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Simulation of scattering in dense medium by Monte Carlo method*

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Abstract: We present a Monte Carlo (MC) method to simulate the scattering for medium within randomly distributed particles, discuss the convergence of this method by varying the size parameter ka, volume parameter η and calculation parameter N_i, then compare this method with the classical iteration method with the same parameters. The calculation results showed that this method has good convergence and accords with the iteration method while consuming less CPU time. At the end of this paper, this method is used to discuss the visual light scatter in the c-Si/α-Si films.

Key words: Monte Carlo (MC), Iteration method, Scattering
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INTRODUCTION

Computing method based on solution of Maxwell's equations is widely used in microwave remote sensing (Tsang *et al.*, 1985) and propagation of light in films. Tsang *et al.*(1992) presented an iteration method to calculate the extinction index of dense medium with randomly distributed dielectric spheres. Akira (2000a; 2000b) also used an iteration simulation method to calculate the light scattering in nano-crystalline films of photoelectrochemical solar cells. But the iteration method consumes plenty of CPU time because $3N$ equations must be solved during every iteration time, where N is the number of particles distributed in the medium, and this method is limited by the initial values and convergence problems.

To avoid these problems, a Monte Carlo (MC) simulation method is presented in this paper to calculate the light scattering of dense medium based on the solutions of Maxwell's equations of a single particle. There is no initial values problem in MC. And the convergence of MC's results is not dependent on the dimension of the problem. Using more random number we can get more accurate results because the precision of MC results is directly proportional to the square root of the random number size. In this paper, we discuss the convergence of this method and compare its results with those of the iteration method. The calculation results showed this MC method accords with those of the iteration method and has good convergence. Especially the MC method consumes less time than the iteration method.

SIMULATION METHOD FOR DENSE MEDIUM

Monte Carlo simulation method

The distributed particles are regarded as dielectric spheres embedded in the medium randomly. MC sampling is used in the ray tracing simulation. The probability of an incident photon scattered by a particle is described by Eq.(1) (Tsang *et al.*, 1985):

$$\sigma = \int_{4\pi} \left| f_{(\hat{i},\hat{o})} \right|^2 \mathrm{d}w \qquad (1)$$

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where $f_{(\hat{i},\hat{o})}$ is the solution of the Maxwell's equations of a single dielectric particle. When a photon is normal to the medium, one MC process begins. The photon keeps propagating until it hits a particle or it goes out of the medium. While it hits a sphere, it will be scattered if a random number in [0,1] generated by the program is smaller than σ. Then we make the photon propagate in a new direction which is decided by the $f_{(\hat{i},\hat{o})}$. If the random number is bigger than σ, the photon will not be scattered and continue propagating in its original direction until it goes out of the medium or hits another sphere. When the photon goes out, the MC process is over. Repeat MC process N_i times and record the number of photons going out of the medium in their original direction as N_o. We define the attenuation index τ by Eq.(2)

$$\tau = -\frac{1}{d}\ln\frac{N_o}{N_i} \tag{2}$$

where N_i is the number of the incident photons, d is the thickness of the dense medium.

Iteration method

In the iteration method, the solution of Maxwell's equations can be cast into Eq.(3) (Tsang *et al.*, 1985; 1992):

$$E_{E,\alpha}^{v} = \sum_{n=1,n\neq\alpha}^{N} E_{s,n}^{v-1} + E_i, \quad E_{s,\alpha}^{v} = \left|E_{E,\alpha}^{v}\right| f_{(\hat{i},\hat{o})}\frac{\exp(ikR)}{R} \tag{3}$$

where the relationship between $E_{s,\alpha}^{v}$ and $E_{E,\alpha}^{v}$ is the solution of Maxwell's equations for a single particle. $E_{s,\alpha}^{v}$, $E_{E,\alpha}^{v}$ and E_i are scattering field, exciting field and the incident field, respectively; k is the wave number. α=1,2,…,N; v denotes the vth-iterated solution. Eq.(3) can be solved by iteration. After choosing a suitable initial value $E_{s,\alpha}^{0}$ for Eq.(3), the solution $E_{E,\alpha}^{v}$ will be obtained after the vth iteration.

Attenuation index τ can be obtained from $E_{E,\alpha}^{v}$, E_i and σ which are defined in Eq.(1) and Eq.(3):

$$\tau = -\frac{1}{d}\ln\left\{\left[\left|E_i\right|^2 - \sum_{\alpha=1}^{N}\left|E_{E,\alpha}^{v}\right|^2\sigma\right]\Big/\left|E_i\right|^2\right\} \tag{4}$$

Then using Eq.(2) and Eq.(4), we can compare the results of the two simulation methods.

SIMULATION RESULTS AND DISCUSSION

In the following simulation, we get some random distribution of dielectric spheres with different volume parameter η (fraction volume). The radius of the spheres is 20 nm. The MC and iteration method use the same distribution of dielectric spheres under the same structure parameters. In the two simulation methods, light absorption by dielectric spheres is neglected.

Convergence of MC

Fig.1 is attenuation index versus number of incident photons with different size parameter ka where a is radius of sphere. The figure shows that the results will converge if enough photons are incident just as MC theory says. And the number of the incident photon to obtain the convergent result is entirely dependent on the size parameter ka. The result conve-

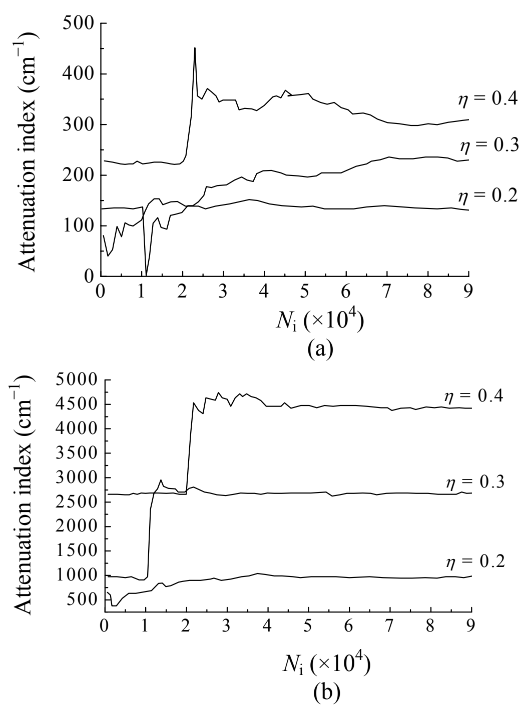

Fig.1 Convergence of attenuation index τ versus N_i, number of incident photons with fraction volume η=0.2, 0.3, 0.4 while the number of spheres is 750, 1100, 1500, respectively. The radius of spheres is 20 nm. The permittivity of the spheres is 13.0 and the refractive index of the matrix is 1.42. The *ka* of (a) and (b) is 0.2 and 0.4, respectively

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rges around $N_i=7\times10^4$ for ka=0.2 but around $N_i=4\times10^4$ for ka=0.4 with different η, respectively. So in the following MC simulation, it is enough that N_i is taken as 10^5 to ensure that the results converge.

Compare with iteration method

Fig.2 is the attenuation index τ versus ka by MC and iteration method. The figure shows that the result of MC accords with that of the iteration method especially for small ka. The poor correspondence between the two results for large ka is probably partly due to errors introduced by $f_{(\hat{i},\hat{o})}$ in Eq.(1) and Eq.(3). Fortunately the range of ka from 0.1 to 0.4 is more important for crystallites in the visual light wavelength range and in this condition $f_{(\hat{i},\hat{o})}$ is accurate enough. The same parameters were used in the comparison, such as η=0.25, a=20 nm, and ε_γ=13.0 while the refractive index of the matrix is 1.42. The number of iterations and the initial value for the iteration method are set as in (Tsang *et al*., 1992). To complete this simulation, MC consumes 990 s while the iteration method consumes 1788 s after 6 iterations on the same machine.

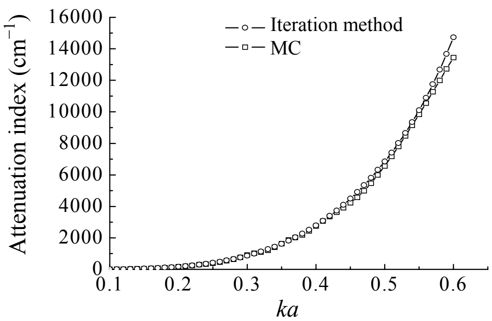

Fig.2 Comparison of MC and iteration method. Fraction volume η is 0.25. Number of spheres is 950. Radius of spheres a is 20 nm. Permittivity of spheres ε_γ is 13.0 and the refractive index of the matrix is 1.42. Number of iterations is 6

Simulation applied in c(crystallite)-Si/α(amorphous)-Si films

The scattering caused by crystallites potentially enhances the anti-reflection optical property of c-Si/α-Si coating glass to solve the "light pollution" problem (Zhang *et al*., 2000). Fig.3 shows the simulation results on the attenuation index of c-Si/α-Si films. In this case silicon crystallites and α-Si matrix are regarded as distributed spheres and medium, respectively. The diameter (radius) of silicon crystallites ranges from 10 (5) nm to 50 (25) nm. The results imply that the scattering can be ignored when the diameter is smaller than 40 nm and that in the short wavelength range the scattering caused by bigger crystallites is strong enough to adversely affect the reflection of films.

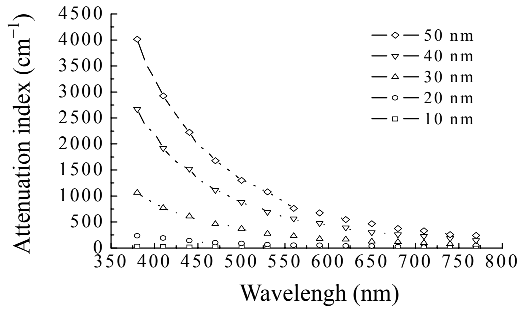

Fig.3 Spectra of attenuation index according to silicon crystallites in c-Si/α-Si matrix. Permittivity of spheres is 13.0 and the refractive index of the matrix is 1.42. Diameter of spheres ranges from 10 nm to 50 nm. Fraction volume η is 0.5

CONCLUSION

This paper presents an MC simulation method to calculate the scattering in dense medium. The simulation results accords with those of the classical iteration method. This MC simulation avoids the initial values problem of the iteration method and has good convergence. At the same time MC consumes less CPU time than the iteration method. The MC method can be used to calculate the scattering of c-Si/α-Si films. The results showed that in the short wavelength range the scattering is strong enough to adversely affect the reflectance of films.

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