very high melting points are sputtered easily.

The MC suite built by Ziegler and Biersack[32-35]. It is therefore important to know the impact of lead substitution on the removal rates of hybrid organic and inorganic halide perovskites. By expansion, it is important to realize if sputter attributes, or modifications in them as certain component of perovskites is altered, has a correspondence with the conversion efficiencies of the perovskites.

In this paper, we used ion-beam machining method to examine the physical features responsible for differences in optoelectronic properties of both lead, lead-free metal halide perovskite materials and magnesium perovskite material in PV applications. And an MC simulation is employed study the sputtering characteristics of ions in lead and these selected lead free metal halide perovskite and perovskite of an alkaline-earth metal ($CH_3NH_3MgI_3$) for ion energies of 1 keV and 5 keV and different angles of incidence, using TRIM. Argon (Ar) and Ne (ion) ions were used to sputter these perovskite.

## 2. METHODOLOGY

The details of our simulation are given in this section and details on theoretical background for the calculation algorithm embedded in TRIM packages are explained in the publications written by Ziegler and Biersack [32-35]. The chosen range as prescribed in ref 29 was use as typical ion energy. TRIM was used to study the rate of removal of atoms of these selected perovskites when bombarded by fast moving argon and neon ions with 1 keV and 5 keV ion energies. The angle of incidence was varied from 0° to 89°. In the set-up, 35 nm was the perovskite thickness used. The magnesium, lead and tin perovskites were built from as 1:3:1:3:1:3 for C, H, N, H, Mg/Pb/Sn and I, respectively. Density of 2.81 g/cm3 was used for magnesium perovskite by using the correction factor suggested ref 29 while. Densities of 4.16g/cm3 [29] and 3.51 g/cm3 [29] were used for the lead and tin perovskites, respectively. Exactly 1000 argon and neon ions were used, each, to hit the perovskite.

## 2.1 Results and Discussion

The outcome of our calculations are reported and explained here. Both results of the two incident ions ($Ne^+$ and $Ar^+$) are presented. Although, higher values of $Ar^+$ sputter yield were found than the corresponding values for $Ne^+$. The simulations were started with neon $Ne^+$ bombardments of the perovskites (Figures 1 - 6). The sputtering yields of magnesium halide perovskite show the same pattern as yields of lead and tin perovskites. Figures 8 – 11 show the result of bombardment of argon $Ar^+$ ion with the selected perovskites. Similar pattern of sputter yield was noticed for magnesium perovskite, also. Although, among the three perovskites, magnesium halide perovskite has the lowest sputter yield. Methylammonium lead iodide has the highest yield while tin iodide perovskite recorded the second highest yield. The yields are inversely proportional to their recorded experimental power conversion efficiencies. Our results showed that magnesium can potentially replace lead in perovskite application.

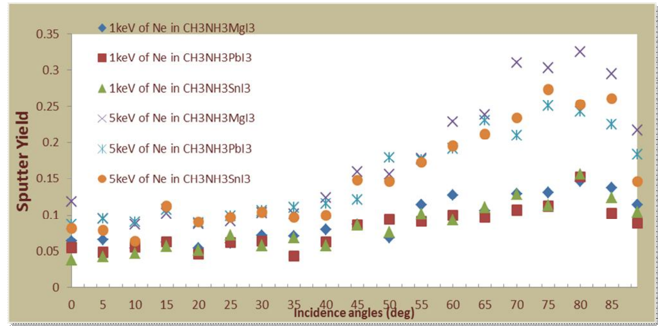


**Figure 1:** Sputter yield of Carbon for the erosion of C atoms from $Ne^+$ bombardment of target perovskites at different angles of incidence, for ion energy of 1 keV and 5 keV

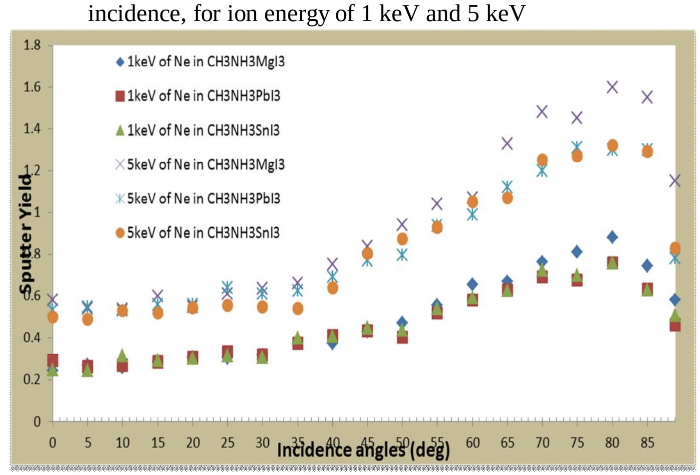


**Figure 2:** Sputter yield of Hydrogen for the erosion of H atoms from $Ne^+$ bombardment of target perovskites at different angles of incidence, for ion energy of 1 keV and 5 keV.

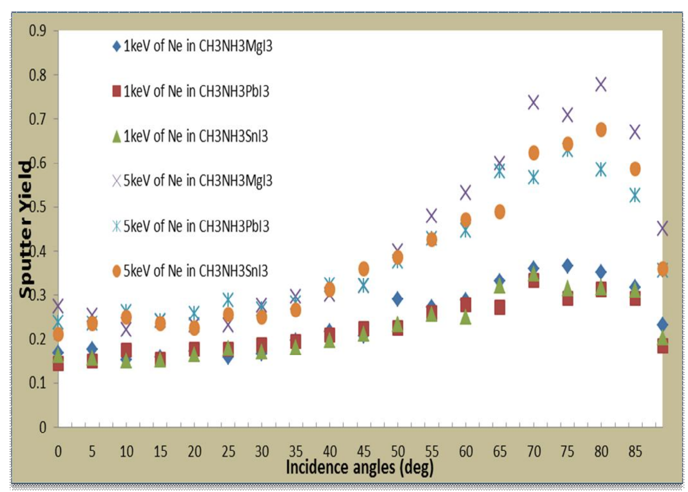


**Figure 3:** Sputter yield of Nitrogen for the erosion of N atoms from $Ne^+$ bombardment of target perovskites at different angles of incidence, for ion energy of 1 keV and 5 keV

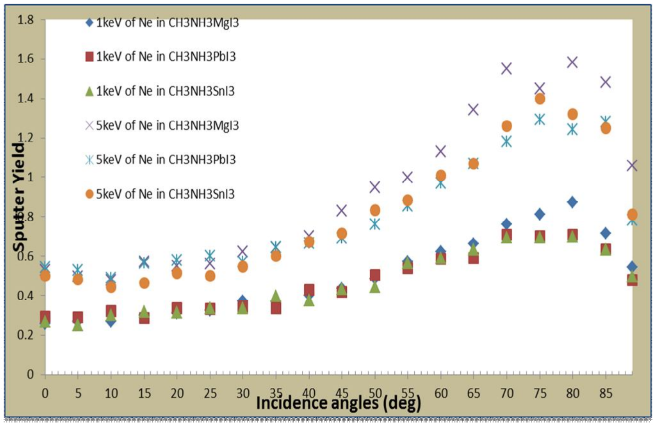


**Figure 4**: Sputter yield of Hydrogen for the erosion of H atoms from $Ne^+$ bombardment of target perovskites at different angles of incidence, for ion energy of 1 keV and 5 keV

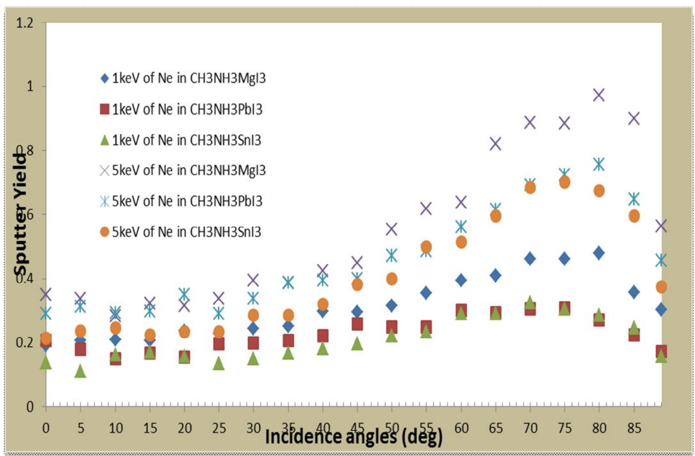


**Figure 5**: Sputter yield of Mg/Pb/Sn for their erosion from $Ne^+$ bombardment of target perovskites at different angles of incidence, for ion energy of 1 keV and 5 keV

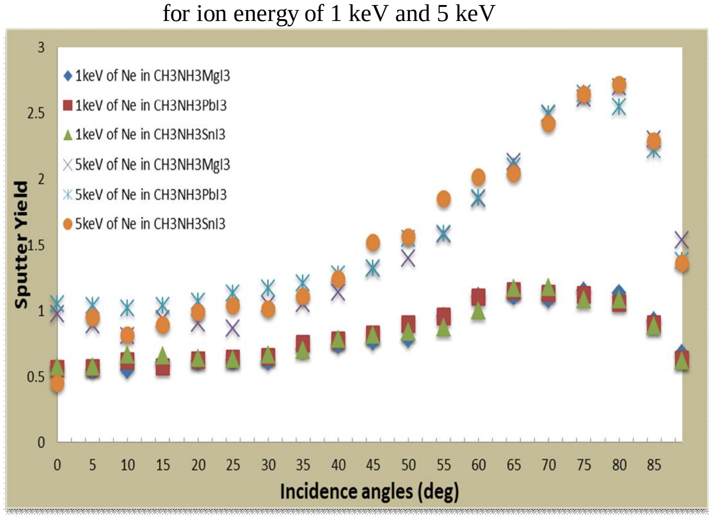


**Figure 6:** Sputter yield of Iodine for the erosion of I atoms from $Ne^+$ bombardment of target perovskites at different angles of incidence, for ion energy of 1 keV and 5 keV.

Results for Ar bombardment results are display below:

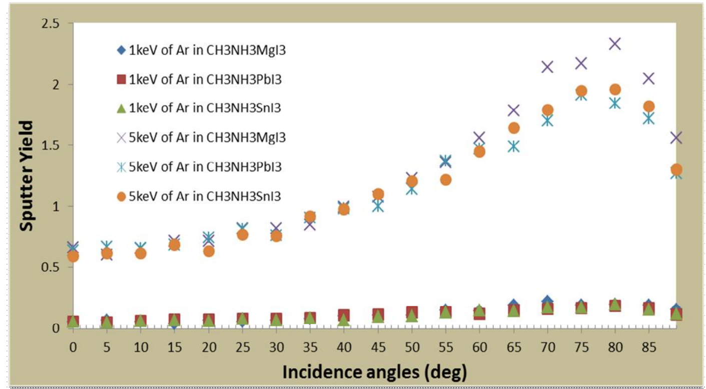


**Figure 7: :** Sputter yield of Carbon for the erosion of C atoms from $Ar^+$ bombardment of target perovskites at different angles of incidence, for ion energy of 1 keV and 5 keV

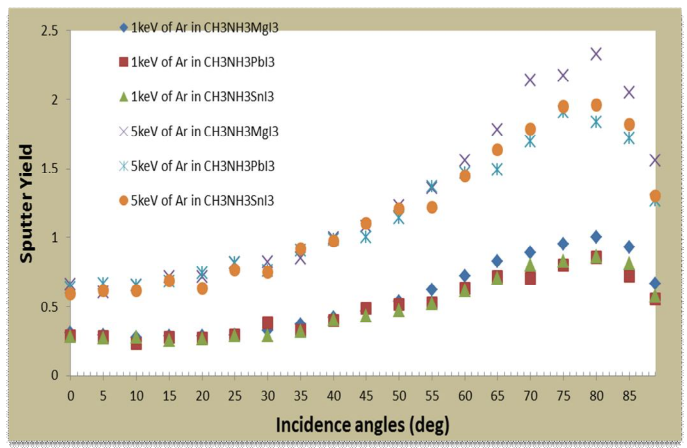


**Figure 8: :** Sputter yield of Hydrogen for the erosion of H atoms from $Ar^+$ bombardment of target perovskites at different angles of incidence, for ion energy of 1 keV and 5 keV.

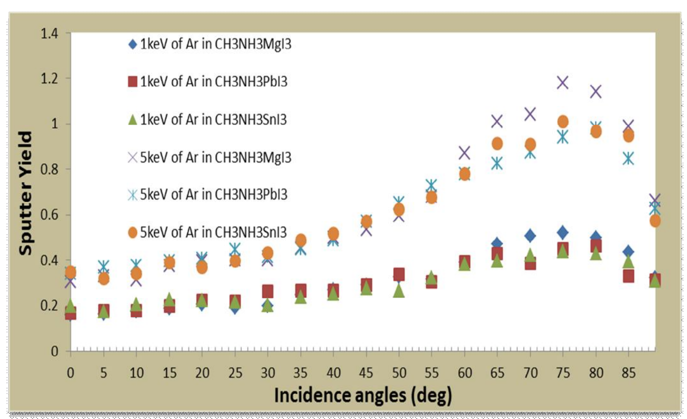


**Figure 9: :** Sputter yield of Nitrogen for the erosion of N atoms from $Ar^+$ bombardment of target perovskites at different angles of incidence, for ion energy of 1 keV and 5 keV

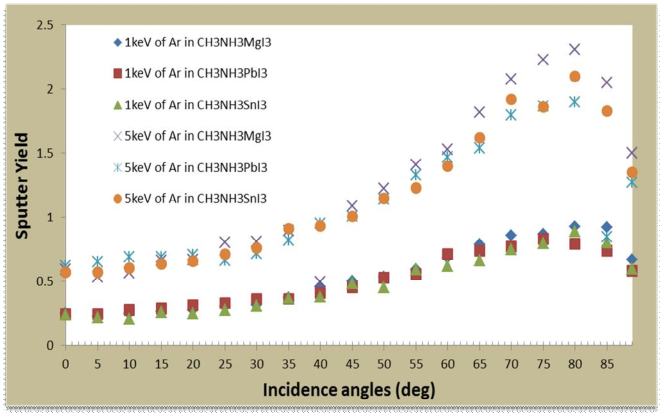


Figure 10: **:** Sputter yield of Hydrogen for the erosion of H atoms from $Ne^+$ bombardment of target perovskites at different angles of incidence, for ion energy of 1 keV and 5 keV

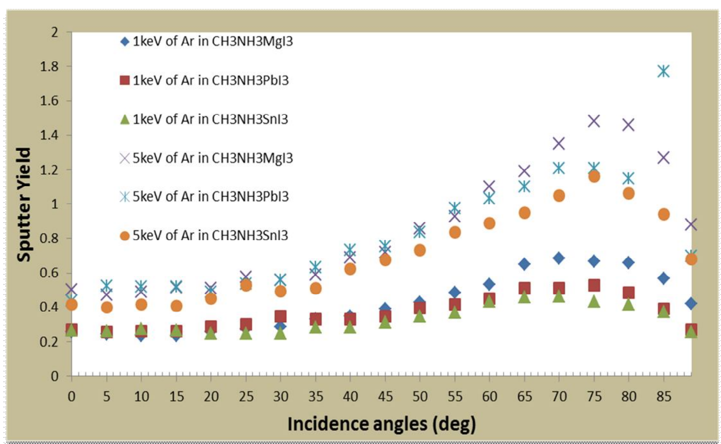


**Figure 11:** Sputter yield of Mg/Pb/Sn for their erosion from $Ar^+$ bombardment of target perovskites at different angles of incidence, for ion energy of 1 keV and 5 keV

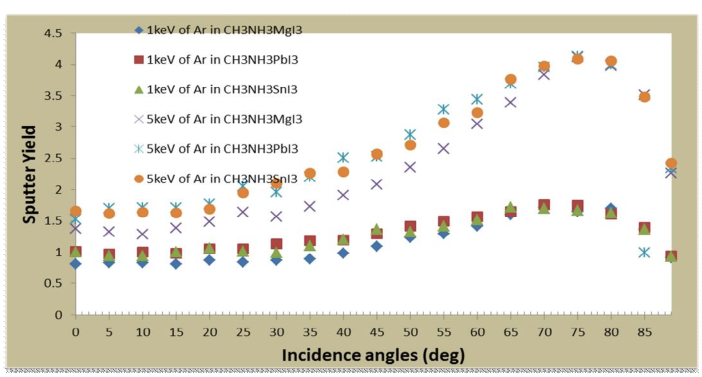


**Figure 12:** Sputter yield of Iodine for the erosion of I atoms from $Ar^+$ bombardment of target perovskites at different angles of incidence, for ion energy of 1 keV and 5 keV.

## 5. CONCLUSION

An ion-beam surface sputtering IBSS approach has been done to examine the physical factors accountable for variations in optoelectronic properties of both lead and lead-free metal halide perovskite materials and magnesium perovskite material in PV applications. And an MC simulation was employed to study the sputtering characteristics of ions in lead and these selected lead free metal halide perovskite and perovskite of an alkaline-earth metal ($CH_3NH_3MgI_3$) as a new viewpoint of confirming if $Mg^+$ in methyl ammonium magnesium iodide has the same sputtering characteristics as $Pb^+$ so as to know if it's a possible substitute for lead.

In this research, it can be concluded that sputtering results of lead perovskite and its best substitute so far, tin perovskite are very similar to magnesium perovskite. Couple with other benefits reported by other researchers, our work further confirms that magnesium can replace lead in lead perovskite, if its power conversion efficiency is not too low.

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