Transfer Matrix Optical Modeling

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This document describes, briefly, how to use the Matlab script, TransferMatrix.m to calculate optical interference and absorption in multilayer stacks. This software uses the transfer matrix method, where transmission and reflection are calculated for each interface in the stack as well as attenuation in each layer. The theory behind this calculation is described in detail in the literature[1, 2] and will not be covered here. This model assumes normal incidence and does not take into account scattering.

The program consists of four files; the TransferMatrix.m file contains the main program as well as three helper functions. Using the program requires no knowledge of the code itself; however we have made every effort to thoroughly comment the code in case the user wishes to modify it. We will focus on how to use the program as designed to calculate optical fields in multilayers.

User definable parameters

All of the user definable parameters are defined at the top of the script:

lambda	array of wavelengths for which all values will be calculated. wavelength values must lie within the bounds of the wavelengths for which the optical constants (*n* and *k*) are defined in *Index_of_Refraction_library.xls*.
stepsize	numerical constant that defines the stepsize (in nanometers) between each point calculated in the spectrum.
plotWavelengths	array of wavelengths for which to plot interference patterns in the device. to add wavelengths, simply add elements to the vector.
layers	cell array of strings corresponding to the materials that compose each layer in the stack. **these strings must correspond to the names used in the *Index_of_Refraction_library.xls* file (minus the '_n' or '_k' extension).** the order of materials matters! light is incident on the stack "from the left"
thicknesses	vector describing the thicknesses of each layer (in nanometers). the thickness value at a given index in this vector corresponds to the thickness of the layer of the same index in *layers*.
plotGeneration	boolean switch. when true, TransferMatrix will include a plot of the generation rate as a function of thickness within the active layer of the device. if *plotGeneration* is set to *true*, *activeLayer* must be defined.
activeLayer	numerical constant that defines the index of the material responsible for photocurrent generation. this index corresponds to the index of the active material in the *layers* and *thicknesses* vectors. for instance, if *layers* = {'material1' 'material2' 'material3'} and material2 is the active layer, then *activeLayer* should be set to 2.

```
33    %----------BEGIN USER INPUT PARAMETERS SPECITIFCATION----------------
34    %
35 -  lambda=350:800; % Wavelengths over which field patterns are calculated
36 -  stepsize = 1;     % The electric field is calculated at a latice of points (nm)
37                      % in the device cross section seperated by this distance
38
39    % plotWavelengths specifies which wavelengths to plot when plotting E-field
40    % intensity distributions (figure 1). Specify values by adding wavelength
41    % values to the array. Values must be within the range of calculated
42    % wavelenths (ie. must be an element of the lambda array). All wavelengths
43    % are in nanometers.
44 -  plotWavelengths = [400 450];
45
46    % Specify Layers in device (an arbitrary number of layers is permitted) and
47    % thicknesses.
48    %
49    % Change these arrays to change the order or number of layers and/or
50    % thickness of layers. List the layers in the order that they appear in the
51    % device starting with the side the light is incident on.  THE NAMES OF THE
52    % LAYERS MUST CORRESPOND TO THE NAMES OF THE MATERIALS IN THE INDEX OF
53    % REFRACTION LIBRARY FILE, 'Index_of_Refraction_library.xls'. The first
54    % layer must be the transparent substrate (glass) or 'Air' if the active
55    % layers are on the reflective electrode (rather than transparent electrode) side
56    % of the device.  The layer thicknesses are in nanometers.
57
58 -  layers = {'SiO2' 'ITOsorizon' 'PEDOT' 'P3HTPCBMBlendDCB' 'Ca' 'Al'}; % Names of layers o
59 -  thicknesses = [0 110 35 220 7 200];  % thickness of each corresponding layer in nm (thic
60
61    % Set plotGeneration to 'true' if you want to plot generation rate as a
62    % function of position in the device and output the calculated short circuit current
63    % under AM1.5G illumination (assuming 100% internal quantum efficiency)
64 -  plotGeneration = true;
65 -  ActiveLayer = 4; % index of material layer number where photocurrent is generated
66    %
67    %----------END USER INPUT PARAMETERS SPECIFICATION--------------------
68
```

All user definable parameters are set within this section of code.

Index of refraction library file

The optical constant data for each available material is defined in the *Index_of_Refraction_library.xls* file. This file consists of wavelength-dependent optical constant data for each material. *n* and *k* are the real and imaginary parts of the complex index of refraction and are defined for each material at each wavelength. The names of the columns containing each set of data must follow the format, *material_n* and *material_k*, where *material* can be any designation for a material and *_n* and *_k* designate which column refers to n and k respectively. The first column must always be domain of wavelengths for which the material optical constants are defined.

We have provided optical constants for the materials we typically use. **Note: many materials' optical properties depend on processing conditions!** ITO deposited under different conditions can have drastically different optical constants and electrical conductivity (in our case, we purchase ITO coated glass substrates from Sorizon technologies and measured the optical constants using variable angle spectroscopic ellipsometry). Similarly, the optical constants of PEDOT:PSS and the P3HT:PCBM blend depend on doping density (in the case of PEDOT:PSS) and deposition technique, solvent, post-annealing temperature and time, and of course material quality (contamination and regioregularity). Therefore, while these results are typical, you may

wish to measure the optical constants of your materials or procure them from a supplier or from the literature.

Index_of_Refraction_library.xls [Compatibility Mode] - Microsoft Excel

H14   0.13

| Wavelength (nm)	Air_n	Air_k	Al_n	Al_k	Ca_n	Ca_k	Ag_n	Ag_k	aSi_n	aSi_k	SiO2_n	SiO2_k
300	1	0	0.27571	3.61265	3.46	0.848	0.13	2.92	1.73	2.77	1.4607	
301	1	0	0.27754	3.62538	3.43	0.85333	0.13	2.92	1.73	2.77	1.4606	
302	1	0	0.27937	3.63812	3.4	0.85867	0.13	2.92	1.74	2.77	1.4605	
303	1	0	0.2812	3.65085	3.37	0.864	0.13	2.92	1.75	2.77	1.4605	
304	1	0	0.28303	3.66359	3.34	0.86933	0.13	2.92	1.76	2.8	1.4604	
305	1	0	0.28485	3.67632	3.31	0.87467	0.13	2.92	1.78	2.8	1.4603	
306	1	0	0.28668	3.68906	3.28	0.88	0.13	2.92	1.795	2.8	1.4602	
307	1	0	0.28851	3.70179	3.25	0.88533	0.13	2.92	1.81	2.82	1.4601	
308	1	0	0.29034	3.71453	3.22	0.89067	0.13	2.92	1.81	2.82	1.46	
309	1	0	0.29217	3.72726	3.19	0.896	0.13	2.92	1.82	2.82	1.46	
310	1	0	0.294	3.74	3.16	0.90133	0.13	2.92	1.83	2.82	1.4599	
311	1	0	0.29596	3.75263	3.13	0.90667	0.13	2.92	1.85	2.82	1.4598	
312	1	0	0.29792	3.76525	3.1	0.912	0.13	2.92	1.85	2.82	1.4598	
313	1	0	0.29988	3.77788	3.07	0.91733	0.13	2.92	1.85	2.82	1.4597	
314	1	0	0.30185	3.7905	3.04	0.92267	0.13	2.92	1.86	2.82	1.4596	
315	1	0	0.30381	3.80313	3.01	0.928	0.13	2.92	1.86	2.85	1.4596	
316	1	0	0.30577	3.81575	2.98	0.93333	0.13	2.92	1.88	2.85	1.4596	
317	1	0	0.30773	3.82838	2.95	0.93867	0.13	2.92	1.9	2.85	1.4595	
318	1	0	0.30969	3.84101	2.92	0.944	0.13	2.92	1.9	2.88	1.4595	
319	1	0	0.31165	3.85363	2.89	0.94933	0.13	2.92	1.91	2.88	1.4594	
320	1	0	0.31361	3.86626	2.86	0.95467	0.13	2.92	1.92	2.88	1.4594	
321	1	0	0.31557	3.87888	2.83	0.96	0.13	2.92	1.94	2.88	1.4593	
322	1	0	0.31754	3.89151	2.8	0.96533	0.13	2.92	1.94	2.88	1.4592	
323	1	0	0.3195	3.90414	2.77	0.97067	0.13	2.92	1.945	2.88	1.4591	
324	1	0	0.32146	3.91676	2.74	0.976	0.13	2.92	1.95	2.88	1.459	
325	1	0	0.32342	3.92939	2.71	0.98133	0.13	2.92	1.97	2.91	1.4589	
326	1	0	0.32538	3.94201	2.68	0.98667	0.13	2.92	1.98	2.91	1.4589	
327	1	0	0.3274	3.95461	2.65	0.992	0.13	2.92	1.99	2.91	1.4589	
328	1	0	0.32944	3.96718	2.62	0.99733	0.13	2.92	2.01	2.91	1.4588	

Example calculation

Suppose we want to calculate the optical properties for a typical poly-3-hexylthiophene:[6,6]-phenyl-C_{61}-butyric acid methyl ester (P3HT:PCBM) solar cell. A typical device structure consists of a glass substrate/ITO/PEDOT:PSS/P3HT:PCBM/Ca/Al (where PEDOT:PSS refers to poly(3,4-ethylenedioxythiophene) poly(styrenesulfonate)). The thickness of the glass substrate is not important as it is thick enough that interference effects have practically no effect. Typical thicknesses for the remaining layers are (in nm), 110/35/220/7/200. We are interested in the visible spectrum where the materials absorb (~350 nm - ~800 nm) and suppose we wish to see the interference patterns of 400, 500, and 600 nm light within the device. We would also like to see the position-dependent generation rate in the device. The user-defined parameters would then take the following values:

3

```
lambda=350:800;
stepsize = 1;
plotWavelengths = [400 500 600];
layers = {'SiO2' 'ITOsorizon' 'PEDOT' 'P3HTPCBMBlendDCB' 'Ca' 'Al'};
thicknesses = [0 110 35 220 7 200];
plotGeneration = true;
activeLayer = 4;
```

The script is then run either by pressing *F5* in the editor or by typing, *TransferMatrix* at the
Matlab command prompt (the current directory must be the directory containing the
TransferMatrix.m file and associated *.xls* files). After a few seconds of computation, the results
are plotted in four figure windows and the predicted short-circuit current (J_{sc}) is output in the
command window (this assumes 100% *internal quantum efficiency* at all wavelengths).

4
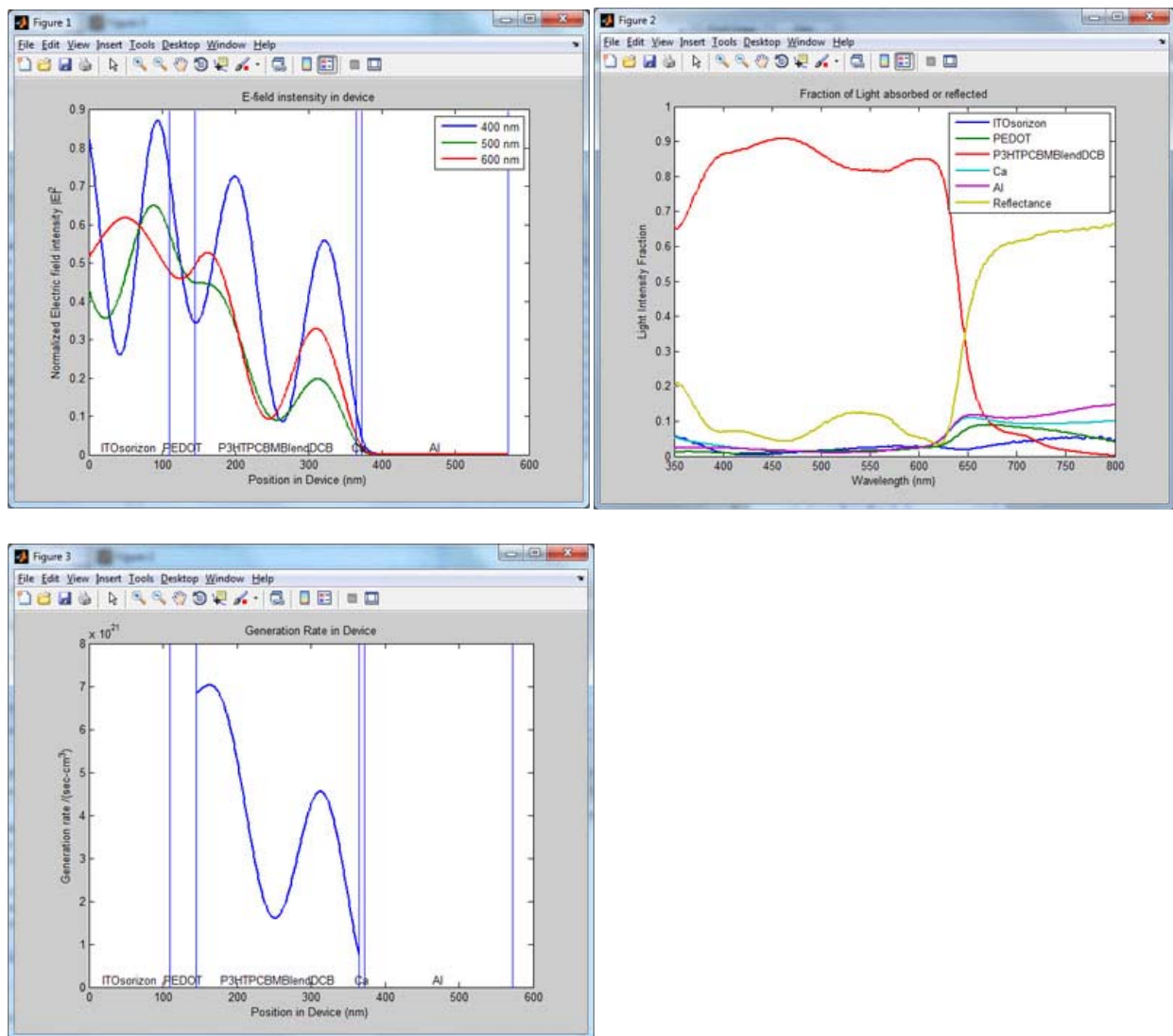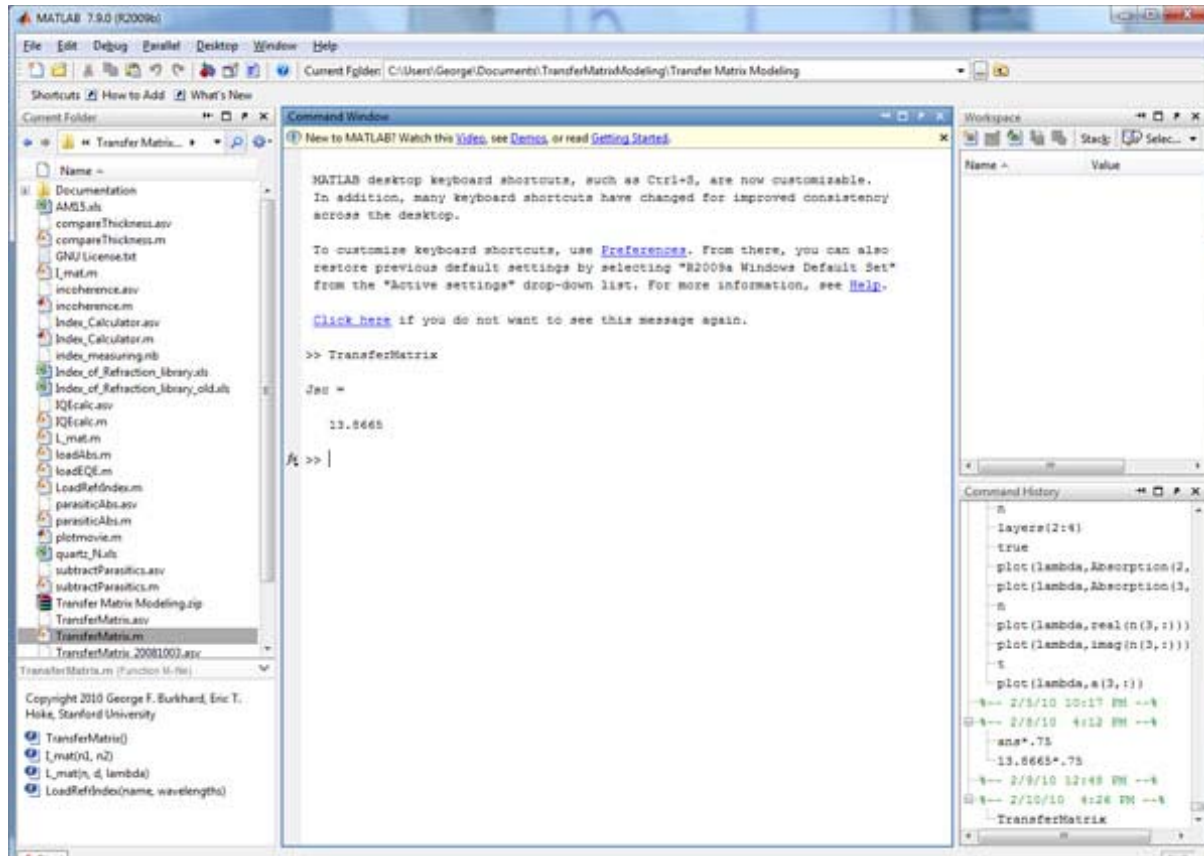
By default, *TransferMatrix.m* creates variables, *absorption*, *reflection*, *parasitic_abs* and *lambda* in the base workspace when run. These arrays contain the absorption data for each material in the stack, the total reflection one would expect to measure from the device, the total parasitic absorption and the list of wavelengths for which these values correspond. This should be sufficient for most users, however, if you wish to output other local variables to the workspace (eg. E-field), you can add more *assignin('base',*variable_name,local_variable*)* commands to the end of the main function.

TransferMatrix_VaryThickness.m

This additional Matlab script calculates the short circuit current that would be obtained if the device had an IQE of 100% as the thickness of one of the layers is varied over values specified by the user. The program generates a graph of the short circuit current (in mA/cm^2) versus the thickness of the layer. It also creates the variables *Jsc* and *Thickness* in the base workspace containing the short circuit current data and the layer thicknesses which the currents correspond to. The methods and parameters are the same as for *TransferMatrix.m* except for the following additional parameters:

LayerVaried	numerical constant that defines the index of the material layer that will be varied in thickness. this index corresponds to the index of the active material in the *layers* and *thicknesses* vectors. for instance, if *layers* = {'material1' 'material2' 'material3'} and

	you want to vary the thickness of material2, then *LayerVaried* should be set to 2.
VaryThickness	numerical constant 1D array that defines the different thicknesses values for the layer which will be varied in thickness (*LayerVaried*). for instance if you would like to calculate the short circuit current for devices where one layer is 50, 60, 70 or 80nm then set *VaryThickness* = [50 60 70 80]; or *VaryThickness* = 50:10:80;

References

[1]   L. A. A. Pettersson, L. S. Roman, O. Inganas, *J. Appl. Phys.* **1999**, *86*, 487.
[2]   P. Peumans, A. Yakimov, S. Forrest, *J. of Appl. Phys.* **2003**, *93*, 3693.