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Analytical considerations of light transport in nanostructured homogeneous/inhomogeneous thin films

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ABSTRACT

Optical thin films are widely used as crucial components in various electrical, optical and photovoltaic devices. Different structural thin films behave different functions; therefore, full understanding of the optical performance of different micro/nano-scale structured thin films is the foundation of designing and optimizing the specific functional devices. In this paper, the optical properties (light reflection, refraction and transmission) in homogeneous and inhomogeneous nanostructures are analyzed and the optical interaction with the nanostructures is investigated.

1. Introduction

Understanding the optical interaction regimes in thin films is the foundation of analyzing the optical characteristics of various electrical, optical and photovoltaic devices. A proper numerical model to investigate the reflection, absorption and transmission of light in different nanostructured thin films is crucial to design and optimize a desirable functional structure. Different structures of thin films may exhibit different optical interaction regimes.

For homogeneous thin films, light propagates in a straight line until it reaches an interface, then it gets reflected or transmitted. Extensive researches have been carried out for the optical interactions inside the homogeneous thin films [1–3]. Based on the previous analysis and the subsequent mathematical derivation, the reflection and transmission of light with different wavelengths could be calculated by using Maxwell's equations [4]. For multi-layer structures, the mathematical formulations can be derived directly from the single-layer film analysis; thus, the optical properties, such as reflection and transmission, can be numerically calculated. The optical properties of the thin films may largely depend on their geometrical structures; in this case, the desirable optical properties could be achieved by varying the thickness of films and the choice of materials. The commonly used photovoltaic materials [5,6], indium tin oxide (ITO), amorphous silicon (a-Si) [7], ZnO, Ag and Al for each layer are used to construct a hetero-structural solar cell model [8]. The mathematical formulations are derived, and the fraction of light absorbed by each layer and the total reflectance are calculated in this paper.

Besides the intrinsic homogeneous thin film structures, it is getting more and more popular to use extrinsic materials to fabricate inhomogeneous films to achieve some highly efficient functions. For inhomogeneous thin films, light would get scattered by some irregularities in the transported films such as the embedded particles and the interfaces between two media [9–11]. The reflectivity of light could be largely reduced since light is trapped by multi-reflections inside the inhomogeneous films. According to the previous research, several scattering models have been established to effectively calculate the scattering intensity of textured surfaces [12] and inhomogeneous structures [13–16]. However, due to the inherent complexity of the optical properties caused by the inhomogeneous structures of thin films, it is difficult to get the specific light transport path inside the thin films. Based on the previous research on light transports in nano-scale textured structure [17], the brief conclusion could be drawn as follows: light would propagate in inhomogeneous film like passing through a graded homogeneous film, regardless of the geometry of the texture and the embedded particles. The optical interactions in thin films could be approximately modelled by using Mie scattering theory. To obtain a precise solution, the thin film is divided into several ultra-thin films and these ultra-thin layers are assumed to be homogeneous in this paper. The volume ratio of particles is linearly distributed and proportional to the distance from the sublayer to the incident front surface (linearly graded). The specific complex dielectric constant can be derived by using of Maxwell–Garnett effective medium theory [18]. As a result, the reflection and absorption of

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light through the nano-scale textured structures could be obtained. Compared with the traditional homogeneous antireflection thin films, the numerical results in this paper show that the linearly graded inhomogeneous surface (by texturing or doping nanoparticles into films) can largely reduce the light reflectivity.

In this paper, the light propagation in homogeneous and inhomogeneous thin films is analyzed; in particular, the numerical models of reflection and transmission of light are established for different structures.

2. Light transport in homogeneous films

2.1. Analysis of optical electric and energy dissipation inside homogeneous structures

Fig. 1 illustrates a beam of p-polarized wave (also known as tangential plane polarized, or said to be the transverse-magnetic wave with the electric vector in the incident plane) propagation through a single layer [19]. The thin film layer is assumed to be homogeneous with the index of refraction n_1 and film thickness of d. The index of refraction of free space and substrate is n_o and n_2, respectively. From the relationship and interaction of electric and magnetic energy of the incident, reflected and transmitted light, the equations of light energy balance in the interfaces of free space/film and film/substrate could be derived.

At the interface 1, the boundary conditions of electric and magnetic fields are given as

$$E_1 = E_0 + E_{r1} = E_{t1} + E_{i1} \quad (1)$$

$$B_1 = B_0 \cos\phi_0 - B_{r1}\cos\phi_0 = B_{t1}\cos\phi_1 - B_{i1}\cos\phi_1 \quad (2)$$

where E and B are the electric field intensity and magnetic field intensity, respectively. The subscripts r, t and i denote the reflected, transmitted and incident part of energy, respectively. ϕ_0 is the angle of incident light, and ϕ_1 is the angle of refraction in the thin film. The Maxwell–Faraday equation $\nabla \times E = -\frac{\partial B}{\partial t}$ denotes the interaction of the perpendicular and tangential components of the electric field and the magnetic field. From Maxwell's equations, the relationship between the electric field and the magnetic field can be obtained, $B = n\sqrt{\varepsilon_0\mu_0}E$. Therefore, from the Eqs. (1) and (2), the link between the electric field and magnetic field energy in boundary 1 is given as

$$B_1 = n_0\sqrt{\varepsilon_0\mu_0}\cos\phi_0(E_0 - E_{r1}) = n_1\sqrt{\varepsilon_0\mu_0}\cos\phi_1(E_{t1} - E_{i1}) \quad (3)$$

When the light propagates to the interface 2, the balance of electric field and magnetic field energy can be expressed as,

$$E_2 = E_{i2} + E_{r2} = E_{t2} \quad (4)$$

$$B_2 = B_{i2}\cos\phi_1 - B_{r2}\cos\phi_1 = B_{t2}\cos\phi_2 \quad (5)$$

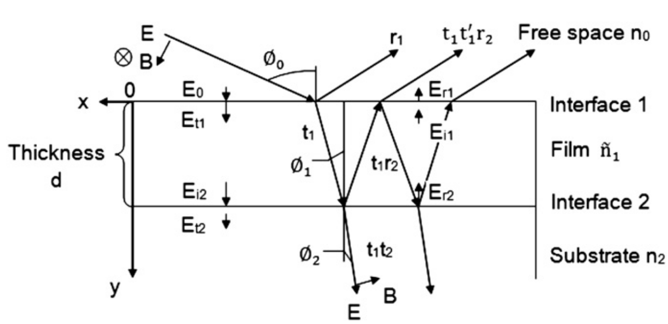

Fig. 1. Light propagation through a single layer homogeneous film.

Similarly, from Eqs. (4) and (5), the following equation can be obtained, as

$$B_2 = n_1\sqrt{\varepsilon_0\mu_0}\cos\phi_1(E_{i2} - E_{r2}) = n_2\sqrt{\varepsilon_0\mu_0}\cos\phi_2 E_{t2} \quad (6)$$

where ϕ_2 is the angle of emergence in substrate, ε_0 is the permittivity of free space (an electric constant) and μ_0 is the permeability of free space (a magnetic constant). After light propagating through the thickness d, there is a phase difference between E_{t1} and E_{i2}, E_{r1} and E_{i1}. According the optical theory [20], the phase difference is given as

$$\delta = \left(\frac{2\pi}{\lambda_0}\right) n_1 d \cos\phi_1 \quad (7)$$

The substitution of these equations into Eqs. (4) and (5) at interface 2 can lead to the following formulations for E-field and M-field energy, respectively,

$$E_2 = E_{t1}e^{-i\delta} + E_{i1}e^{i\delta} = E_{t2} \quad (8)$$

$$B_2 = n_1\sqrt{\varepsilon_0\mu_0}\cos\phi_1\left(E_{t1}e^{-i\delta} - E_{i1}e^{i\delta}\right) = n_2\sqrt{\varepsilon_0\mu_0}\cos\phi_2 E_{t2} \quad (9)$$

To simplify the expression, we assume $\chi_0 = n_0\sqrt{\varepsilon_0\mu_0}\cos\theta_0$, $\chi_1 = n_1\sqrt{\varepsilon_0\mu_0}\cos\theta_1$ and $\chi_2 = n_2\sqrt{\varepsilon_0\mu_0}\cos\theta_2$. The relation between the electric field energy and magnetic field energy before and after light transport through the thin film can be expressed in a matrix shown as

$$\begin{pmatrix} E_1 \\ B_1 \end{pmatrix} = \begin{pmatrix} \cos\delta & \frac{i\sin\delta}{\chi_1} \\ i\chi_1\sin\delta & \cos\delta \end{pmatrix}\begin{pmatrix} E_2 \\ B_2 \end{pmatrix} \quad (10)$$

Matrix $M_1 = \begin{pmatrix} m_{11} & m_{12} \\ m_{21} & m_{22} \end{pmatrix} = \begin{pmatrix} \cos\delta & \frac{i\sin\delta}{\chi_1} \\ i\chi_1\sin\delta & \cos\delta \end{pmatrix}$ is the transfer matrix of a single layer film.

To realize anti-reflection, it always uses the quarter-wave thick film. When the film thickness $d = \frac{\lambda_0}{4n_1}$, then $\delta = \pi/2$ and $R = \left(\frac{n_0 n_2 - n_1^2}{n_0 n_2 + n_1^2}\right)^2$. Hence, the reflectance is only determined by the material of the film.

If the Fresnel coefficients are small, then their product can be neglected. Also if the absorption in the film is high, the multiple reflection could be neglected. In that case, the expression of transmission and reflection can be simplified as

$$r = \frac{E_{r1}}{E_0} \quad (11)$$

$$t = \frac{E_{t2}}{E_0} \quad (12)$$

For a multi-layer film, the transfer matrix is given as [21]

$$\begin{pmatrix} E_1 \\ B_1 \end{pmatrix} = \overline{M}\begin{pmatrix} E_N \\ B_N \end{pmatrix} \quad (13)$$

And

$$\overline{M} = \prod_{i=1}^{N} M_i \quad (14)$$

2.2. Modelling results

A typical heterostructural solar cell usually utilizes indium tin oxide (ITO) as the front transparent conducting layer, a-Si as the active layer, ZnO as the n-type material, silver and aluminium as the back conducting layer. In order to achieve the best performance of the solar cell, besides the material selection, it needs to adjust the thickness of