Determination of optical properties and thickness of optical thin film using stochastic particle swarm optimization

Zhao-Hui Ruan, Yuan Yuan *, Xiao-Xian Zhang, Yong Shuai, He-Ping Tan *

School of Energy Science and Engineering, Harbin Institute of Technology, 92, West Dazhi Street, Harbin 150001, PR China

Abstract

The wavelength-selective properties of optical thin films offer a sensible solution to the problems of effective wavelength-selective use of solar energy. However, the design of the optical constants of these optical thin films is crucial to the study of the film's optical properties. To address this problem, we introduced stochastic particle swarm optimization (SPSO) to an inverse model of the optical constants and thicknesses of optical thin films in this paper. Initially, we discussed the anti-error capacity of the Cauchy dispersion model, and we then discussed the importance of the parameters used in the Forouhi–Bloomer dispersion model, before modifying the Forouhi–Bloomer dispersion model on this basis. We also discussed the influence of the measured error on the inversion effects of each parameter in the modified model. Finally, we inverted the measured transmittance data using the Cauchy dispersion model, the Forouhi–Bloomer dispersion model and a modified Forouhi–Bloomer dispersion model, and the effectiveness and the feasibility of SPSO when applied to the determination of optical constants is verified.

1. Introduction

Energy sources have an enormous impact on the lives and productivity of human beings. To satisfy the growing demand for energy sources, the speed of development and use of fossil fuels such as coal, petroleum and natural gas was greatly increased (Panda et al., 2014; Nicoletti et al., 2015). However, the combustion products of fossil fuel shave also accelerated global warming. Solar energy stands out as an alternative with several advantages, i.e., providing a clean and renewable energy source with rich

reserves, becoming apparent over the past few decades (Zhang et al., 2015; Ceballos-Mendivil et al., 2015), and solar technology therefore has experienced rapid development (Li et al., 2015). At present, the comparatively simple and effective method of solar energy utilization is with solar cells and photovoltaic (PV) devices (Perez and Fthenakis, 2015). However, there are many problems with the devices used for solar energy utilization, including how to collect the sun's rays effectively (Wang et al., 2015a,b), and how to use solar energy in a wavelength-selective manner (Zheng et al., 2015). Optical thin films are viewed favorably because of their good optical properties, and many researchers have made great progress in applying these films to solar energy systems (Kim et al., 2015; Cuevas et al., 2015; Huang et al., 2015; Ma et al., 2015;

* Corresponding authors.
  E-mail addresses: yuanyuan83@hit.edu.cn (Y. Yuan), tanheping@hit.edu.cn (H.-P. Tan).

Nomenclature

a	vector of optical constants and thickness
c	speed of light
c_1, c_2	two acceleration coefficients
d	thickness of optical thin film
d_s	thickness of substrate
f_{fitness}	objective function
h	planck constant
k	extinction coefficient of optical thin film
n	refractive index of optical thin film
n_s	refractive index of substrate
n_p	number of reference points
A_1, B_1, A_2, B_2	constants in Cauchy dispersion model

$n(\infty), E_g, A, B, C$	constants in Forouhi–Bloomer dispersion model
$T_{\text{cal}}(i, \mathbf{a})$	inverse calculation value
T_{est}	inverse result
T_{exact}	exact value of the forward problem
wt	inertia weight coefficient

Greek symbols

γ	measured error
λ	wavelength (μm)
ε_{rel}	relative error
ς	a standard normal distribution random variable
σ	standard deviation

Wakefield et al., 2015). It is therefore necessary for us to perform further research on the method of the determination of the optical properties of optical thin films to enable them to be used more effectively.

The optical properties of an optical thin film are mainly determined by the film's optical constants (refractive index n and extinction coefficient k) and thickness (d). The research to date on optical thin films is mainly divided into two parts. On one hand, if it is assumed that the optical constants and the thickness of the film are known, then the optical properties can be determined. On the other hand, if an optical thin film already exists and it is necessary to detect its optical properties, the optical constants and the thickness of the film can be determined by inversion of transmittance data, which can be obtained experimentally; we can also design optical thin films in this manner. Many researchers have studied the determination of the optical constants and thicknesses of optical thin films over recent decades. Manifacier et al. (1976) proposed a traditional method to determine the optical constants and thicknesses of optical thin films that are deposited on non-absorbing substrates based on their transmission spectra. Swanepoel (1984) proposed a method to calculate both the refractive index n and the thickness d of the weakly absorbing region based on the maximum and the minimum of the interference fringes, and the extinction coefficient k could be calculated from the transmission spectra of the weakly absorbing and strongly absorbing regions. Demiryont et al. (1986) proposed a method to determine the optical constants and thicknesses of optical thin films in which only the transmittance data was required. As time has passed, increasing numbers of methods have been proposed. Ahmadi et al. (2015) proposed a method to determine the optical constants and thicknesses of optical thin films using the Levenberg–Marquardt algorithm. Atyia and Hegab (2014) determined the optical properties of Ge$_{15}$Se$_{60}$Bi$_2$ thin films using their transmittance and reflectance data. Le et al. (2014) proposed an effective statistical method to optimize indium tin oxide (ITO) thin films based on the Taguchi method and gray relational analysis. Khawaja et al. (2000) also proposed a simple method to determine the optical constants and thicknesses of optical thin films that had been applied to gold films and that had performed very well.

In this paper, to determine the optical constants and thicknesses of optical thin films, we first establish an inverse model of the optical constants and the thickness of the film of interest. We then introduce stochastic particle swarm optimization (SPSO), which enables us to solve the problem using inversion. On this basis, we discuss the influence of the measured error on the inversion accuracy when using the Cauchy dispersion model and the Forouhi–Bloomer dispersion model separately. Then, we discuss the effects of each parameter in the Forouhi–Bloomer dispersion model and the influence of different points selection strategies on the inversion effect. We also offer an optimization approach for the Forouhi–Bloomer dispersion model.

2. Methods

2.1. Forward transmission problem

Assuming that the incident light irradiates the thin film vertically, and that the refractive index values of the substrate and of the surrounding air are n_s and 1, respectively, then the refractive index and the extinction coefficient of the thin film are n and k, respectively. If the thickness of the weakly absorbing thin film is much less than that of the substrate (d_s), i.e., $k^2 \ll n^2$ and $d \ll d_s$, then the relationship among the transmittance T, the refractive index n, the extinction coefficient k and the thickness d will be as shown below (Márquez et al., 1997; Marquez et al., 1992; Heavens, 1991):