Mie Scattering of Electromagnetic Waves

Sergei Yushanov, Jeffrey S. Crompton[*], and Kyle C. Koppenhoefer
*Corresponding author
AltaSim Technologies, 130 East Wilson Bridge Rd, Suite 140, Columbus, OH,
jeff@altasimtechnologies.com

Abstract: Scattering of electromagnetic waves by spherical particles is described by the Mie solution to Maxwell's equations. Illumination of an obstacle by an electromagnetic wave excites electric charges in the obstacle to oscillate due to interaction with the electric field of the incident wave. The oscillating charge radiates electromagnetic energy in all directions; this secondary radiation is the radiation scattered by the obstacle. In addition, the excited elementary charges may absorb radiation and transform part of the incident energy into other forms, such as thermal energy. Both scattering and absorption remove energy from a beam of light and the beam is attenuated.

In this work, scattering of an incident electromagnetic wave by a spherical particle has been analyzed using COMSOL Multiphysics. The nature of the interaction has been considered for materialswith three different properties: metallic, magnetic and dielectric. The solutions provide details of the absorption, scattering, extinction, pressure cross-sections, back-scattering and radiation force exerted on the particle by an incident plane wave.Results of these analyses are compared against the Mie analytical solutions.

Keywords: electromagnetic scattering, angle-resolved low-coherence interferometry, Mie solution, Maxwell's equations

1. Introduction

The Mie solution to Maxwell's equations provides the basis for measuring the size of particles through the scattering of electromagnetic radiation. Applications include dust particles in the atmosphere, oil droplet in water, and cell nuclei in biological systems (e.g., cancer research).

The Mie solution, also called Lorenz-Mie theory or Lorenz-Mie-Debye theory, provides an analytical solution of Maxwell's equations for the scattering of electromagnetic radiation by spherical particles in terms of infinite series [1-3].

Scattering may be defined as the redirection of radiation from the original propagation direction typically due to interactions with molecules and particles. Reflection, refraction etc. represent specific forms of scattering. Electromagnetic waves scatter when they meet an obstacle due to the electric charges in the obstacle being oscillated by the electric field of the incident wave. Accelerated charges radiate electromagnetic energy in all directions; this secondary radiation is referred to as radiation scattered by the obstacle. Thus, charge excitation and re-radiation of the electromagnetic energy constitutes scattering.

In addition to re-radiating electromagnetic energy, the excited elementary charges may transform part of the incident energy into other forms, e.g. thermal energy, via absorption. Both scattering and absorption remove energy from an electromagnetic wave, thus attenuating the beam. This attenuation, which is called extinction, consists of scattering and absorption:

$$\text{Extinction} = \text{scattering} + \text{absorption}$$

Scattering and absorption are not mutually independent processes. This paper considers elastic scattering only: the frequency of the scattered wave is the same as that of incident wave. Thus, ineleastic scattering phenomena such as Brillouin and Raman scattering are excluded from this paper.

2. Theory

In scattering problems, the total wave decomposes onto incident and scattered waves:

$$\mathbf{E} = \mathbf{E}_{inc} + \mathbf{E}_{sca} \qquad (1)$$

$$\mathbf{H} = \mathbf{H}_{inc} + \mathbf{H}_{sca} \qquad (2)$$

Maxwell's wave equation is solved with respect to scattered electric field:

$$\nabla \times \left(\frac{1}{\mu_r} \nabla \times \mathbf{E}_{sca} \right) - k_0^2 \left(\varepsilon_r - j \frac{\sigma}{\omega \varepsilon_0} \right) \mathbf{E}_{sca} = 0 \quad (3)$$

The scattered magnetic field is calculated from Faraday's law:

$$\mathbf{H}_{sca} = -\frac{1}{j\omega\mu} \nabla \times \mathbf{E}_{sca} \quad (4)$$

The Time-average Poynting vector for time-harmonic fields gives the energy flux:

$$\mathcal{P} = \frac{1}{2} \text{Re} \left[\mathbf{E} \times \mathbf{H}^* \right], \quad \left[W / m^2 \right] \quad (5)$$

For an incident plane wave, the magnetic field is related to the electric field by:

$$\mathbf{H}_{inc} = \frac{1}{\eta} \hat{\mathbf{k}} \times \mathbf{E}_{inc} \quad (6)$$

where $\hat{\mathbf{k}}$ is direction of the incident wave propagation, $\eta = \sqrt{\mu / \varepsilon}$ is characteristic impedance, ε is permittivity and μ is permeability of ambient medium. Hence, incident energy flux is calculated as

$$\mathcal{P}_{inc} = \frac{1}{2\eta} \left| \mathbf{E}_{inc} \right|^2 \hat{\mathbf{k}} = \frac{1}{2} c\varepsilon \left| \mathbf{E}_{inc} \right|^2 \hat{\mathbf{k}} \quad (7)$$

where $c = \sqrt{1 / \varepsilon \mu}$ is speed of light.

2.1 Cross-Section Calculations

Important physical quantities can be obtained from scattered fields. One of these is the cross section, which can be defined as the net rate at which electromagnetic energy (W) crosses the surface of an imaginary sphere centered at the particle divided by the incident irradiation $(\mathcal{P}_{inc})$. To quantify the rate of the electromagnetic energy that is absorbed (W_{abs}) and scattered (

W_{sca}) by the particle, the absorption (σ_{abs}) and scattering (σ_{sca}) cross section can be defined:

$$\sigma_{abs} = \frac{W_{abs}}{\mathcal{P}_{inc}}, \quad \sigma_{sca} = \frac{W_{sca}}{\mathcal{P}_{inc}} \quad (8)$$

where

$\mathcal{P}_{inc}$ is incident irradiance, defined as energy flux of the incident wave, $\left[W / m^2 \right]$

W_{abs} is energy rate absorbed by particle, $\left[W \right]$

W_{sca} is scattered energy rate, $\left[W \right]$

The total scattering cross-section, or *extinction* cross-section, is the amount of energy removed from the incident field due to absorption and scattering. By energy balance, the extinction cross-section is a superposition of the scattering and absorption cross-sections:

$$\sigma_{ext} = \sigma_{abs} + \sigma_{sca}, \quad \left[m^2 \right] \quad (9)$$

The energy loss rate in a particle is:

$$Q_{loss} = \frac{1}{2} \text{Re} \left[\mathbf{J}_{tot} \cdot \mathbf{E}^* + j\omega \mathbf{B} \cdot \mathbf{H}^* \right], \quad \left[W / m^3 \right] \quad (10)$$

Where the total current is a superposition of conduction and displacement currents: $\mathbf{J}_{tot} = \sigma \mathbf{E} + j\omega \mathbf{D}$. Thus, Eq. (10) includes conduction, polarization, and magnetic losses. The total absorbed energy is derived by integration of energy loss over the volume of the particle:

$$W_{abs} = \iiint_{V_P} Q_{loss} dV = \quad (11)$$

$$\frac{1}{2} \iiint_{V_P} \text{Re} \left[(\sigma \mathbf{E} + j\omega \mathbf{D}) \cdot \mathbf{E}^* + j\omega \mathbf{B} \cdot \mathbf{H}^* \right] dV, [W]$$

The scattered energy is derived by integration the Poynting vector over an imaginary sphere around the particle:

$$W_{sca} = \oiint_S \mathcal{P}_{sca} \cdot \mathbf{n} dS = \quad (12)$$

$$\frac{1}{2} \oiint_S \text{Re} \left[\mathbf{E}_{sca} \times \mathbf{H}_{sca}^* \right] \cdot \mathbf{n} dS, [W]$$

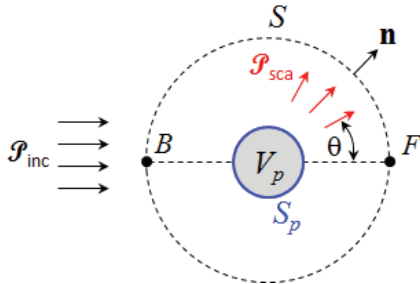where **n** is unit vector normal to the imaginary sphere.

Figure 1. Imaginary sphere S around a particle volume V_p enclosed by surface S_p. **Scattering amplitude is evaluated in the forward direction at point** F.

2.2 Optical Theorem

In physics, the optical theorem is a general law of wave scattering theory, which relates the forward scattering amplitude to the total cross section of the scattering object. The optical theorem has a long history and is common to all kinds of seemingly disparate scattering phenomena involving acoustic waves, electromagnetic waves and elementary particles. The theorem can be derived directly from a treatment of a scalar wave [1]. Scattering is a superposition of the incident and scattered waves, as schematically shown in Figure 2.
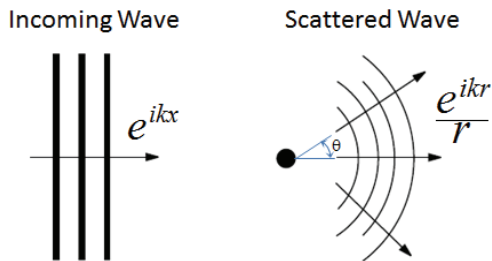

Figure 2. Generic scattering geometry. An incoming plane wave e^{ikx} scattered off a particle. A great distance away scattered wave is approximated by a spherical wave e^{ikr}/r.

If a plane wave is incident on an object, then the wave amplitude a great distance away from the scattering object, neglecting higher order terms, is given by:

$$\psi(\mathbf{r}) \approx e^{ikx} + f(\theta)\frac{e^{ikr}}{r} \tag{13}$$

where f is the *scattering amplitude*, θ is scattering angle, and $k = \omega/c$ is the wave vector.

The optical theorem states that the relation between the total cross section and the scattering amplitude. It is usually written in the form:

$$\sigma_{ext} = \frac{4\pi}{k} \operatorname{Im}\{f(0)\}/E_{inc} \tag{14}$$

where $f(0)$ is the scattering amplitude in the forward direction $\theta = 0°$. Thus, the optical theorem relates extinction cross-section to the imaginary part of the scattering amplitude evaluated in the forward direction. Yet, extinction is due to the scattering and absorption. Scattering involves all directions whereas absorption is often independent of direction, so why should the optical theorem depend on only the forward direction, and how is absorption involved? Berg, and Sorensen [4] provide a physical explanation of these features of the optical theorem.

COMSOL includes a built-in far-field computation node that automatically calculates the far-field variables defined as:

$$\mathbf{E}_{far} = \lim_{r \to \infty} r\mathbf{E}_{sca} \tag{15}$$

The far-field variables, e.g., E_{far}, represent the *scattering amplitude* rather than the physical electric field and are measured in units $[E_{far}] = [m \cdot V / m] = [V]$.

Thus, the extinction cross-section can be directly calculated, without evaluation of absorption and scattering cross-sections, as:

$$\sigma_{ext} = \frac{4\pi}{kE_{inc}} \operatorname{Im}\{E_{far}(0)\}, \quad [m^2] \tag{16}$$

2.3 Radiation Pressure Cross-Section

In addition to energy, the electromagnetic wave carries momentum $\mathcal{P}/c$; therefore, a beam of light that interacts with a particle will exert a force on the particle, called *radiation pressure*. Debye, in 1909, was probably the first to calculate the radiation force on a small particle. By integrating the Maxwell stress tensor over the surface of the sphere, he demonstrated that:

$$\sigma_{pr} = \sigma_{ext} - \langle\cos\theta\rangle\sigma_{sca}, \quad [m^2] \quad (17)$$

where σ_{pr} is the *pressure cross-section*, and

$g = \langle\cos\theta\rangle$ is so called *asymmetry parameter*. This expression for pressure cross-section holds for any small particle illuminated by a beam of light [2]. The radiation cross section is directly related to the radiation force.

The asymmetry parameter g can be interpreted as the mean direction of the scattered light and is defined as an average of the scattering angle weighted with respect to scattered power flow:

$$\langle\cos\theta\rangle = \frac{\oiint\limits_{S} \cos\theta(\mathcal{P}_{sca}\cdot\mathbf{n})dS}{\oiint\limits_{S}\mathcal{P}_{sca}\cdot\mathbf{n}dS} \quad (18)$$

where $\cos\theta = \mathbf{n}\cdot\hat{\mathbf{k}}$ is directional cosine between vector normal to the surface S and direction of incident plane wave.
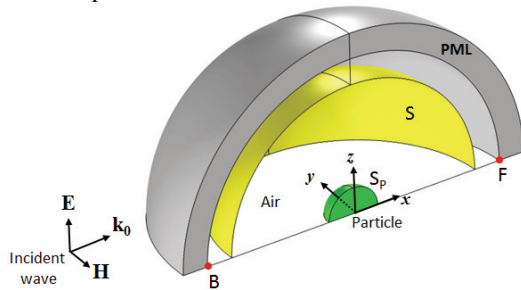

Figure 3*: Model geometry for Mie scattering by a spherical particle.

For a particle that scatters light isotropically (i.e., the same in all directions), the factor g vanishes; it also vanishes if scattering is symmetric about a scattering angle of $\theta = 90°$. If the particle scatters more light towards the forward direction ($\theta = 0°$), the factor g is positive. The factor g is negative if the scattering is directed more towards the back direction ($\theta = 180°$).

2.4 Radiation Force

The radiation pressure cross section can be used to calculate force that a particle experiences in the incidence direction [5]:

$$\mathbf{F} = \frac{1}{c}\sigma_{pr}\mathcal{P}_{inc}, \quad [N] \quad (19)$$

Where the pressure cross-section is given by Eq.(17). Alternatively, this force can be calculated by integration of Maxwell's stress tensor over the surface of the particle. The time-averaged Maxwell's stress tensor is:

$$\hat{\mathbf{T}} = \frac{1}{2}\text{Re}\left[\mathbf{E}^*\mathbf{D} + \mathbf{H}^*\mathbf{B} - \frac{1}{2}\left(\mathbf{E}^*\cdot\mathbf{D} + \mathbf{H}^*\cdot\mathbf{B}\right)\hat{\mathbf{I}}\right], \quad [Pa] \quad (20)$$

where $\mathbf{D} = \varepsilon E$ is electric flux density, $\mathbf{B} = \mu\mathbf{H}$ is magnetic flux density, and $\hat{\mathbf{I}}$ is unit tensor of second rank.

The total time-averaged force $\mathbf{F}$ acting on a particle illuminated with light can be calculated using the surface integral:

$$\mathbf{F} = \oiint\limits_{S_P}\hat{\mathbf{T}}\cdot\mathbf{n}dS_P, \quad [N] \quad (21)$$

where S_P is surface enclosing particle volume V_P, and $\mathbf{n}$ is unit normal vector to surface S_P. Calculating the force based on Eq. (18) or Eq. (21) gives the same result.

3. Use of COMSOL Multiphysics

This model solves for the scattering off the spherical particle with radius of $a = 0.1\mu m$. The model geometry is shown in Figure 3. Two symmetry planes enable modelingonly one-quarter of the sphere. The air domain is truncated by a perfectly matched layer (PML), andfar-field calculationsare done on the inner boundary of

thePML domain. The surface S is used to calculate total scattered energy.
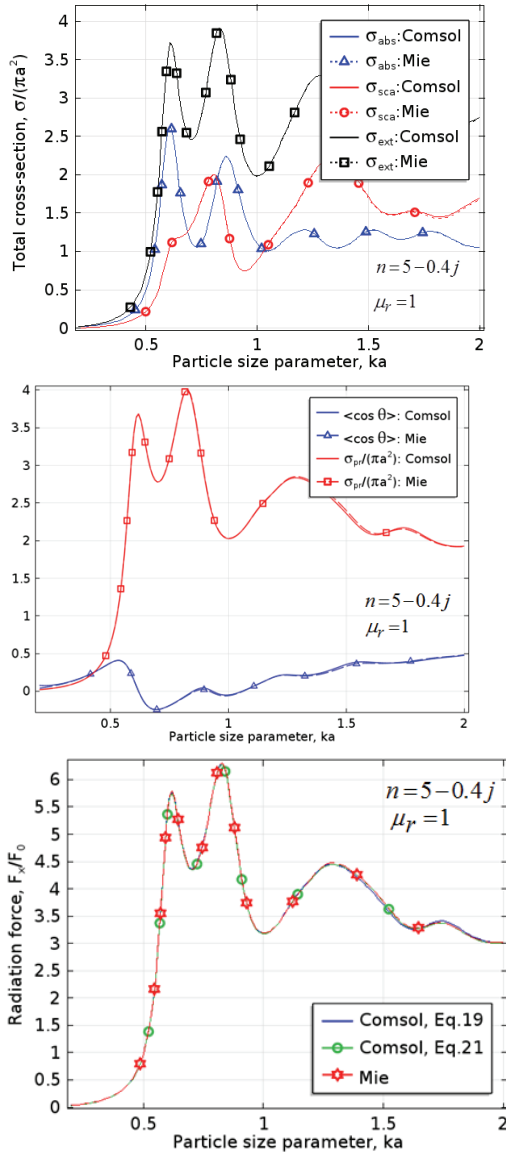

Figure 4. Cross-section parameters and radiation force for dielectric particle.

An incident plane wave travels in the positive x-direction, with the electric field polarized along the z-axis. This imposes the following boundary conditions on the symmetry planes:

Symmetry in electric field:

$$\mathbf{n} \times \mathbf{H}\big|_{y=0} = 0 \quad (\text{PMC})$$

Symmetry in magnetic field:

$$\mathbf{n} \times \mathbf{E}\big|_{z=0} = 0 \quad (\text{PEC})$$

For the scattered field formulation, Eqs.(1) and(3)are used in the model setup. The background incident plane wave is defined as:

$$\mathbf{E}_{inc} = \left\{0, 0, E_0 e^{-jk_0 x}\right\} \qquad (22)$$

where E_0 is plane wave amplitude, $k_0 = \omega / c$ is wavevector in the air, ω is circular frequency and c is speed of light in air.

The incident energy flux amplitude follows from Eq. (7):

$$P_0 = \left|\boldsymbol{\mathcal{P}}_{inc}\right| = c\varepsilon E_0^2 / 2 \qquad (23)$$

The convenient normalization factor for radiation force is defined as:

$$F_0 = \varepsilon_0 \left(aE_0\right)^2, \quad [N] \qquad (24)$$

4. Results

The following particles of radius $a = 0.1\mu m$ are considered: dielectric, magnetic, and metal (silver). Material properties of the dielectric particles are: $\varepsilon_r = \left(5 - 0.4j\right)^2$, $\mu_r = 1$, $\sigma = 0$ .Material properties of the magnetic particle are: $\varepsilon_r = 1$, $\mu_r = 8 - 2j$, $\sigma = 0$. At optical frequencies, the metal particle is modeled as a dielectric having a complex valued permittivity. The real and imaginary parts of the complex permittivity of silver are extracted using complex refractive index frequency-dependent data [5].

Scattering characteristics for three types of particles considered are shown in Figure 4, Figure 5, and Figure 6. Numerical results are compared with analytical solutions obtained with Matlab code developed by Mätzler [6]. All results are in good agreement with analytical solution based on Mie theory.

5. Summary

A solution of the scattering of electromagnetic waves has been developed using COMSOL Multiphysics. The results assume elastic

scattering only and do not include Brillouin or Raman scattering. The results developed from the COMSOL Multiphysics model are compared with the Mie analytical solution. In all cases considered, the analysis shows good agreement with the Mie solution.
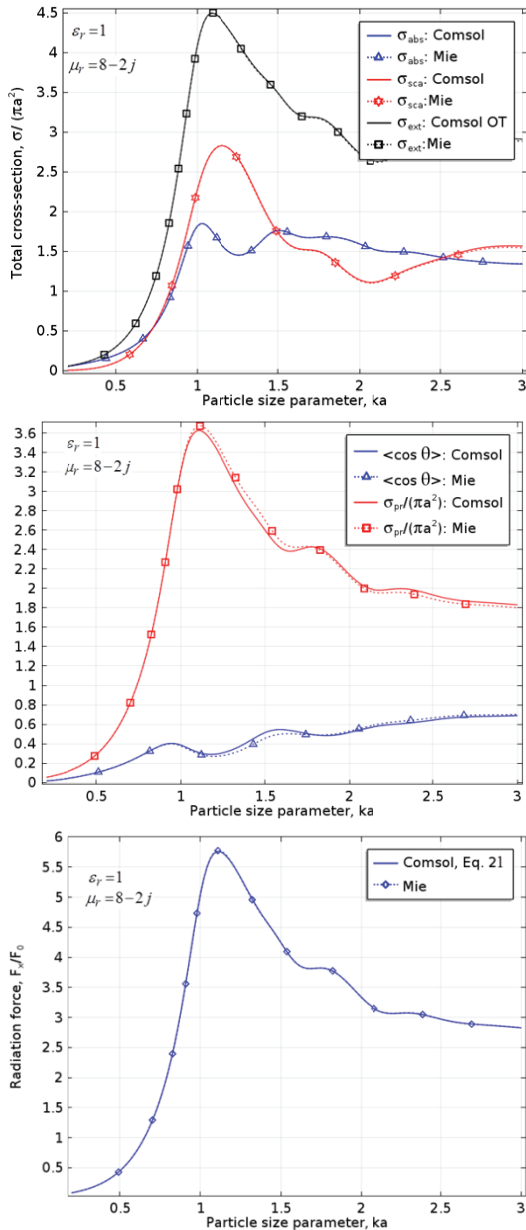

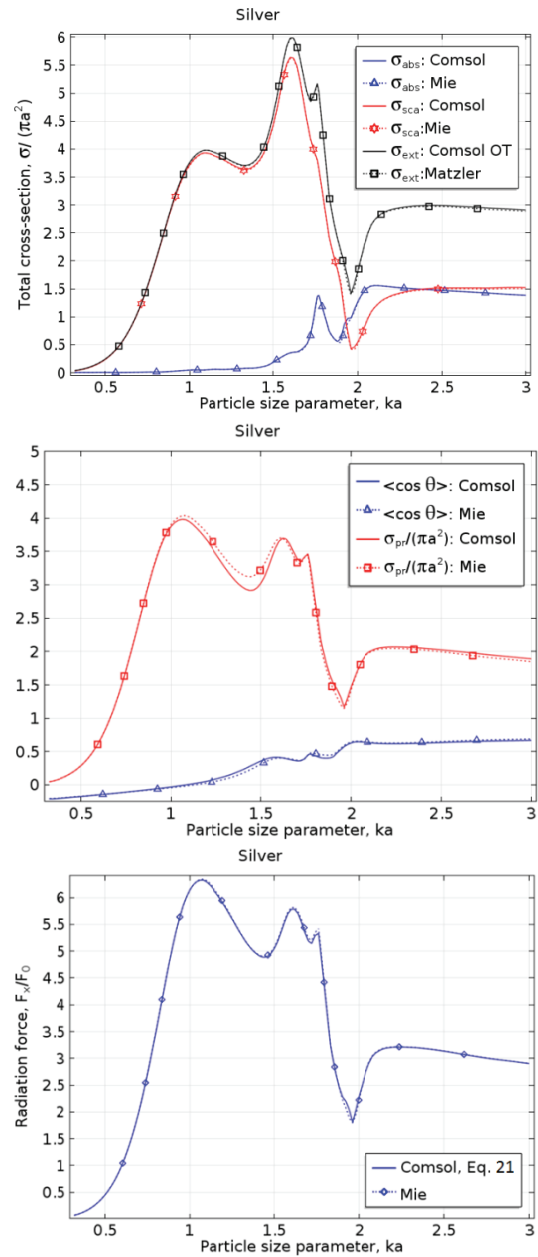**Figure 5. Cross-section parameters and radiation force for magnetic particle.**

Figure 6. Cross-section parameters and radiation force for silver particle with dielectric constants shown in Fig. 7.
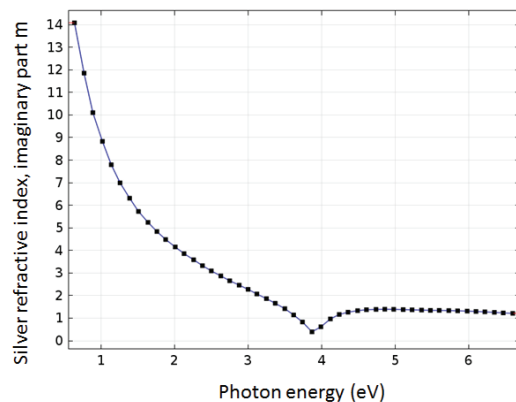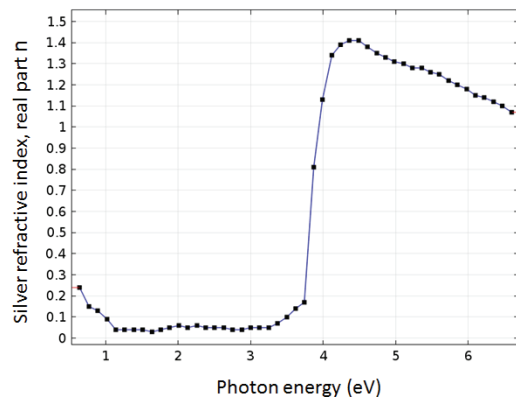
Figure 7.Dielectric constants for silver as a function of photon energy: Data from Ref. [5].

8. Acknowledgements

9. References

1. van de Hulst, *Light Scattering by Small Particles,* Dover, New York, 1981.

2.Bahrem, C.F., and Huffman, D.R., *Absorbing and Scattering of Light by Small Particles*, Wiley, New York, 1983.

3. Quinten, M. *Optical Properties of Nanoparticle Systems: Mie and Beyond*, Wiley, New York, 2011

4.Berg, M. J., Sorensen, C. M., and Chakrabarti, A., "Extinction and the Optical Theorem. Part I.

Single Particles*", J. Opt. Soc. Am.A 25*, pp. 1504-1513 (2008).

5. Johnson, P.B. and Christy, R.W. "Optical Constants of the Noble Metals", *Phys. Rev. B*, vol. 6, pp. 4370−4379, 1972.

6. Mätzler, C.: *MATLAB Functions for Mie Scattering and Absorption, Version 2*, IAP Research Report, No. 2002-11, InstitutfürangewandtePhysik, Universität Bern, 2002.