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ORIGINAL ARTICLE

Estimation and prediction of optical properties of PA6/TiO2 nanocomposites

Amir Rastar [a,*], Mohamad E. Yazdanshenas [b], Abusaeed Rashidi [a], Seyed M. Bidoki [c]

[a] *Department of Textile Engineering, Science and Research Branch, Islamic Azad University, Tehran, Iran*
[b] *Department of Textile Engineering, Yazd Branch, Islamic Azad University, Yazd, Iran*
[c] *Department of Textile Engineering, Yazd University, Yazd, Iran*

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Abstract Nanocomposites are used in many scientific and industrial applications in recent times. In polymer nanocomposites, nanoparticles are used as the main component in creation which has always been considerable. Nano TiO2 as a nanoparticle has a very strong light scattering effect which can replace the ordinary TiO2 in less amounts of usage.

In this research, optical properties of the PA6/nano TiO2 nanocomposite are studied using Mie scattering theory. Mie theory uses the relative refractive index of a small particle to calculate the light scattering efficiency of a material. At first, experimental and estimated properties of a nanocomposite film containing nano TiO2 particles with 40 nm radius are compared. Optical properties of nanocomposites are then predicted with various particle sizes as a result of this research.

Results show that by taking the refractive index as an intrinsic property of a particle, it is possible to estimate the optical properties with a defined size and in addition it can help to predict these properties for different particle sizes.

1. Introduction

Optical properties of particles are studied from very old time until recent years as one of their main characteristics. There are several theories and models alongside experimental tries in order to measure or calculate this property. Many general definitions are made for various conditions in which the particle and its medium take part in the light scattering. These conditions include single and multiple scattering, absorbent or nonabsorbent media, regular or irregular shaped particles and nonlinear optics. A common base for all these theories is the Maxwell's equations for electromagnetism as the light is an electromagnetic wave. These theories include Mie and Rayleigh light scattering models, effective medium theories (EMT), anomalous diffraction theory (ADT), T-Matrix, Monte-Carlo approximations and vice versa (Ulrich, 2006; Nelson and Deng, 2007; Bohren and Huffman, 1983; van de Hulst, 1957; Mishchenko et al., 2004; Mie, 1908; Kokhanovsky, 2010; Şahin and Miller, 1997).

* Corresponding author.
E-mail address: amir.rastar@gmail.com (A. Rastar).
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Mie theory is widely used among all those mentioned in order to obtain scattering properties of a single spherical particle. Therefore it can be used for single scattering where light scattering happens only from a single particle with no relation to neighboring ones. The fact is, Mie theory is a very complicated calculation and it can only be done by some modifications and restrictions (Mie, 1978). On the other hand in a material there are many scattering particles interacting with each other in light scattering so it is multiple scattering which really happens in the material. Researches usually combine a simple form of Mie theory for a single particle with a multiple scattering theory like Kubelka–Munk in order to calculate the scattering of the whole collection (Quinten, 2001).

In this study Mie's results are used as an input to the Kubelka–Munk theory in order to calculate the reflectance factor of the nanocomposite. These theories are briefly described in next sections.

2. Refractive index

Many of the previously explained theories act upon the material's refractive index as a basic input for their calculations. Refractive index is used in Mie theory in order to evaluate its coefficients and then those coefficients are the key parameters for calculating the Mie scattering efficiencies. Refractive index are measured or calculated in various ways such as ellipsometry as an instrumental method. However there are some theoretical methods for this purpose one of which is presented here (Azzam and Bashara, 1988).

Materials especially metals have a complex refractive index. This index contains two parts, a real and an imaginary part. The imaginary part of refractive index can be calculated from the Beer–Lambert's law of transmittance. According to this law, transmittance is related to the extinction coefficient and the number of absorbent particles.

$$T = 10^{-\varepsilon c l} \tag{1}$$

where T is transmittance, ε stands for the extinction coefficient, c is the concentration of absorbing material and l is the path length for the incident light.

From the above equation:

$$\varepsilon = \frac{4K}{\lambda} \tag{2}$$

where λ is the wavelength and K is the imaginary part of the refractive index.

Fresnel law is the scattered light from the surface of materials relevant to the refractive index. According to this law when the light is entering an environment perpendicularly, the reflected light intensity is:

$$R = \frac{[(n-1)^2 + K^2]}{[(n+1)^2 + K^2]} \tag{3}$$

where n is the real part of refractive index.

3. Mie theory

Mie theory is one of the most basic theories among the light scattering models presented about a hundred years ago. It returns to 1908 when Lorentz Mie published an article about optical properties of spherical metal particles based on their complex refractive index. In this theory from the relative refractive index and size of the particle, two main coefficients are derived and used to calculate the optical parameters of the material like optical efficiencies, cross sections and patterns (Bohren and Huffman, 1983).

$$Q_{ext} = \frac{2}{x^2}\sum_{n=1}^{\infty}(2n+1)\Re(a_n + b_n) \tag{4}$$

$$Q_{sca} = \frac{2}{x^2}\sum_{n=1}^{\infty}(2n+1)(|a_n| + |b_n|) \tag{5}$$

$$Q_{abs} = Q_{ext} - Q_{sca} \tag{6}$$

$$x = \frac{2\pi r}{\lambda} \tag{7}$$

in above formulas, Q_{ext} is the extinction efficiency, Q_{sca} is the scattering efficiency, Q_{abs} is the absorption efficiency, r is replaced by the particle radius and x represents the size parameter which is a factor of particle size and the incident light's wavelength.

a_n and b_n are Mie coefficients and n is the number of iterations in these functions where its maximum number is calculated according to Bohren and Huffman as below (Matzler, XXXX):

$$n_{max} = x + 4x^{1/3} + 2 \tag{8}$$

Mie coefficients can be estimated as the Bessel functions of the particle's relative complex refractive index.

$$a_n = \frac{m^2 j_n(mx)[xj_n(x)]' - j_n(x)[mxj_n(mx)]'}{m^2 j_n(mx)\left[xh_n^{(1)}(x)\right]' - h_n^{(1)}(x)[mxj_n(mx)]'} \tag{9}$$

$$b_n = \frac{j_n(mx)[xj_n(x)]' - j_n(x)[mxj_n(mx)]'}{j_n(mx)\left[xh_n^{(1)}(x)\right]' - h_n^{(1)}(x)[mxj_n(mx)]'} \tag{10}$$

From efficiencies, cross sections which are the area in which the light has its effects efficiently are calculated.

$$Q_{ext} = \frac{C_{ext}}{G}, Q_{abs} = \frac{C_{abs}}{G}, Q_{sca} = \frac{C_{sca}}{G}, Q_{ext} = Q_{abs} + Q_{sca} \tag{11}$$

and G is the particle's cross sectional area.

Finally the scattering patterns which demonstrate the amount of light scattering in different angles around the particles in the scattering plane are calculated from above formulas (Matzler, XXXX).

4. Kubelka–Munk theory

When multiple scattering occurs a single particle takes part in its own scattering behavior while in the light scattering of many neighbor particles. Kubelka–Munk theory is a multiple scattering theory which calculates the reflectance factor of a matter or semi-transparent material using its scattering (S) and absorption (K) coefficients.

$$\frac{K}{S} = \frac{(1-R)^2}{2R} \tag{12}$$

R is the reflectance factor in formula 12.

These coefficients can be calculated by the efficiencies of other single scattering theories like Mie theory as an input.

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