

Low Cost Solar Cell Technology for Heterogenously Integrated Systems

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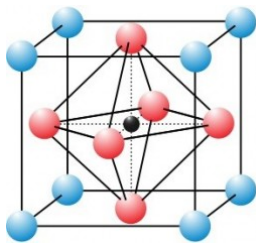
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Abstract:

Perovskite Solar Cells (PSCs) are an area of study that has grown exponentially in the past decade. Their sudden popularity is due to several factors; most notably that they are highly effective in increasing power conversion efficiency of solar cells, and are low-cost. A perovskite material is simply a specific crystalline structure, which is shown to the left, in figure 1 (Korjus [CC BY-SA 3.0 (<https://creativecommons.org/licenses/by-sa/3.0/>)]). The general formula is ABX_3 . A and B are cations, where A is greater in size than B, and X is an anion bonded to both cations. They are generally a hybrid organic-inorganic lead/tin halide, and are desirable for their flexibility, ease of management, low cost, and lightweight nature. This project focuses on optimizing this material to achieve the greatest power conversion efficiency, while also keeping production costs low. Several different factors are considered when researching which material is ideal, such as challenges to be overcome; voltage current density hysteresis, and long-term stability/lifetime. Numerous perovskite materials and their material properties were reviewed, and Methylammonium tin tri-chloride was chosen as the preliminary ideal perovskite layer material, due to its low production costs, chemical and thermal stability, and overall increased efficiency of PSCs. The final step in the project was to create and simulate the 2D device using TCAD Sentaurus Software. Once the material's properties were added, the mesh was built. The simulations run relay information about the electron and hole transport in the device. Due to time constrictions, the TCAD simulations were not run.



Introduction:

The goal of this project was to complete a literature study on PSC technology, and to develop a conclusion as to whether or not it can be integrated into other optoelectronic devices, such as lasers, and light-emitting diodes. The literature study was primarily done on scientific and

academic journals/papers, which focused on several different aspects of the PSCs; such as device structures, characteristics of the different perovskite layer materials, and environmental impacts.

There were three phases to this project. The first was to complete the research of the different materials, and their properties. The second phase was to formulate and understand a plan of how to produce the material, and the actual device. The third and final step was to run simulations of the 2D mesh device in TCAD Sentaurus software.

Two main challenges were found when attempting to complete this project. The first, is the presence of current density-voltage hysteresis. This is the phenomenon where the voltage drop measured from the open circuit to the short circuit is not equivalent to the voltage drop measured from the short circuit to the open circuit. Though there is no clear scientific reasoning for this, it is ambiguously approximated to be due to ion migration, or capacitance leakage. The second challenge faced is broader than the first; which is the overall stability of the devices. This is determined through several factors; including, but not limited to, structure of the device, how it reacts to harsh conditions, and the device's purpose.

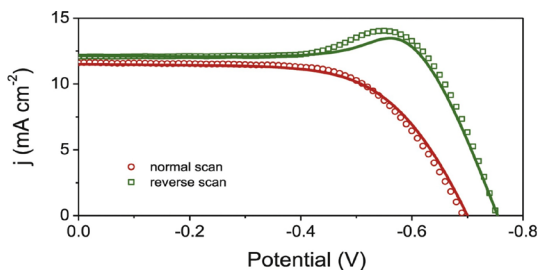
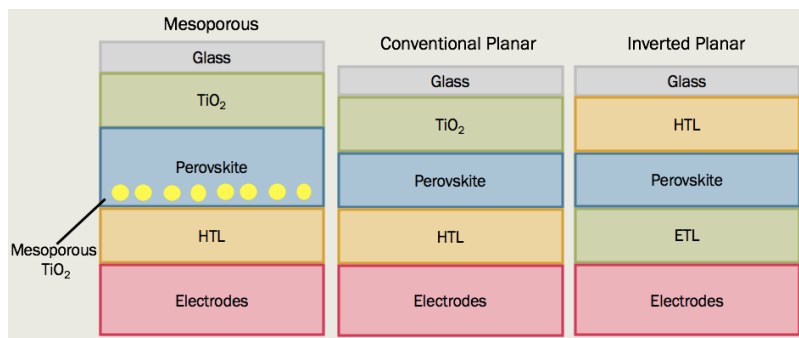


Figure 1, shown to the left, is a graph depicting the current density-voltage hysteresis effect, and the discrepancy that occurs between the “normal” scan and the “reverse” scan.

Kang, Dong-Ho and Nam-Gyu Park. “On the current-voltage”. *Advanced Materials*. 2019.

Phase 1:

Throughout the process, several different materials for the perovskite layer were researched, most consisting of the same organic component, with varying halide material. Due to the vast amount of information available through the papers, a checklist of the ideal perovskite material was devised. Several different factors were present on it, such as the material's chemical and thermal stability (long-term), whether or not the material increases efficiency, its operability in



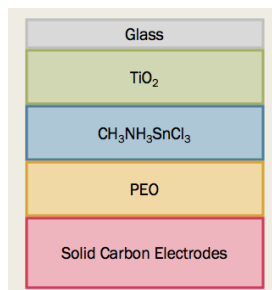
harsh conditions, lack of electrode degradation, and minimal current density-voltage hysteresis. Additionally, due to its toxicity, any material consisting of lead was annexed as an option. The three different structures that were compared for efficiency and viability are shown to the left in Figure 2.

The three different structures are (left to right) mesoporous, conventional planar, and inverted planar. These structures are roughly the same, with only minor differences. For example, the mesoporous and conventional planar are identical, except the mesoporous has a mesoporous

layer of TiO_2 embedded in the perovskite layer. Similarly, the inverted and conventional planar are almost the same, except for the inverted planar has the Electron Transfer Layer (ETL) and Hole Transfer Layer (HTL) switched. The conventional planar and mesoporous structures are most commonly used, though they both have advantages and disadvantages. For example, the mesoporous structures require a higher temperature in production, which means they cost more to produce. Conversely, the conventional planar structure results in increased hysteresis activity.

Based on this checklist, the final ideal material was determined to be methylammonium tin tri-chloride. Through experimental results, it has shown to be chemically and thermally stable long-term, and significantly increases power conversion efficiency in PSCs.

Phase 2:



The final device structure is shown to the left in Figure 3. The most commonly used method for producing PSCs is spin coating, as the devices produced via this method have been shown to have long-term stability, for a relatively low cost. Therefore, this method was determined to be used for creating this device.

The most challenging aspect of this phase was finding literature about the production of methyl ammonium tin tri-chloride. Though the other layers of the device are relatively common in the production of PSCs, methyl ammonium tin tri-chloride is lesser known, and lacks significant coverage in literature in regard to its production. Once information was found, the procedure was dependent on whether a crystalline or powder structure was desired. Ultimately, the crystalline product procedure was chosen, as it is more cost-effective.

Phase 3:

Due to time constraints, the simulations were unable to take place. However, the first step in the TCAD Sentaurus software integration was to input the material's properties and write a code for building the mesh (device), which was completed. These simulations were primarily used to evaluate the potential and feasibility of this specific PSC and its accompanying technology into other optoelectronic devices, to determine whether or not widespread integration is possible. This would be done through electron and hole carrier activity information relayed through the simulations and its data via electric field.

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