ISSN Print: 2394-7500
ISSN Online: 2394-5869
Impact Factor: 5.2
IJAR 2020; 6(3): 09-11
www.allresearchjournal.com
Received: 10-01-2020
Accepted: 13-02-2020

Dr. Shimpy Kumari
Research Scholar, Department of Physics, L.N.M.U., Darbhanga, Bihar, India

Correspondence Author:
Dr. Shimpy Kumari
Research Scholar, Department of Physics, L.N.M.U., Darbhanga, Bihar, India

MIE theory for study of optical anisotropy of crystals

Dr. Shimpy Kumari

Abstract
In this study, to quantify the accuracy of the finite element method, it is useful to compare results obtained using the finite element method for scattering by an isotropic sphere to the exact results obtained using Mie theory. To compute the Mie theory results presented below, we have employed the BHMIE computer code provided by Bohren and Huffman, with additional code introduced for computation of the asymmetry parameter. In this computational approach, series expansions are performed to compute the scattering cross section and asymmetry parameter at far field.

Keywords: MIE theory, optical anisotropy, crystals

Introduction
Attempts to use Mie theory to predict the light scattering properties of a rutile titanium particle require approximation to address the optical anisotropy of the crystal. Rutile titanium is uniaxial, exhibiting its ordinary refractive index for light polarized parallel to either axis of the crystal and its extraordinary refractive index for light polarized perpendicular to the axis. The light scattering properties of optically anisotropic spheres of rutile titanium have been computed directly for using the time-domain finite element approach. Two methods for approximating rutile as an isotropic material have been proposed in the literature. One approach has been to compute the mean of the refractive indices along the three crystal axes at the light wavelength of interest and subsequently apply Mie theory to compute far-field scattering parameters. This is the average index approximation. For the light wavelength 560 nm, the average refractive index of rutile titanium is 2.74. In these computations, the refractive index of the surrounding medium is 1.51, representing a typical palm resin. The greatest S values occur for sphere diameters in the range 0.18-0.30 are, with maximum value of $S=27.74\mu^{-1}$ for the diameter 0.272am. The maximum value of the angle-weighted scattering coefficient $\sigma=12.17\mu m^{-1}$ occurs for the sphere diameter 0.20 am. A second method for approximating the scattering behaviour of rutile titanium using isotropic materials has been to compute separately far-field scattering parameters tier an isotropic sphere having the ordinary and extraordinary refractive indices of rutile titanium, and subsequently compute the weighted sum of these separate far-field results [22]. The weighted sum consists of two-thirds the result for the ordinary refractive index plus one-third the result for the extraordinary refractive index. This is the weighted sum approximation. The results of Mie theory computations for the scattering coefficient S using the weighted sum approximation exhibits less pronounced resonant peaks in S than the analogous plot generated using the average index approximation. This is expected, since the resonant peaks in the two individual curves used to form the weighted sum are systematically offset from one another. The maximum S values for the weighted sum approximation occur in the range 0.18-0.3am, as with the average index approximation. The maximum value $S = 25.08\mu m^{-1}$ occurs for the diameter 0.270am, about 10% lower than the maximum value $S = 27.74\mu m^{-1}$ observed in the case of the average index approximation. The angle-weighted scattering coefficient σ using the weighted sum approximation is in close agreement with that computed using the average index approximation. In the case of the weighted sum approximation, the maximum value of the angle-weighted scattering coefficient $\sigma = 11.71\mu m^{-1}$ occurs for the sphere diameter 0.204 am, about 4% lower than the maximum value of the angle-weighted scattering coefficient $\sigma=12.17\mu m^{-1}$ observed in the case of the average index approximation. The average index anisotropic spheres of rutile titanium computed using the time-domain finite element method.

Results obtained using the finite element method contain the effects of the optical activity of the uniaxial crystal, unlike the results of the average index or weighted sum approximations based upon scattering by isotropic spheres.

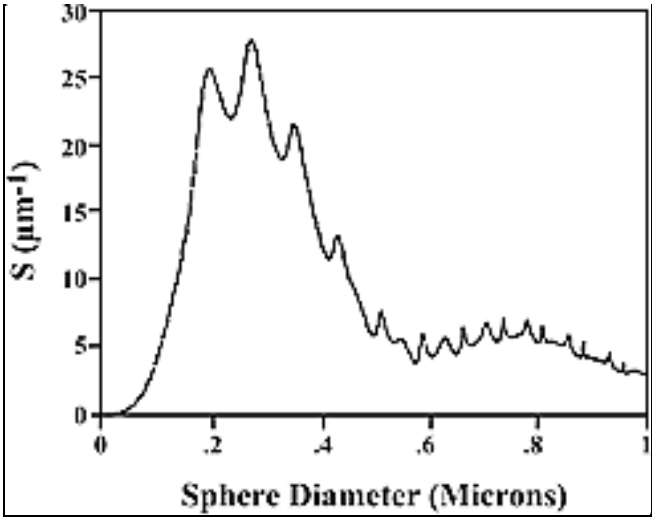

Fig 1: Scattering coefficient S versus sphere diameter for an optically isotropic sphere from Mie theory, using the average index approximation

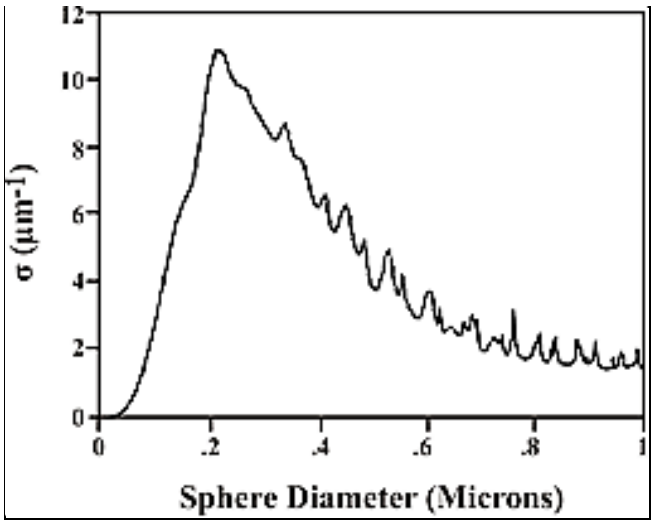

Fig 2: Angle-weighted scattering coefficient σ versus sphere diameter for an optically isotropic sphere from Mie theory, using the weighted sum approximation

The light scattering properties of anisotropic, high-index spheres assigned the optical constants of rutile titanium with diameters in the range 50-350nm have been computed using the finite element method. The light wavelength used in these computations is 560 nm. At this wavelength, the ordinary refractive index of rutile titanium is 2.64, while the extraordinary index is 2.94 [17]. The spatial symmetry elements of an anisotropic, uniaxial sphere include an equatorial mirror plane and a cylindrical rotation axis perpendicular to this mirror plane. The complete light scattering behavior of such a system can therefore be sampled through a series of illuminations along any are connecting one pole of the sphere to the equator. Two mutually perpendicular polarizations (parallel and perpendicular to the optic axis of the sphere) are used for each illumination direction, resulting in a total of 12 individual illuminations per sphere. The far-field scattering parameters S and σ are computed for each sphere by computing the averages of these two quantities, weighting the individual results by the probabilities of their occurrence under conditions of random illumination. As a result of the cylindrical rotation axis parallel to the optical axis of these spheres, illumination directions nearly perpendicular to the optic axis are significantly more probable than those nearly parallel to the optic axis.

The finite element models for each of the spheres studied consisted of a spherical particle at the center of a cubic finite element model. In each case, the sphere is surrounded by an optically isotropic medium with refractive index n = 1.514, representative of an acrylic, alkyd paint resin [7]. The finite element mesh density differs from model to model but is typically ρ = 50-60 elements per wavelength in the highest index material in the model. In the case of the 0.2–μm sphere, for example, the cubic element edge length is 3.87 nm. Accuracy analysis of the time-domain finite element approach [11, 12]. Suggests that the error associated with each of the calculations in this study should be less than 2% the full near-field results of a finite element computation performed on the anisotropic titanium sphere with diameter 0.2μm. In this computation, the incident light in the +x direction, and the incident polarization is parallel to the y direction. The incident intensity of the light is equal to unity. The scattered intensities observed in the model are as much as 4.3 times greater than the incident intensity. The far-field parameters S and σ have been computed for a series of anisotropic spheres of rutile titanium with diameters in the range 0.05-0.35am. The data exhibit a sharp increase in S as the sphere diameter is increased through the Rayleigh scattering from 0.05-0.2am, beyond which resonant peaks are observed with diameter. The σ data exhibit the same sharp increase the same sharp diameters increases from 0.05-0.2. For sphere diameters greater than 0.2μm, the σ data in decrease without the same pronounced resonant peaks observed in the S data.

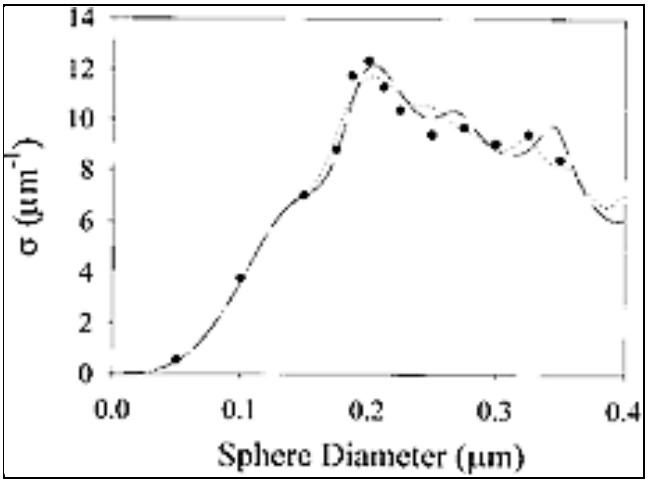

Fig 3: The angle-weighted scattering coefficient σ as a function of sphere diameter computed using the finite element method (solid points) for anisotropic spheres of rutile titanium embedded in a medium with n = 1.514. The illumination wavelength is 560 nm. The long dashed curve corresponds to the average index approximation, which the dotted curve corresponds to the weighted sum approximation.

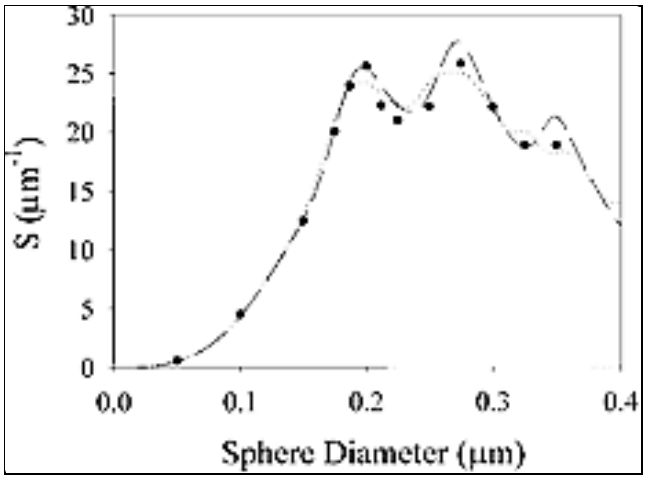

Fig 4: The scattering coefficient S as a function of sphere diameter computed using the finite element method for anisotropic spheres of rutile titanium embedded in a medium with n = 1.514. The illumination wavelength is 560 nm. The long dashed curve corresponds to the average index approximation which the dashed curve corresponds to the weighted sum approximation

Table 1: Scattering coefficients S and σ computed for anisotropic spheres of different diameters using the finite element approach.

Diameter (μm)	S (μm^{-1})	σ (μm^{-1})
0.050	0.578	0.564
0.100	4.52	3.79
0.150	12.50	7.03
0.175	20.06	8.82
0.187	23.94	11.73
0.200	25.62	12.34
0.212	22.27	11.30
0.225	21.01	10.37
0.250	22.17	9.04
0.275	25.83	9.68
0.300	22.10	9.07
0.325	18.89	9.43
0.350	18.91	8.44

For this particular rutile titanium particle, at least, the scattering properties of the equivalent volume sphere computed using the two approximations and Mie theory are the finite element result.

Conclusion

In the study described here, the problem of light scattering by anisotropic rutile titanium spheres. Efforts to model the light scattering properties of rutile titanium have typically relied upon Mie theory, which is limited to the description of a single, isotropic sphere. This approach requires simplifying approximations to address the optical anisotropy of the particles. We observed resonances in the far-field scattering coefficients that depend upon sphere diameter, in analogy with approximations based on Mie theory. The results of this numerical approach are compared to the two usual Mie theory approximations used to address the anisotropy of rutile titanium.

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