Final Scientific/Technical Report

Project Title: Solar Power Generation Development

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Executive Summary: This project centered on creating a solar cell prototype enabling significant reductions in module cost and increases in module efficiency. Low cost was addressed by using plentiful organic materials that only comprise 16% of the total module cost, and by leveraging building integrated PV concepts that reduce the cost of key module components to zero. High efficiency was addressed by implementing multiband organic PV, low cost spectral splitting, and possibly integrating photovoltaic and photothermal mechanisms. This research has contributed to the design of multiband organic PV, and the sealing of organic PV cells. If one assumes that the aggregate multiband efficiency can reach 12%, projected cost would be \$0.97/W. If the sealing technology enables 10 to 20 year lifetimes, the LCOE will match that of domestic coal. The following sections describe progress towards these goals.

Project Activity Overview:

Original hypotheses and planned approaches

PV systems must become more efficient and less costly in order to be widely accepted in the marketplace. Our design will surpass known theoretical limitations of single junction collectors by combining a low cost PV cell (10% efficiency) with a cost-effective PT design (30% efficiency). The resulting 40% integrated efficiency will reduce payback times to about 5 years with collector area compatible with residential applications. Our ultimate goal is to integrate PV and PT collection into residential building materials.

Omega's approach leverages significant thin film and materials expertise. PV cells will be formed by depositing optimized low cost organic thin films between two properly chosen metallic thin films. The potential of low cost organic PV materials has not been widely realized because of low and highly variable efficiency. The organic transistor literature indicates that carrier mobility can vary over several orders of magnitude. We contend that organic thin film deposition parameters can be adjusted to optimize carrier mobility, improve excitonic diffusion, and maximize PV efficiency. Further, organic materials can be configured to harvest multiple spectral bands. We plan to separate these bands via spectral splitting for efficient collection by the appropriate material.

Problems encountered
Based on extensive literature research, optimization of organic PV efficiency was an expected challenge. We have progressed from Schottkys with low efficiencies (less than 0.01%) to heterojunctions in both red and blue bands with efficiencies in the one to three percent range. Photothermal collection efficiency reached 50% despite a number of physical leaks from the unoptimized design and assembly scheme and an uninsulated back surface.

Impact of problems
Our red absorbing PV cell attained 3.1% while the blue absorbing cell attained 1.6%. Similar cells reported in the literature indicate that the red cell should attain 8.3% and the blue cell should attain 3.9%. Our spectral splitting models predict that these two cells reported in the literature can be combined to reach an aggregate efficiency of 10.2% - which would have exceeded our goal. The following section lists several adjustments that we plan to address to bring our cells up to values reported in the literature. Further, we have not been able to test our sealed cells for enough time to project lifetimes, though early tests are promising.

Departure from plan
Our primary departure centers on planned product embodiments. Ideal BIPV designs may prevent the PV/PT integration that we originally envisioned.

Ongoing Solar R&D at Omega Optical:
This grant has allowed Omega to enter the solar field. Rapid progress has been made over the last two years, but much remains to be done. We have attained an aggregate PV efficiency of about 4% without trying the following enhancements – which should allow us to reach an aggregate efficiency of at least 10 to 12%.

- Fabricate, measure and seal devices under dry, oil free and inert conditions to control the effects of oxygen and water vapor.
- Optimize thickness of the absorber layers and find the balance between higher absorption and efficient exciton diffusion.
- Improve crystallinity of the thin films which would result in higher mobilities.
- Optimize transport layers for efficient charge transport and collection.
- Investigate growth on templates
- Fabricate bulk hetero junctions to achieve higher charge dissociation.

- Harness the near IR region with additional organics.
- Doping of the transport layers and absorbing layers.
- Investigate tandem structures
- Explore alternative transparent electrodes

Omega Optical will proceed with this effort - addressing the above list, performing accelerated lifetime tests, and defining product embodiments.

Comparison of Accomplishments with Original Goals & Objectives: The following tasks match those identified in our statement of project objectives. The bullets and figures describe to what extent each objective was met.

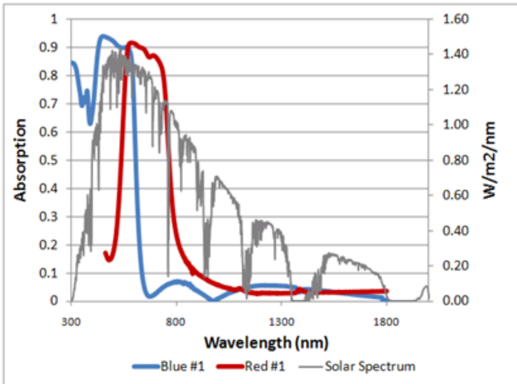
PHASE 1 (First Year Program)

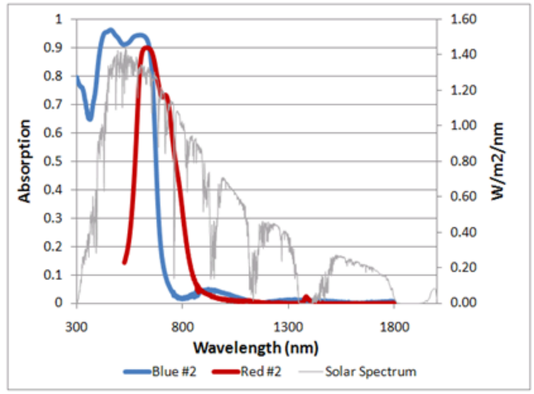
Year 1Task 1: Assess Thin Film Properties (August 2009 – January 2010)

- Acquired and set up 3 full vacuum deposition systems for the deposition of transparent conducting oxides, organic materials and metals. Systems are equipped with temperature control, thickness monitors and methods of applying electric fields during depositon.
- Installed optoelectronic test instrumentation - including a Kelvin Probe (for work function), a Keithley test system (for resistivity, trap density, work function, V_{oc}, I_{SC}, FF), and a magnet (for mobility)
- Developed other characterization methods (optical microscopy, UV/VIS/NIR transmission and reflectance, FTIR)
- Software has been written for extracting optical constants and thickness from reflectance/transmittance data
- Established a relationship with University of Vermont for thin-film characterization by XRD, SEM

Task 1.1: Deposition and evaluation of key organic semiconductors

- Ten different red-absorbing metallic phthalocyanines have been deposited and characterized including p-type semiconductors: MPc:H (where M = Cu, Fe, Co, Ni, TiO, Ag, Zn, and Mn), and n-type semiconductors: MPc:F (where M = Cu, Co).
- Deposited blue and near-infrared absorbing organic compounds including: CuPc:Cl, CuPc:Cl/Br, naphthalocyanines, diindenoperylene (DIP), perylene tetracarboxylic dianhydride (PTCDA), perylene tetracarboxylic diimide derivatives (PTCDI), diketo pyrrolo pyrrole (DPP), and quinacridone (QA).
- Narrowed down the possible organic compounds to two classes that span the visible spectrum- the phthalocyanines, perylenes and perhaps the DPPs.





- Investigated the relationship between film morphology/ device performance and deposition parameters by varying deposition rate, substrate temperature, field strength and annealing processes (using heat or solvent).
- Observed a correlation between organic crystal size and charge mobility.

Device Structure	Purity (%)	Treatment	Mobility (cm2/Vs)	Crystal size (micron)	Crystal form (X-ray Data)
ITO/CuPc/Ag	97	As deposited	2.00E-06	0.05	alpha
ITO/CuPc/Ag	99.99	As deposited	1.60E-03	0.05	alpha
ITO/CuPc/Ag	99.99	Post Deposition Anneal	8.20E-02	20	beta

<u>Task 1.2</u>: Deposition and evaluation of metals for electron and hole collection

- Deposited Cu, Al, Ag, Mg, and Zn films
- Chemically treated purchased ITO-coated glass to adjust the work function from roughly 4.2 to 5.6 eV to match the organic semiconductors of interest

<u>Year 1Task 2</u>: Device Design (November 2009 – January 2010)

<u>Task 2.1</u>: Model and/or evaluate optical absorption and carrier transport

- Module-level optimization
  - The efficiencies of three different module geometries were modeled using *Essential MacLeod* software and *TF Calc Thin Film* calculator.
  - Models matched transmission and absorbance spectra of copper phthalocyanine and numerous blue absorbers.
  - Absorption by active layers was calculated to exceed 67% of the light between 300 and 850 nm in our best geometrical arrangement.
  - Other photovoltaic geometries investigated varied in their absorbance efficiency between 300 and 850 nm from 41% to 62%.

- The estimated production of free carriers at the cell-level as a function of time was determined at different light levels using *Mathematica 6.0*. This model was adapted from the literature (Terao, Sasabe & Adache. Applied Physics Letters 90, 2007). Calculated free carriers were consistent with observed results.

<u>Task 2.2</u>: Model and/or evaluate optical absorption and thermal transfer

- Developed a Microsoft Excel-based finite-difference method for predicting temperature distributions in the substrate and underlying liquid.

- The finite-difference method is a well-established numerical approach that approximates the solutions to differential equations. It employs the use of "nodes" or points in space where discrete numerical values are calculated. There is a 2D array of nodes in the substrate and because thorough mixing of the liquid is assumed, a 1D array of nodes in the fluid beneath the substrate

- Standard, well-established equations for convective, surface-to-surface radiative and conductive heat transfer are utilized to generate the boundary conditions

- Assumptions include a flat-plate geometry and no thermal loss from the back of the module. Any solar load impinging on the system is assumed to either be absorbed by the substrate or by the underlying liquid.

- The Excel model was validated with a full computational fluid dynamics (CFD) treatment. Agreement was within 1% between the two approaches.

- Data from our photothermal prototype was fed into the model using ambient temperature and wind speed acquired from a nearby weather station.

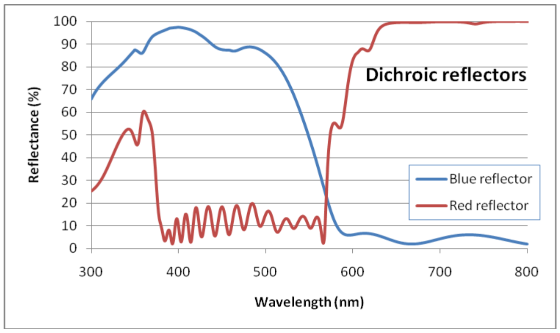
- Predicted temperature changes from the model were 20-30% higher than measured. This is not unexpected since our prototype was not insulated and the model assumes there is no heat loss from the backside of the channel.

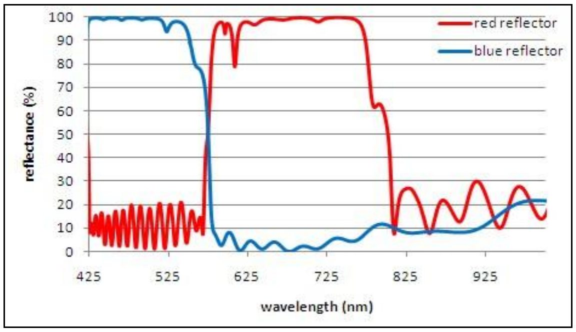
<u>Year 1 Task 3</u>: Prototype Fabrication and Test (February 2010 – July 2010)

<u>Task 3.1</u>: Fabricate PV cell structure

- Schottky cells (Al/CuPc/ITO/glass) were fabricated with a series of organic thicknesses. Our results are similar to those reported in the literature (Kwong et al, Proc SPIE Vol 4801, p. 7, 2003) for the thicker films.

- Constructed spectral splitting dichroic mirrors which will be used in a v-shaped module to direct the light onto the appropriate blue- or red-absorbing cell. Dichroic mirrors can be designed with a small number of layers to minimize production time and cost. Four different designs are shown below.





- Designed gold / dielectric stacks with induced transparency as an alternative to ITO for use as a transparent electrode. These stacks need to be built so their suitability as electrodes can be assessed.

Task 3.2: Fabricate PV/PT cell structure

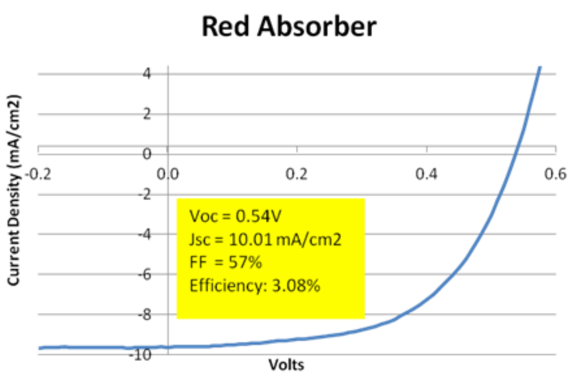
- Two photothermal prototypes were assembled- 1) a glass–covered PVC channel through which water flows, and 2) an aluminum fin attached to a copper pipe containing flowing water
- Two experiments were carried out, one with just the PT component (control structure), and one which was painted with clear polyurethane containing microcrystals of OPV molecules in suspension, to mimic the effect of having an OPV stack adhered to the surface.
- With the control structure, we observed maximum temperature changes of 2.9 and 4.4 ^{o}C/m for the glass and Cu structures respectively. With the simulated OPV top layers, we observed a slight increase in maximum temperature changes of 3.3 and 5.1 degrees per meter for the glass and Cu - presumably due to heat transfer from the absorbing OPV layers into the cooling water
- Calculated peak efficiency (based on comparison with the photothermal model) is on the order of 50%. Many commercially available PT systems have a certified efficiency in the 70-85% range.
- We were unable to integrate functional PV cells with PT components within the contract period.

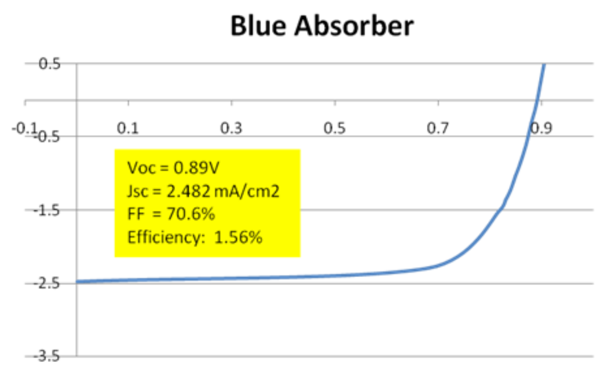
Year 1 Task 4 – Project Planning and Reporting (August 2009 – July 2010)
Reports and other deliverables were provided in accordance with the Federal Assistance Reporting Checklist following the instructions included therein.

PHASE 2 (Second Year Program)

Year 2 Task 1: Optimize Cell Level Fabrication (August 2010 – January 2011)

- Investigated relationship between film morphology, substrate temperature and electric field strength and orientation
- Set up and utilized tube furnace for organic molecule purification.
- Began to optimize several organic heterostructures, including both small-molecule and polymeric systems.





- Deposited ITO films with resistivity in the 100s of micro ohm cm range.
- Metallic pads were deposited for in-situ tests at the cell level.
- Typical R&D cells are 2 by 2 mm in size. Larger cells are being deposited on our own ITO layers.

Year 2 Task 2: Module Design and Fabrication (February 2011 – April 2011)

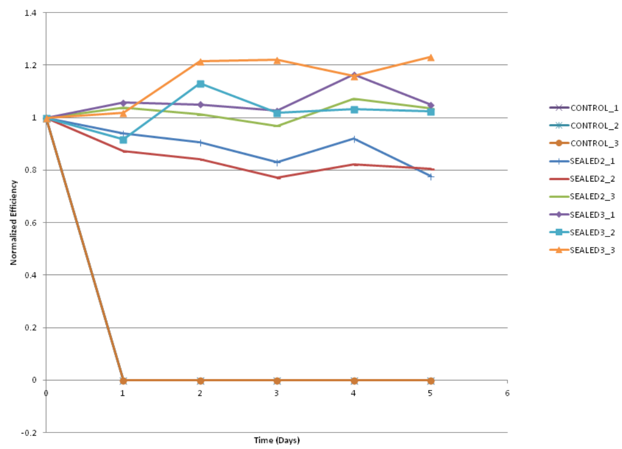
- Modeled the angular performance of various folded spectral splitting designs over various sun positions.
- Estimated the performance of a transmissive spectral splitting design to be 12%, assuming an 8% efficiency of both red and blue absorbers. For reference - Heliatek has published single cell results above 8%, and our original PV goal is 10%.
- Investigated sealing options including SiO_x thin films, epoxies with desiccants, athermal laser welding, and window assembly techniques. Athermal glass-to-glass welding has been demonstrated on several pieces of our glass. A three step OPV sealing method has been established.

- We will integrate our PV and PT systems when larger PV cells become available.

Year 2 Task 3: Module Prototype testing (May 2011 – July 2011)

- Expose module prototype to initial temperature/humidity and UV stress tests
  PV devices were sealed with our three step process and tested daily.

- Evaluate V_{OC}, I_{SC}, Fill Factor as a function of time and environmental stress - see figure below. Unprotected cells fail rapidly, while the protected cells are unchanged within measurement accuracy. We plan to continue these tests for longer intervals and under accelerated conditions.



- Consider module design iterations based on organic degradation mechanisms
  This will be addressed going forward.

- Measure spectrally resolved efficiency (η_{PV} goal is 10%, η_{PT} goal is 30%)
  We have met the PT goal and see a path towards the PV goal.

Year 2 Task 4 – Project Planning and Reporting (August 2010 – July 2011)

Reports and other deliverables were provided in accordance with the Federal Assistance Reporting Checklist following the instructions included therein.

Patents: Two patentable concepts are under consideration:

Method for hermetic sealing of thin film photovoltaics

Low cost spectral splitting in organic photovoltaics