Sensitivity analysis for characterization of gold nano-particles via surface wave scattering

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Abstract

A preliminary sensitivity analysis is performed for surface wave scattering by gold nano-particles. Sensitivities of the normalized scattering matrix elements, M_{ij}, to the diameter of the particle and its distance above the substrate, is calculated and reported as a function of the observation angle in the far-field.

1 Introduction

It is well known that nano-particles have different properties than their bulk materials counterparts, and their uses allowed to obtained unique optical, electrical, and structural properties. To control the nano-scale fabrication process, the composition, structure, shape and size distributions of such nano-particles or colloids need to be known; there is consequently a need to develop real-time non-intrusive visualization tools.

Since the wavelength of light is much greater than the typical size of nano-structures, a non-intrusive characterization method using evanescent waves/surface plasmons has been proposed recently [1, 2]. The cases considered in these papers consists of a thin metallic film (medium 1) placed on a quartz layer (medium 0); metallic spherical nano-particles are located on, or above, the surface of the thin metallic film in air (medium 2). A radiation beam is incident on the interface 0–1, at an angle equal or greater than the critical angle for total internal reflection. This leads to surface waves in medium 2 which are tunneled to the particle (or agglomerates), and then scattered. The idea is to use the far-field scattered polarized light to characterize these metallic nano-particles.

The mathematical model has been described in details for a single nano-particle [1], and for agglomerates [3], and is not repeated here; only the general ideas are presented below. The far-field scattered electric field is related to the incident electric field by the amplitude scattering matrix:

$$\begin{pmatrix} E_\theta^{sca} \\ E_\phi^{sca} \end{pmatrix} = \frac{\exp(ikr)}{-ikr} \begin{bmatrix} S_2 & S_3 \\ S_4 & S_1 \end{bmatrix} \begin{pmatrix} E_{TM}^{inc} \\ E_{TE}^{inc} \end{pmatrix} \tag{1}$$

The elements of the amplitude scattering matrix are calculated from the scattered field expansion coefficients, which in turn are found from the incident field expansion coefficients and the T-matrix of the particle/agglomerate.

Results previously obtained [2, 3] have shown that angular variations of the normalized scattering matrix elements, M_{ij}, provide significant information about the size, shape, and orientation of particles/agglomerates. These observations have been done mostly in a qualitative manner, and there is a need to quantify the sensitivity of the system to the parameters to be characterized. A sensitivity analysis is of primary importance in order to determine the conditions for which a particular parameter can be estimated, and is a necessary step, with the experimental validation of the forward numerical model, of the development of inversion techniques.

In this paper, the basics of a sensitivity analysis are discussed and preliminary results are presented; more particularly, sensitivity of M_{11}, M_{12}, M_{33}, and M_{34} to the diameter of the particle and its distance above the metallic film is performed.

2 Sensitivity analysis

The sensitivity of a measurement to the parameters to be estimated is given by the sensitivity coefficients. In the frame of this study, the normalized sensitivity coefficients are written following [4]:

$$X_{\psi_k}^{norm}[M_{ij}](\eta, \psi) = \left| \frac{\partial M_{ij}(\eta, \psi)}{\partial \psi_k} \psi_k \right| \quad (2)$$

and provides the variation of an output (normalized scattering matrix elements, M_{ij}) associated to a relative variation of one parameter of the system (ψ_k), when all other parameters (known η or to be estimated $\psi_{l,l\neq k}$) are fixed. In a general way, the estimation of a parameter is considered to be conceivable when the normalized sensitivity coefficients are greater than 0.1 [4].

In this paper, it is assumed that there is a distribution of single spherical nano-particles (no agglomerates) of varying diameters (d_m) and distances relative to the surface of the thin metallic film (h). To calculate the global sensitivity of a given configuration to a parameter to be estimated, averaged normalized sensitivity coefficients are defined as follows:

$$X_{\psi_k}^{norm,avg}[M_{ij}](\eta, \psi) = \sum_{k=1}^{K} w_k \left| \frac{\partial M_{ij}(\eta, \psi)}{\partial \psi_k} \psi_k \right| \quad (3)$$

where w_k is a weighting factor associated with the number of particles characterized by the parameter ψ_k relative to the total number of particles (i.e., w_k is given by a distribution function). By the same way, averaged M_{ij} are defined following the distribution of particles, and are calculated accordingly.

Due to the complexity of the mathematical model, averaged normalized sensitivity coefficients (Eq. (3)) are calculated numerically using a finite difference scheme. Also, this preliminary study is restricted to gold nano-particles located on, or above, a thin gold film having a thickness of 20 nm. The wavelength of the incident radiation beam is taken as 515 nm, and therefore the real and imaginary part of the complex refractive index of gold are 0.279 and 1.039, respectively. The angle of incidence of the beam on the interface 0–1 is 23.3° (the critical angle for this particular case is 17.1°).

Sensitivities of M_{ij} to the diameter is now considered ($\psi_k = d_m$) for two size distributions of particles; the first involved a uniform distribution of single spherical particles having diameters from 10 to 15 nm, and the second a uniform distribution of diameters from 45 to 50 nm. For both configurations, all particles are located on the surface of the substrate (gold thin film); averaged scattering profiles (not shown) and averaged normalized sensitivity coefficients (Fig. 1) are calculated in function of the observation angle in the far-field (θ).

It can be seen that for both configurations, sensitivities of the normalized scattering matrix elements are highly dependent of the angle θ. For a uniform distribution of particles having diameters from 10 to 15 nm (Fig. 1(a)), the sensitivity is generally low (below 0.1, margin represented by a dashed line); averaged normalized sensitivity coefficients of M_{12} are greater than 0.1 for angles from 0° to 10°, and 145° to 180°, approximately. In the case of particles having diameters from 45 to

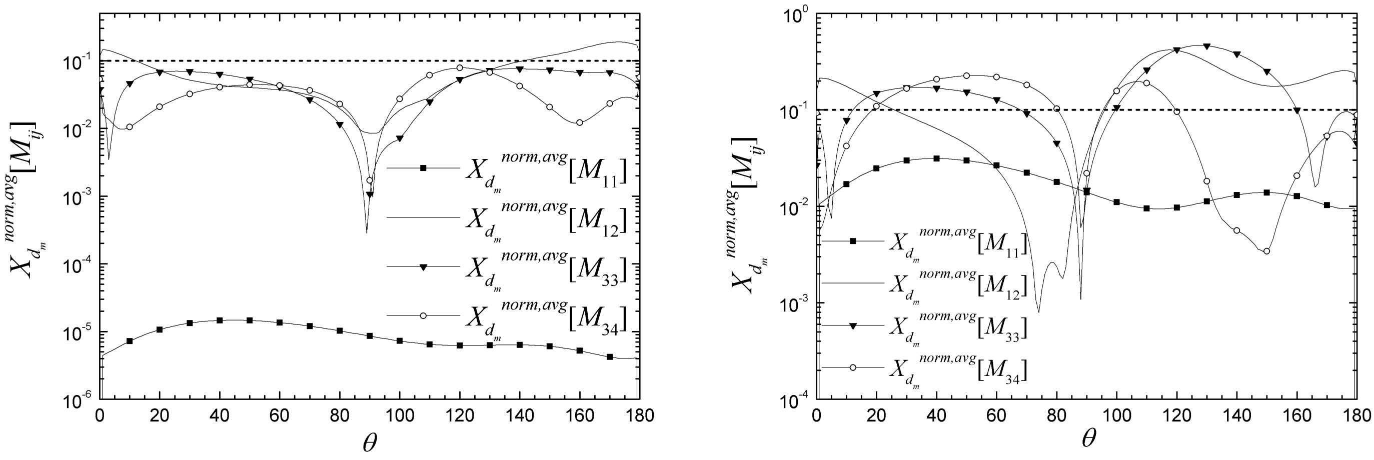

Figure 1: Averaged normalized sensitivity coefficient to d_m ($h = 0$). (a) Uniform distribution of particles with d_m from 10 to 15 nm. (b) Uniform distribution of particles with d_m from 45 to 50 nm.

50 nm (Fig. 1(b)), the sensitivity of all parameters is considerably increased; this can be explained by the fact that as the diameter increases, more energy is tunneled to the particle, which in turns increase the amount of energy scattered. For this configuration, M_{12}, M_{33}, and M_{34} reached, for certain ranges of angle, a sensitivity higher than 0.1. It is interesting to note that for both cases, the sensitivity of M_{11} is low, regardless of the observation angle, θ. Moreover, the sensitivity of M_{12}, M_{33}, and M_{34} is minimal in the vicinity of an angle of 90°.

The same kind of analysis is repeated next, but by considering the sensitivity of M_{ij} to the distance of the particle relative to the substrate ($\psi_k = h$). A uniform distribution of spherical particles of equal diameter (15 nm), and with h varying from 0 to 25 nm, is considered; averaged normalized scattering elements (not shown), and averaged normalized sensitivity coefficients (Fig. 2) are calculated as a function of the observation angle in the far-field (θ).

It can be seen that M_{ij} are sensitive to h, for a wide range of observation angles θ. As for the previous cases, the sensitivity of M_{11} is very low; at the opposite, the sensitivity of M_{33} reach an interesting peak for θ from 120° to 140°, approximately.

3 Conclusions

A preliminary sensitivity analysis for the design of a nano-particle characterization tool, using evanescent waves/surface plasmons, has been presented in this paper. Sensitivities of the normalized scattering matrix elements, M_{ij}, to the diameter of the particle, and its distance above the substrate, have been reported. It has been shown that sensitivities of the M_{ij} elements are highly dependent of the observation angle in the far-field, and are in general sufficiently sensitive to the parameters to be estimated. However, for all cases, results have revealed that M_{11} is of low interest for the characterization of the diameter of a particle, and its distance above the substrate.

Results presented here are preliminary, and restricted to gold nano-particles on, or above, a gold thin film. Therefore, the basics of the sensitivity analysis presented above need to be extended. Sensitivity to other parameters, such as the wavelength of the incident beam, is crucial and must

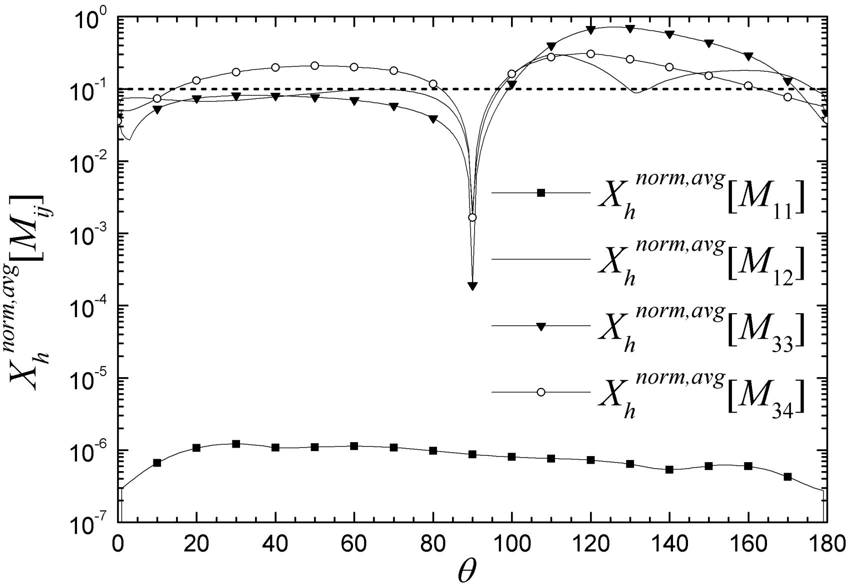

Figure 2: Averaged normalized sensitivity coefficient to h ($d_m = 15$ nm). Uniform distribution of particles with h from 0 to 25 nm.

be considered. Also, only uniform distribution of single particles has been considered, and further efforts must be devoted to more realistic configurations, involving agglomerates and non-uniform distributions.

Acknowledgments

This work is partially sponsored by a National Science Foundation grant (NSF-NER DMI-0403703, 2004). MF is grateful to the Natural Sciences and Engineering Research Council of Canada (NSERC) for their financial support (ES D3 scholarship). Additional funding is received for PGV from the Department of Mechanical Engineering, University of Kentucky.

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