

Open Science Hardware Setup for investigating the Stability of Organic Solar Cells - Interim Report

Samuel Mendis

Department of Engineering Science, University of Oxford

Department of Physics, University of Oxford

12th January 2021

Chapter 1

Mechanical Design

1.1 Introduction

The design of the container was a process that encompassed several months. This chapter will go through the entire mechanical design process, outlining the key aims, decisions and analysis behind the container design.

During the mechanical design process, there were two different software's used: OpenSCAD and SOLIDWORKS. OpenSCAD is an open source software which is compatible with all major computer operating systems. This enabled the start of the design process to occur before the beginning of the Michaelmas Term. Furthermore, as mentioned in the introduction, using opensource software is a key tenant of this project as it needs to be replicable for teams worldwide. SOLIDWORKS however, is not open source, but was still used. This is because there is some key functionality in SOLIDWORKS which helps reduces the time needed on a few of the important steps (such as rendering photos, heat simulations and producing engineering drawings). However, as I will lay out further in the chapter, the main designs were completed on OpenSCAD, and they do hold enough information for a group elsewhere to replicate without significant difficulty.

A key consideration was what processes would be needed for the manufacturing of the container. The engineering department has different facilities which could be useful including: a workshop with a CNC machine, multiple different 3D printers, a mechanical workshop which I would be able to use along with an electrical workshop. These all were considered when designing the container and each will be mentioned during this chapter.

1.2 Specification

The first stage of the design process was to outline a specification for the testing container. These specifications were drawn from the project brief, the literature review and discussion with my supervisor Professor Moritz Riede. The specification of the design is outlined below:

1. The container must be able to accommodate a 30 mm x 30 mm substrate provided by AFMD research group.
2. The container must be leakproof to outside air.
3. The container must allow electrical connections from outside to connect to the substrate for measurements.
4. The container must enable the substrate to be heated to a given temperature¹.
5. The container must have a window allowing light to be shone into the box.
6. The container must contain a gas inlet.
7. The container should fit into the small glovebox inlet with diameter 150 mm.

This specification is a clear guide to what functionality there needs to be within the container, as well as any size limitations. As mentioned in both the introduction and literature review, it is essential for the container to be leakproof, to ensure that the solar cell does not degrade due to atmospheric O₂ and water vapour. This would result in flawed results due to the cell having some unmeasured degradation before the experiments even begin. Another important point in the specification is the ability of the cell to be heated to a given temperature*. This functionality is important as its role is to attempt to emulate a lifetime (20 years) of temperature degradation in the space of 3 months.

The gas inlet is another feature to enhance the degradation. This will be used to create a ‘cocktail’ of different gases (guided by the literature) to try and emulate lifetime degradation of the solar cell. The last point on the specification is to ensure the ease of use with the AFMD research group. The gloveboxes they use have a small inlet with a diameter of 150 mm, using this would vastly reduce the time needed to insert the solar cell into the testing container.

Along with the specification, some further goals were drawn up to provide aims that would provide important functionality but were not essential for the solar cell. These are shown below:

- Build a Python based GUI (Graphical User Interface) to enable programmatic testing of the solar cell
- Enable a programmable atmosphere for the box which should be embedded into the GUI built.

¹The reason for a none specific temperature

These goals are important to ensure the ease of use of the box, as well as to reduce the amount of time needed for setting up and running the container. The programmatic testing of the cell, along with a programmable atmosphere is useful as it enables the researchers to simply input time, temperature and what combination of gases, which then allows the system to run a test, all the time measuring the outputs and logging it for further analysis.

1.3 Initial Design

This specification provided the structure for the testing container. Using work done in the literature review, it was clear that this type of testing container is unusual for the market, thereby requiring innovative design. I was put in contact with Karl-Augustin Zaininger - a Physics researcher who had developed a simplified version of this device – to discuss viable methods for achieving the specifications. This conversation allowed me to create an extremely simple first iteration of the outer shell of the design shown in Figures 1.1 and 1.2.

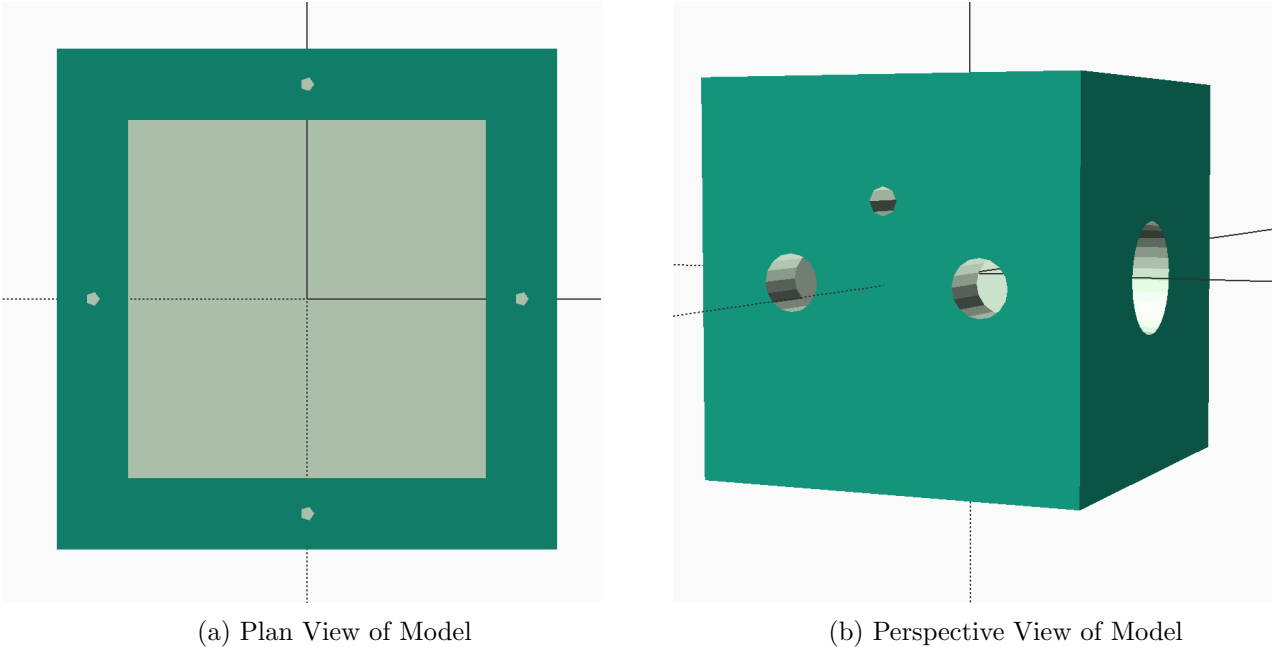


Figure 1.1: Showing a Plan and Perspective view of the First Iteration of the Outer Shell

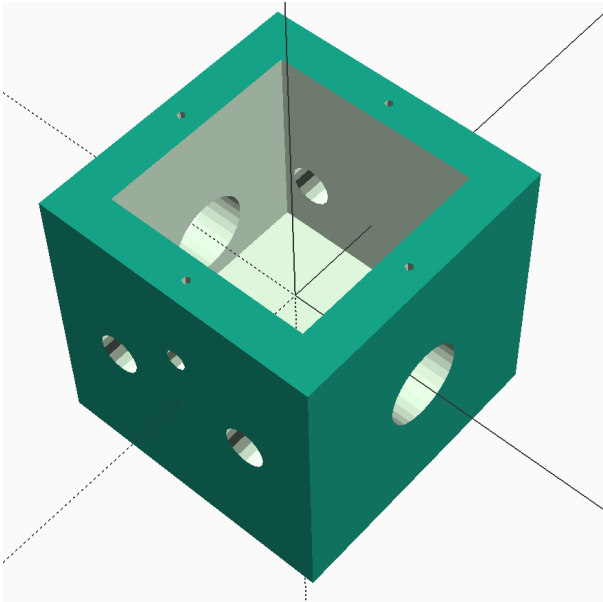


Figure 1.2: Showing Isometric View of the Outer Shell

This model is supposed to coincide with a smaller module named the Substrate Holder, which is designed to sit within the outer shell, holding the substrate, temperature sensor and heater, shown in Figure 1.3. The substrate holder is designed to be a removable component which can be edited to match the substrate provided. During the design process, this module was designed to be 3D printed to ensure low costs and easy modification.

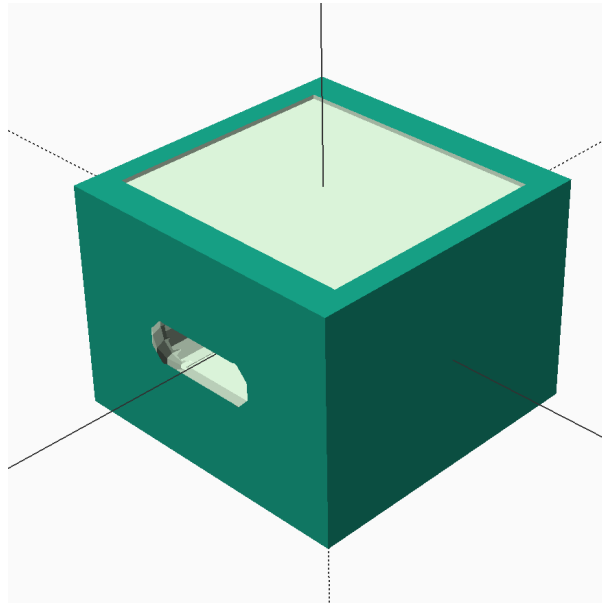


Figure 1.3: Showing the Isometric view of the first iteration of the Substrate Holder

Both the substrate holder and Outer Shell were 3D printed to provide a physical representation of the model (with a photo shown in Figure 1.4), where it became possible to see some of the flaws that were hidden by the virtual design. The first thing was that this design was very small, making it difficult for use within the glovebox. This was a problem as all assembly needed to occur within a glovebox to ensure there would be no unwanted oxygen or water residue able to degrade the cell. Adding to this, it seemed that there wouldn't be enough room to wire the components in the container, this would cause significant problems as the modularity of the design would be compromised. This would go against one of the tenants of the project (modularity) which would be a problem when thinking of using this set up on different substrate layouts.

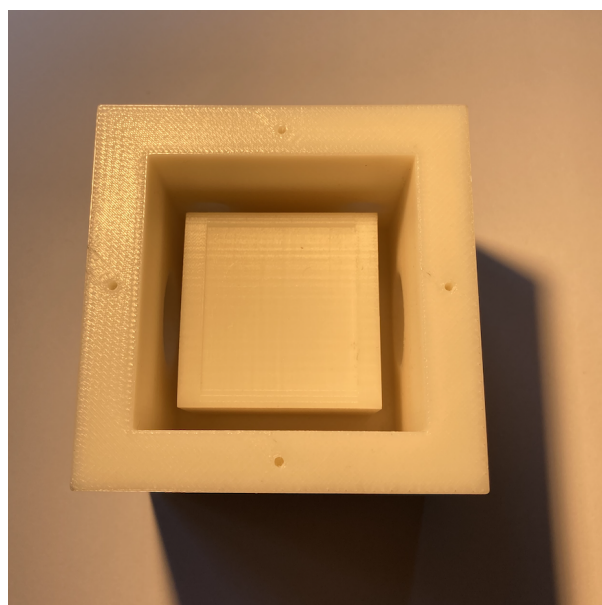


Figure 1.4: Showing the result of the first 3D print of the model

1.4 Final Models

These problems caused a redesign of the container, resulting in the model shown in figure (n). The Outer Shell is larger in this model with dimensions 100 mm* 110 mm* 77 mm, with a wall thickness 16 mm, resulting in more space within the container. Additionally, there was a rethink of the sealing method, to eliminate the need of directly screwing onto glass, risking a break, therefore a lid was constructed for the substrate holder, which would cause the glass window to be sandwiched between 2 O-rings creating an airtight seal. The changes to the outer shell can be seen in Figure 1.5.

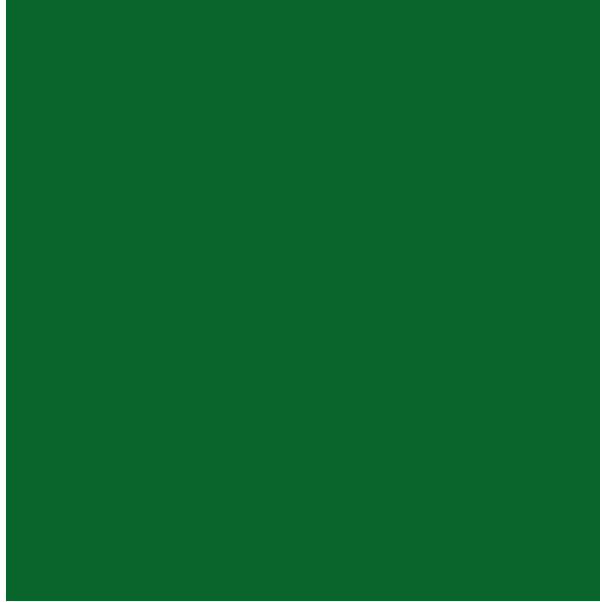


Figure 1.5: The Final Outer Shell model.

The substrate holder was also modified with the intention of being unique to this particular substrate layout resulting in a more detailed design. The substrate layout was provided to me by Dr. Grey Christophoro, a researcher working in the Physics department, and can be seen in Figure 1.6.



Figure 1.6: Showing the substrate layout provided by Dr. Christophoro.

As shown in Figure 1.6 the substrate has x contact points and y cells, meaning that the substrate holder needs to provide a method to cleanly contact the contact points, without hindering the flow of air around the cell, or blocking the light incident on the cell surface. The solution was to develop a small lid which would be screwed into the substrate holder, thereby providing downward pressure onto the substrate to ensure clean contacts with the pins. This lid was designed so that the outline did not block any light

being incident on the cells. The lid outline can be seen in Figure 1.7.

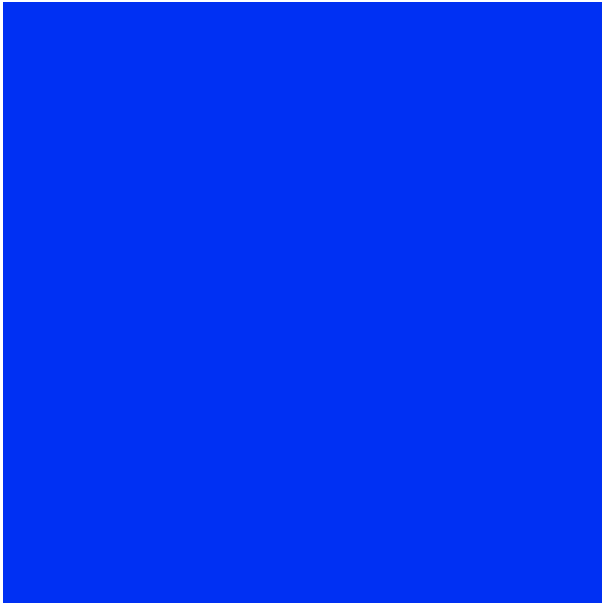


Figure 1.7: Showing the lid used to exert downward pressure on the substrate.

Another important consideration was the ability for the substrate holder to be easily attached to the outer shell within the glovebox. Therefore, the substrate holder needs to have electrical wiring within it, to easily connect up the solar cell with the monitoring device. This process required more time than planned as it was surprisingly difficult to come up with a viable idea. However, conversations with the electrical workshop helped me come up with a simple idea of creating a ‘plug’ which would enable the substrate holder to be connected to wiring that in turn would be connected with the monitoring device. This will be spoken about in the later chapter on electrical design, however, required the altering of the substrate holder so that pins could be placed at the top and the bottom with wires running through the container.

Moreover, when speaking to Professor Riede, he pointed out that there needs to be air flow below the substrate for the mixture of gases to have any substantial effect on the degradation of the solar cell. This led to a slight change which can be seen in figure n of 2 holes below where the substrate is meant to sit, which lead to empty space where there can be a good range of mixing to encourage degradation. Another issue was where the heater and temperature sensor would sit. This lead be to place the two holes running through the substrate holder one on top of the other to place the sensor and the heater. These holes were positioned there tactically so that the sensor temperature could be correlated with the predicted substrate temperature by modelling and testing *Link to different chapter*. These changes are shown and labelled in Figure 1.8.



Figure 1.8: The Final Substrate Layout