S4: Stanford Stratified Structure Solver

I. Introduction

S4 is a frequency domain code to solve layered periodic structures. Internally, it uses Rigorous Coupled Wave Analysis (RCWA; also called the Fourier Modal Method (FMM)) and the S-matrix algorithm. S⁴ was developed by Victor Liu of the Fan Group in the Stanford Electrical Engineering Department [1].

http://www.stanford.edu/group/fan/S4/#main

The S4sim developed at Purdue University uses S4 as an engine for fast, accurate calculation of optical propagation through complex 3D structures. It can rapidly solve optical problems involving thin films that occur in our daily life – for example, antireflection coatings for glasses and solar cells, or pavement marking for highways. It is also suitable for producing publication-quality optical research simulation results. This tool allows users to enter parameters to define multilayered structures with their physical dimensions. S4 has also been combined with a comprehensive materials database known as PhotonicsDB, which incorporates materials optical data drawn from carefully vetted sources.

II. Graphical User Interface Description



Figure 2.1 Simulation options page

A. Simulation options

First, the user should select simulation input type:

- "Graphical interface" for ease-of-use parameter-input interface.
- "S4 input deck" for advanced users control-file-input interface.

B. Parameters

1. If the user selects "Use Graphical Interface":

(a) Material selection

🗙 54	
<u>F</u> ile	
Simulation Option + 2 Parameter + 6 Simulate Load Example	S
Loader	
Example: New	
Materials Layers Simulation	
Select the Number of Materials: 3	
Material #1 Material #2 Material #3	
Category: Dielectric	<u> </u>
Dielectric	
Material: Crystalline Silicon	
Symbol: Si Description: Crystalline Silicon Range (nm): 163-2479 Provider: http://www.sopra-sa.com Interpolation method: Cubic spline interpolation with quadratic end points.	Select categories and materials from photonicsDB or select user-defined materials.
< Simulation Option	Simulate >

Figure 2.2 Materials selection page

At the top, there is a loader providing several examples for users to simulate some common or important structures.

After selecting number of materials used in the structure, the user can select Category and specific materials from PhotonicsDB to see the material descriptions. The user can also opt to manually define the relative permittivity of the material.

(b) Layer configuration

With all the materials chosen, the user should then set the layers of the structure using the "Layer" tab.

🗙 S4		
<u>F</u> ile		
Simulation Option + 2 Parameter + 3 Simulate		
Loader		
Example: New	•	
Materials Layers Simulation		
Set basis vectors		
 Notice: ~ Be careful of the relationship between the basis vector, thickness of the layers and the size of the patterns inside each layer. ~ Be careful of the correlation between the basis vector, wavelength range and reduced units. coordinate of the first lattice base vector: (x1 = 270 mm, y1 = 0 mm) coordinate of the second lattice base vector: (x2 = 0 mm, y2 = 270 mm) 		
Select Number of layers: 6	•	
Repeated layers		
Do you need to repeat a range of layers?: • m no		
repeated layers from: 1		
to: 10		
Times the layers are copyed:		
		M
< Simulation Option	Simulate >	

Figure 2.3 Layer configuration page (1)

🗙 S4	
<u>F</u> ile	
O Simulation Option → ② Parameter	+ () Simulate
Disable Layer #1	1: • ves ; #2: • ves ; #3: • ves
Disable Laver	
	re. • • • • • • • • • • • • • • • • • • •
Disable Layer #7: 🔘 📖 🗍	no ; #8: •no ; #9: •no ; #10: •no
Semi-Infinite Top Layer Layer 4	Layer 6 Semi-Infinite Bottom Layer
Thickness of the laye	r: 500nm
Material #	t: 3 + -
Select Number of patterns in this laye	r. 2 + -
Pattern 1 Pattern 2	
Select the shap	e of the pattern: Circle
	Material #: 1
	Center: ({ 0 , 0 })
Parameters setting for each laver	Radius: 0
	Angle: 0
	of the polygon: [x1,y1,x2,y2,]
·	
	Get poynting flux: Select desired output for each
	Get Electromagnetic energy: • • • no layer
	li v
< Simulation Option	Simulate >

Figure 2.4 Layer configuration page (2)

The user can define the size of the lattice and select number of layers. The S4 graphical interface supports a maximum of 10 unique layers. The user can also repeat a range of layers with a maximum of 10 periods.

All the layers can be disabled or enabled for quick modification of the design. In each layer, a maximum of 2 patterns can be set.

Furthermore, for each layer, the Poynting flux with respect to a user-defined offset, as well as the electromagnetic energy integrated over the volume can be simulated. All the desired outputs need to be selected here.

(c) General simulation setting

After settings of the layers, general simulation setting can be made under "Simulation" tab.

🗙 S4	
<u>F</u> ile	
① Simulation Option → ② Parameter → ③ Simulate	
Loader	
Example: New	•
Materials Layers Simulation	
Max Fourier expansion orders: 1	+ -
Set Excitation Planewave	
Planewave angles: phi= 0 , theta= 0	
S-wave: $ E_s = 1$, phi_s= 0	
P-wave: E_p = 1 , phi_p= 0	
Output Frequency Setting	
default	
reduced units -> period: type in a number or the word "default". Default means to set the period to 0.9 " wavelengthmin. If you set it to 1, the frequency will have a unit of chrm, where c is the speed of light.	
The wavelength range is: min= 300nm , max= 1100nm , step= 2nm	
Smooth the resulted curves?: 💿 📰 🔄 no	
Smoothing range of moving average (nm): 10	
Note: Be aware of the value in reduced unit. The change in reduced unit will affect the value of electromagnetic energy but not Poynting flux. This is because the energy is a integral of the whole layer's volume, while the flux is normalized by the incidence flux. Also be aware of the wavelength range of each material. The setting of wavelength canbe exceed the wavelength range of all materials used. The maximum wavelength can be set is 1 nm; The maximum wavelength can be set is 3000 nm. If you encounter error, please check the wavelength range of all materials under "Materials" tab.	
< Simulation Option	Simulate >

Figure 2.5 General Simulation setting page

The maximum number of Fourier components, the nature of the excitation plane wave (including its amplitude and polarization) and the frequency range can all be set here. The user can also select to smooth the output spectra and decide the smoothing moving average. This will only change the output curves but not the output log.

(d) Parameter setting complete

After finishing all the parameter settings, click "Simulate" button to run the program.

2. If the user selects "S4 input deck":

(a) Input control file code

K 54	
File	
Simulation Option Parameter Simulate Load examples, upload or download contrrol file	
Example: binary_grating	-
<pre>Input deck In a 1D pattern, the pattern should be specified only with rectangles. The y-dimension of the rectangles is ignored. S = 54. NewSimulation() S:SetUmulation() S:SetUmulation(27) Material definition S:AddMaterial("Silicon", (12,0)) real and imag parts S:AddMaterial("Silicon", (12,0)) real and imag parts S:AddMaterial("Vacuum", (1,0)) S:AddMaterial("Vacuum", (1,0)) S:AddLayer('AirAbove',name 0, thickness 'Vacuum')background material S:AddLayer('Slab', 0.5, 'Vacuum') S:SetLayerPattenRectangle('Slab', which layer to alter 'Silicon', material in rectangle (0,0), center 0, tilt angle (degrees) S:AddLayerCopy('AirBelov', new layer name 0, thickness 'AirAbove') layer to copy</pre>	
Choose "Upload" to upload your script from local disk	N.
Options	
Number of processors: 1	+ -
Walltime: 2h	
< Simulation Option Sin	nulate >

Figure 2.6 S4 input deck page

The user can select examples, upload a control file, write their own control file code, and/or download the control file in the input deck.

(b) Parameter setting complete

After the user finishes entering the control file code, he or she can click the "Simulate" button to run the program.

C. Simulation Results

Three types of results will be displayed after simulating the structure: the control file (input or generated by S4sim), the output log from S4, and the spectral curves.

× 54				
File				
Simulation Option + ② Parameter + ③ Simulate	Download the control file			
Result Control File				
<pre>S = S4.NewSimulation() S:SetLattice({1.000000, 0.000000}, {0.000000, 1.000000}) S:SetNumG(1)</pre>				
S:AddMaterial("vacuum", {1.000000,0.000000}) S:AddMaterial("SICR", {7.720210,41.651648}) S:AddMaterial("material_3", {-100.000000,-14.000000}) S:AddMaterial("material_4", {1.795600,0.000000}) S:AddMaterial("material_5", {5.712100,0.000000}) S:AddMaterial("material_6", {14.364100,0.000000})	Select output type			
S:AddLayer('Layer_Above', 0.000000, 'vacuum') S:AddLayer('layer_1', 0.337037, 'material_4') S:AddLayer('layer_2', 0.196667, 'material_5') S:AddLayer('layer_3', 0.110741, 'material_6') S:AddLayer('layer_4', 7.407407, 'SICR') S:AddLayer('layer_6', 1.851852, 'material_3')	Lua Control file generated			
S:AddLayerCopy('Layer_Below', 0.000000, 'Layer_Above')				
S:SetExcitationPlanewave({0.000000,0.000000}, {1.000000,0.	.000000}, (1.000000, 0.000000})			
<pre>frequency = {0.900000, 0.894040, 0.888158, 0.882353, 0.87 real_eps_1 = {1.000000, 1.000000, 1.000000, 1.000000, 1.0 imag_eps_1 = {0.000000, 0.0000000, 0.0000000, 0.000000, 0.000000, 0.0000000, 0.00000000</pre>	76623, 0.870968, 0.865385, 0.859873, 0.854430, 0 000000, 1.000000, 1.000000, 1.000000, 1.000000, 000000, 0.000000, 0.000000, 0.000000, 0.000000,			
<pre>real_eps_2 = {7.720210, 9.109094, 10.172001, 11.006612, 1 imag_eps_2 = {41.651648, 40.225378, 38.941339, 37.806615,</pre>	11.692610, 12.252476, 12.749287, 13.193563, 13.5 , 36.803512, 35.926192, 35.192912, 34.561095, 34			
real_eps_3 = {-100.000000, -100.000000, -100.000000, -100 imag_eps_3 = {-14.000000, -14.000000, -14.000000, -14.000	0.000000, -100.000000, -100.000000, -100.000000, 0000, -14.000000, -14.000000, -14.000000, -14.00			
<pre>real_eps_4 = {1.795600, 1.795600, 1.795600, 1.795600, 1.7 imag_eps_4 = {0.000000, 0.000000, 0.0000000, 0.000000, 0.0</pre>	795600, 1.795600, 1.795600, 1.795600, 1.795600, 000000, 0.000000, 0.000000, 0.000000, 0.000000,			
<pre>real_eps_5 = {5.712100, 5.712100, 5.712100, 5.712100, 5.7 imag_eps_5 = {0.000000, 0.000000, 0.000000, 0.000000, 0.0</pre>	712100, 5.712100, 5.712100, 5.712100, 5.712100, 0.000000, 0.000000, 0.000000, 0.000000, 0.000000, 0.0000000,			
Find: 🔰 🔮 🕢	Select All			
1 result	Clear			
< Parameter				

Figure 2.7 Control file



Figure 2.8 Output Log



Figure 2.9 Spectral Curves

Spectra for reflection, transmission, and integrated layer electromagnetic energy can be generated here.

The raw text output or images can be downloaded here.

A clear button on the bottom right could be used to clear the plots and the simulation. It is recommended to clear the result after each simulation before going back and changing the parameters for best performance.

III. Case Study





IV. Conclusion

This new S4 GUI has been demonstrated to be capable of reproducing published research results as shown in Section III, Case Study. The user interface is extremely flexible and allows a wide range of optical structures in 1D, 2D, and 3D. Users are strongly encouraged to test advanced optical problems of interest, and communicate their results and challenges with the authors.

References:

1. Victor Liu and Shanhui Fan, "S⁴: A free electromagnetic solver for layered periodic structures," *Computer Physics Communications* **183**, 2233-2244 (2012) <u>http://dx.doi.org/10.1016/j.cpc.2012.04.026</u>.

2. M. Ghebrebrhan, P. Bermel, Y. Avniel, J. Joannopoulos, and S. Johnson, "Global optimization of silicon photovoltaic cell front coatings," *Opt. Express* **17**, 7505-7518 (2009).