

Claudio make
perovskite solar cells
very commercially
attractive.



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Claudio Mastrocinque 12/1/17 Physical Chemistry Term Paper The Future of Solar Cells Silicon-based solar cells have been a dominant force in the solar energy field due to their exceptional efficiencies. However, the high manufacturing costs of these photovoltaic cells have motivated researchers to seek cheaper alternatives. Despite a lack of efficiency, perovskite solar cells show much more promise than its silicon counterparts.

The power conversion efficiency of perovskite solar cells has increased up to 21% in only 3 years, making it the fastest-advancing solar technology to date⁵. Furthermore, its low production costs and simple construction make perovskite solar cells very commercially attractive. Although perovskite solar cells have recently exhibited significant advancements, skepticism has surrounded these photovoltaic cells. Currently, the applications of perovskite solar cells are limited due to the toxicity that accompanies them. The lead composition of these cells make them hazardous to the environment, and therefore lessen their appeal. Fortunately, the reduction of lead content in perovskite solar cells has become a popular area of research. Elements such as tin, germanium, and copper have been investigated as possible alternatives to lead. Multiple Sn perovskite solar cells have recently emerged; reaching power conversion efficiencies of up to 6%¹.

Clearly, the efficiencies of Sn perovskite solar cells currently do not compare to its lead counterparts. However, Sn perovskite solar cells appear to be the most viable substitute for lead. In the paper titled "Highly Efficient Perovskite Solar Cells with Substantial Reduction of Lead Content," Liu, Fan, Li, Zhang, and Mai developed organometal halide perovskite solar cells in hopes of considerably reducing the lead content, as the title suggests.

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Through solvent engineering, $\text{CH}_3\text{NH}_3\text{Pb}(1-x)\text{Sn}_x\text{I}_3$ ($0 \leq x \leq 1$) perovskite thin films with varying Pb and Sn concentrations were obtained. A fluorine doped tin oxide-coated glass was cleaned, dried, and treated under oxygen plasma. Poly(3, 4-ethylenedioxythiophene) polystyrene sulfonate (PEDOT: PSS) was spun on the as-prepared substrate, and the thin film was annealed.

PEDOT: PSS is a transparent polymer that can be used to increase conductivity and surface photovoltage within the cell. PbI_2 and SnI_2 were separately dissolved in a mixed solvent system containing DMF and DMSO. Once the solutions were heated and mixed, the precursor solution was spun on the PEDOT: PSS layer. The DMSO intercalated with the $\text{PbI}_2/\text{SnI}_2$ through this solvent mediation, producing the $\text{PbI}_2/(\text{SnI}_2) \cdot (\text{DMSO})_x$ complexes.

Then, a methylamine hydroiodide (MAI) solution was spun on the substrate, and the thin films were annealed. Since MAI has a higher affinity for $\text{PbI}_2/\text{SnI}_2$ than that of DMSO, MAI exchanges DMSO and gives rise to $\text{CH}_3\text{NH}_3\text{Pb}(1-x)\text{Sn}_x\text{I}_3$ ($0 \leq x \leq 1$) perovskite thin films. The 6, 6-phenyl-C61-butyric acid methyl ester (PCBM) dissolved in dichlorobenzene was spun on the top of the perovskite layers.

Lastly, 6 nm $2,9$ -dimethyl- $4,7$ -diphenyl- $1,10$ -Phenanthroline (BCP) was deposited by thermal evaporation, followed by the deposition of an Ag electrode. A variety of techniques and instruments were used for characterization, including X-ray diffraction, photoluminescence, FT-IR, UV-vis, SEM, and XPS. By examining the crystallinity of $\text{CH}_3\text{NH}_3\text{Pb}(1-x)\text{Sn}_x\text{I}_3$ ($0 \leq x \leq 1$) thin films, the X-ray diffraction patterns displayed the structural differences of the films at varying volumes of Sn in the precursor solution.

First, Liu et al. observed the diffraction patterns for $x = 0$ and $x = 1$. The results showed that the perovskite phase changed from tetrahedral phase, $\text{CH}_3\text{NH}_3\text{PbI}_3$ ($x = 0$), to cubic phase, $\text{CH}_3\text{NH}_3\text{SnI}_3$ ($x = 1$). The researchers then observed the X-ray diffraction patterns of the perovskite between $x = 0$ and $x = 1$.

As shown in the figure below, the (110) peak of the perovskite shifted towards the (100) plane of the cubic phase as the amount of Sn increased, while the fluorine doped tin oxide (FTO) peak remained constant. Although not shown in the figure, the (211) and (202) peaks merged into a single peak corresponding to the (113) plane in the cubic phase as the Sn amount increased. These values refer to miller indices, a type of notation for planes of crystal lattices that is used in crystallography². The X-ray diffraction patterns suggested that Sn was involved in the alteration of the perovskite phase. The crystal structures of $\text{CH}_3\text{NH}_3\text{Pb}(1-x)\text{Sn}x\text{I}_3$ for $x < 0.5$ and $x > 0.5$, and a potential mechanism are provided below.

The stability of the $\text{CH}_3\text{NH}_3\text{Pb}(1-x)\text{Sn}x\text{I}_3$ ($0 \leq x \leq 1$) perovskite films were observed using X-ray photoelectron spectroscopy (XPS). XPS is a technique that is used to analyze the surface chemistry of a material, providing information such as the binding energy of the elements involved. When Sn was introduced, the Sn peak was fitted into two peaks at 455.

8 eV and 486.8 eV within the XPS spectra, corresponding to Sn^{+2} and Sn^{+4} respectively. As the Sn content increased, the Sn^{+2} tended to decrease, whereas the Sn^{+4} increased. The oxygen peak, fitted to SnO_2 , also increased as the Sn amount increased. Oppositely, the Pb peaks tended to

decrease as the Sn content increased. Therefore, Liu and his team concluded that Pb stabilizes Sn in its +2 state more readily, and that $\text{CH}_3\text{NH}_3\text{Pb}(1-x)\text{Sn}_x\text{I}_3$ ($0 \leq x \leq 1$) films prefer to be oxidized when the Pb content decreases. The XPS spectra provided in the figure below also suggest that the introduction of Sn^{+2} alters the coordination environment of Pb and I.

The UV-vis absorbance of $\text{CH}_3\text{NH}_3\text{Pb}(1-x)\text{Sn}_x\text{I}_3$ ($0 \leq x \leq 1$) was recorded at increments of $x = 0.125$. The optical absorbance band-edge was recorded, where the optical band edges refer to the lowest energy state of an electron in the valence band, and the highest energy state of that in the conduction band.

The optical absorbance band-edge of the perovskite film displayed an infrared-shift as the Sn amount increased. In addition, the photoluminescence was also recorded and displayed a similar infrared shift as the Sn content increased. However, the PL spectrum shifted to a shorter wavelength when $x = 1$, which corresponded to $\text{CH}_3\text{NH}_3\text{SnI}_3$ (no lead content). This unexpected phenomenon can be attributed to the tunable bandgap that occurs in the presence of multiple metals. Thus, the presence of both lead and tin in the perovskite film may have induced the infrared shift, and therefore the pure $\text{CH}_3\text{NH}_3\text{SnI}_3$ complex did not follow this trend. Images of the $\text{CH}_3\text{NH}_3\text{Pb}(0.$

$75)\text{Sn}_0.25\text{I}_3$ thin film were taken using a scanning electron microscope (SEM), along with elemental mappings of Pb, Sn, and I. The topography and composition of the thin film's surface can be obtained using a SEM. A beam of electrons scan the surface of the sample and interact with its atoms,

releasing secondary electrons in unique patterns. Backscattered electrons, electrons that come directly from the electron beam, and X-rays are also detected.

The signals given by the detectors are unique to the sample, and provide the user with high-resolution images of the shapes of the object⁴. According to the energy-dispersive X-ray spectroscopy (EDS), the Sn, Pb, and I appeared to be homogeneously distributed throughout the $\text{CH}_3\text{NH}_3\text{Pb}_{0.75}\text{Sn}_{0.25}\text{I}_3$ thin film. EDS analysis was performed, and the results infer that there was less Sn in the final perovskite film than the amount added in its preparation, which was likely due to a solubility issue. The SEM images illustrated the enlarged grain sizes of the $\text{CH}_3\text{NH}_3\text{Pb}_{(1-x)}\text{Sn}_x\text{I}_3$ ($0 \leq x \leq 1$) thin films with increasing Sn content.

The pure $\text{CH}_3\text{NH}_3\text{SnI}_3$ thin film exhibited poor coverage compared to the films containing Pb. Therefore, the SEM images confirm that Pb plays a key role in stabilizing the perovskite thin films.