Incoherent Propagation of Light in Coherent Models

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Abstract: In the finite element based modeling and simulations only the coherent propagation of light is considered. However, in reality when light passes the thick layer it loses the phase information and its coherent nature due to the spatial, temporal or spectral incoherence. In this work, we present two methods to include the incoherent layer in coherent based simulations: (a) phase matching and (b) phase elimination approach. Additionally, appropriate scaling down of incoherent layer thickness from mm range to few hundred nm range is shown. Methods are implemented in COMSOL multiphysics and verified on bare glass substrate and on complete thin film amorphous silicon solar cell in superstrate configuration.

Keywords: Solar cells, surface textures, incoherent light

1. Introduction

In studying different optoelectronic devices, the supporting thick layers (e.g., glass layer in thin-film solar cells) in mm range are presenting the challenge to include them in the finite element method (FEM) based simulations. The first issue is the thickness of the layer which might be too thick to be appropriately discretized and effectively included in simulations. In 3-D simulations the number of mesh elements would easily increase over the limit set by the numerical solvers or available resources in modern workstation computers. The second issue is how to include the incoherent propagation in the coherent FEM-based model. It is well know the light might lose its coherent nature and the reason might be spatial or/and spectral incoherent source (e.g. tungsten lamp, spectral width of laser source). Since the coherence length of such sources are usually much smaller than thicknesses of mm thick supporting layers in optoelectronic devices, such as solar cells, we have to consider the incoherent propagation of light in those layers. The main idea is to eliminate the interface term [1] in Poynting vector of backward and forward propagating wave regardless the reason for incoherence.

Eq. 1 describes the simplified Poynting vector for forward and backward propagating wave in arbitrary isotropic media.

$$\mathbf{EE}^* = \left(\mathbf{E_0}e^{jk\mathbf{r}} + \mathbf{E_1}e^{jk\mathbf{r}-\mathrm{jk2d-j\varphi}}\right)\left(\mathbf{E_0}e^{jk\mathbf{r}} + \mathbf{E_1}e^{jk\mathbf{r}-\mathrm{jk2d-j\varphi}}\right)^* = |\mathbf{E}_0^2| + |\mathbf{E}_1^2|e^{Re[-jk]4d} + \underbrace{|\mathbf{E_0}\mathbf{E}_1^*|e^{-jk2d-j\varphi} + |\mathbf{E_0}\mathbf{E}_1^*|e^{jk2d+j\varphi}}_{interference\ term} \quad (1)$$

Where **E** is electric field strength of forward ($\mathbf{E_0}$) and backward ($\mathbf{E_1}$) propagating wave(s), **r** is position vector at the front interface inside of incoherent layer, *k* is the wavenumber (in case of an absorbing medium a complex value which is wavelength dependent), φ is the phase shift due to reflectance at the subsequent layers and *d* is the thickness of the incoherent layer. The last term in Eq. 1 describes the interference term which has to be 0 in case of incoherent propagation of light.

2. Theory

The interference term can be nullified in means of proper variation of the thickness *d* for very small value. We present two approaches for eliminating interference term (a) phase matching and (b) phase elimination approach [2] and the method to decrease the thickness of thick incoherent layer from mm range to few hundred nm range.

2.1 Phase Matching Approach

In this approach the interference term is directly eliminated in one simulation run, first by finding the phase shift φ of the common electric field of reflected waves (in this approach it is assumed φ is known) and then to adjust the thickness to nullify the interference term.

$$2kd + \varphi = \frac{\pi}{2} + m\pi,\ \mathrm{m} = 0, \pm 1, \pm 2, \dots \quad (2)$$

The new thickness is calculated based on equation (2) by selecting the integer *m* in the way the modified thickness (*d*’) is as close as possible to original thickness (d) so we do not introduce additional error due to shorter/longer path that may affect absorptance in layer, Eq. 3.

$$d' = Re\left[\frac{\frac{\pi}{2}+m\pi-\varphi}{2k}\right],\ \ \mathrm{m} = 0, \pm1, \pm2, \ldots \qquad (3)$$

The derivation with the exact and not simplified Eq. 3 can be found in our published article [2].

2.2 Phase Elimination Approach

In this approach we do not need the knowledge about the phase of backward propagating wave, thus it is much easier to implement this method to the structure where the layers and/or structure is complex (e.g. random textures at interfaces of thin-film solar cells). This approach is also suitable for rough interfaces of incoherent layer. Approach is based on eliminating the phase in Eq. 1 in two steps. In the first step we calculate the solution at original thickness and in second step we modify the thickness in the way the superposition of results eliminates the interference term [2], the second thickness is given by Eq. 4 for perpendicular incidence of light.

$$d' = d - Re\left[\frac{\lambda}{4N(\lambda)}\right] \qquad (4)$$

where N is the wavelength (λ) dependent complex refractive index of the incoherent layer.

2.3 Thinning down the incoherent layer

Since the incoherent layers are usually very thick (up to a few mm) and thus are not suitable for inclusion in FEM based simulations. The mesh of incoherent layer would present in most cases more than 99% of all mesh, thus we have developed the approach to thin down the incoherent layer. In the case of incoherent layer from the Eq. 1 only the propagation term is left, Eq. 5.

$$\mathbf{EE}^* = |\mathbf{E}_0^2| + |\mathbf{E}_1^2| e^{Re[-jk]4d} \qquad (5)$$

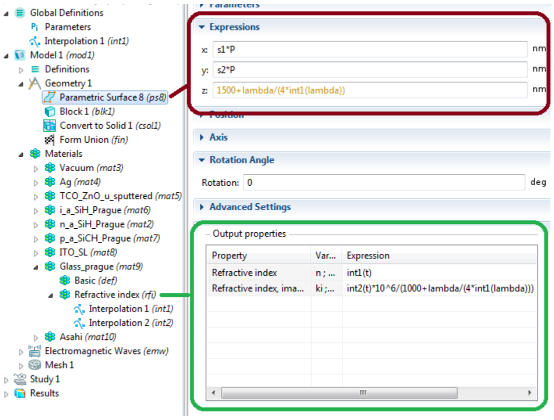
If we scale down the incoherent layer the exponent should remain the same, thus, the extinction coefficient (κ, included in wavenumber k) has to be increased by the same factor this way the Poynting vector remains the same. By thinning down the thickness we have to operate with modified-thinner thickness in equations 3 and 4. However the one has to be careful that modified extinction coefficient is not to large, it has to be much lower compared to real part of refractive index other way the modified extinction might influence the reflectance and transmittance at the interfaces.

3. Results

The numerical models were prepared for a COMSOL simulation software version 4.3b with a Radio Frequency (RF) module, however, the new Wave Optics module can be used as well. Two 3-D numerical models are presented one with the bare glass layer with thickness of 1 mm and one with the thin-film amorphous silicon solar cell (a-Si SC).

3.1 Numerical model of bare glass layer

In the first model build for glass substrate we have applied both methods for incoherent propagation of light in COMSOL, additionally the coherent simulation of glass was performed in order to compare the methods. Perpendicular incidence of light is considered in simulations, the glass was thinned down from thickness of 1 mm to ~1 µm. Since the thickness obtained from methods is changing with the wavelength, we have built the dynamic model that changes the thickness and extinction coefficient of incoherent layer automatically.



x: s1*P nm
y: s2*P nm
z: 1500+lambda/(4*int1(lambda)) nm

Rotation: 0 deg

Property	Var...	Expression
Refractive index	n ; ...	int1(t)
Refractive index, ima...	ki ;...	int2(t)*10^6/(1000+lambda/(4*int1(lambda)))

Figure 1. Settings of parameters related to phase elimination approach in COMSOL.

In Figure 1 settings for phase elimination approach are presented. The parametric surface position is changed dynamically according to wavelength (lambda) and the imaginary part of refractive index (int1). In material parameters we had to change extinction coefficient (int2) due to scaling of thickness by factor of 1000 and due to phase elimination approach, Eq. 4.

The reflectance (*R*) and transmittance (*T*) of 1 mm thick glass layer were measured with Perkin Elmer Lambda 950 spectrophotometer in the wavelength region of 300 to 900 nm, with the step size of 10 nm. The simulations were done in the same wavelength region with the same step size. In order to reduce computation time the mesh was generated at every wavelength, with the discretization of at least 10 elements per effective wavelength (wavelength in the material). This way the mesh was greatly reduced for higher wavelengths. Very good agreement is obtained between measured values and values obtained by both modeling approaches, Fig. 2. Additionally, the coherent simulation with thickness of 1 mm was performed (black dashed curve) with different wavelength steps. In order to reproduce all the interferences the wavelength step size was reduced from 10 nm to 0.025 nm, the right graph of Fig. 2, where only a small wavelength region was simulated 650-652 nm.

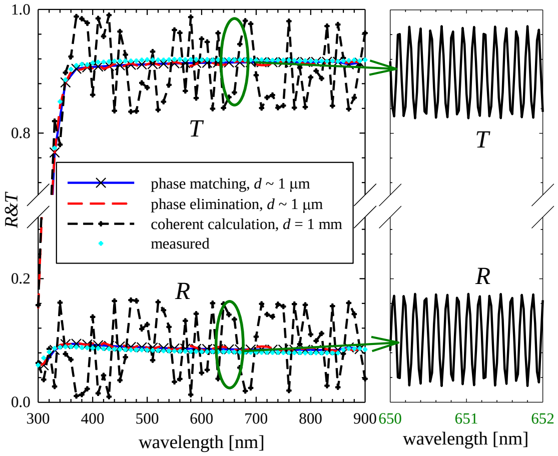


Figure 2. Measured *R* and *T* of glass substrate (symbols) compared to simulated *R* and *T* (lines). The right graph shows the very dense interferences obtained by coherent simulations of glass using very small wavelength step of 0.025 nm.

3.2 Numerical model of thin-film amorphous silicon solar cell

The second model is based on realistic thin-film amorphous silicon solar cell (TF a-Si:H SC). The structure of the a-Si:H SC is shown in Fig. 3. Looking from the incidence of the light the solar cell is composed of the following layers 1 mm thick incoherent glass layer, SnO_2:F transparent conductive oxide (650 nm), p-a-Si:H (10 nm), i-a-Si:H (300 nm), n-a-Si:H (20 nm) and opaque Ag layer as a back contact. SnO_2:F transparent conductive layer introduces its own texture which is transferred to subsequent interfaces of the cell. Calibrated non-conformal layer growth model was used to describe the interfaces after deposition of individual layers [3], which appears to be crucial for accurate simulation. Since the random roughness scatters the light in all directions the domain was closed on the top by perfectly matched layer (PML), which has very good absorption of incident waves for all scattered directions [4]. Excitation was generated bellow the PML layer by using Lumped port (RF module) or Surface current (wave optics module). Since the textured surface is isotropic, only one polarization was used in simulations. The size of surface considered in simulation domain was 1x1 µm.

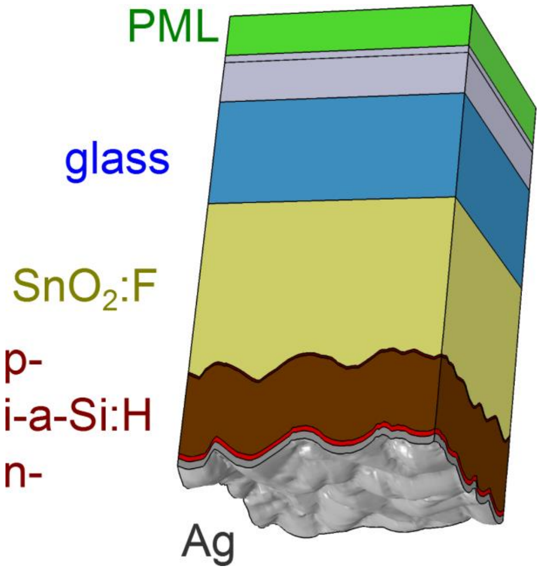


Figure 3. Realistic thin-film solar cell modeled in COMSOL.

The external quantum efficiency (*EQE*) of a-Si:H SC was measured in the wavelength range from 400 nm to 800 nm with the step size of 10 nm. 3-D optical simulations were performed in the same wavelength range, while the absorptance in i-a-Si:H layer was equaled to *EQE* [5]. Simulations show very good agreement between measured and calculated *EQE*, Fig. 4. In this case the phase elimination approach with two runs was considered. Since the structure is complex (random rough texture) it is hard or impossible to determine the phase of back propagating wave and thus phase matching approach was not considered in this case. By reason of the model dimensions, we could not simulate the complete 1 mm thick glass layer. However, the coherent simulation of 5 µm thick glass layer was considered (green curve) which shows many of interference fringes and even more interference fringes are expected for thicker glass. The method shows to be very reliable in eliminating the interference fringes which are the consequence of specular part of coherent propagation of light inside the glass layer. The scattered light from the rough surface already has incoherent nature, many random angles and phases, which compensate the coherent nature of scattered waves.

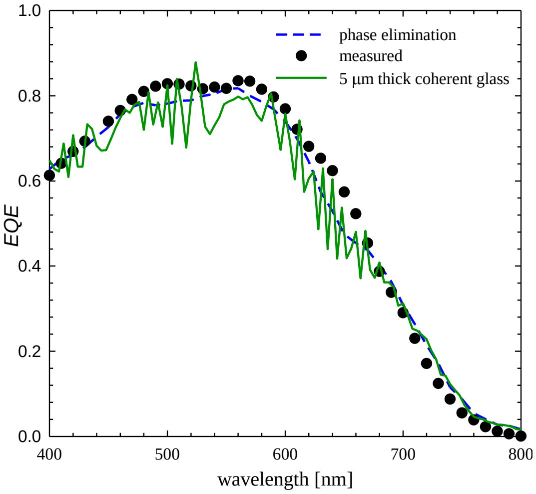


Figure 4. Measured and simulated *EQE* of a-Si:H TF solar cell. Additionally coherent simulation of solar cell with 5 µm thick glass is shown.

4. Conclusions

We have presented two approaches to include the thick incoherent layer into the coherent model. Additionally we presented the method to decrease the thickness of rough surface. All methods were implemented in the simulation of thick glass layer and thin-film a-Si:H solar cell. Good agreement is obtained between measurement and simulations for both cases.

5. References

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