Light scattering simulation by concave, peanut-shaped silver nanoparticles modeled on Cassini-ovals

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Abstract

Light scattering is a useful tool in particle characterization. The simulation of light scattering processes can help to understand scattering characteristics and from this information about particle sizes, materials or shapes can be retrieved. In this paper we demonstrate the application of the Nullfield Method with Discrete Sources for light scattering by concave, peanut-shaped silver nanoparticles. Additionally we use the Discrete Sources Method for result validation. For the shape model a Cassini-oval based model is used, which accords to two sintered silver spheres. This model is compared to a simpler two-sphere approach by calculating the corresponding scattering patterns.

1 Introduction

With the increasing interest in nanotechnology also the interest in light scattering by such nanoparticles increases, as it can help to understand their sometimes complex characteristics and interactions. Often systems or clusters of single nanoparticles are the topics of interest. For metal nanoparticles with their luminous optical properties Gunnarsson et al. [1] point out, that the localized surface plasmon resonance has a key role in nanoparticle optics and that this is connected with the shape of the particles. So suitable particle and cluster models are needed and this includes an adequate description of the connection between two or more single particles. The easiest connection model is made from single spheres touching each other at one point. But this might be a too general approach; the resulting shape of two metallic particles sintered together should be more complex, as e.g. was demonstrated by Shimosaka et al. [2]. Because of this light-scattering studies can lead to wrong interpretations as soon as the intersection of such combined particles has an influence on the scattering pattern. This influence is investigated in this work; it is a preliminary study for better cluster models. We compare light scattering by two identical spheres with optical properties of silver with a more realistically shaped model based on a three-dimensional Cassini-oval. For light-scattering calculations we use an advanced T-matrix approach, the Nullfield Method with Discrete Sources (NFM-DS). Unlike the conventional T-matrix theory the NFM-DS allows to calculate light-scattering by such concave particles. A detailed description of the NFM-DS together with computer codes can be found in the book by Doicu et al. [3]. To make sure that we get reliable results by the NFM-DS we compare the calculated results with those we get from the Discrete Sources Method (DSM). More information about the DSM can be found in the book chapter by Eremin et al. [4]. The approach to check the validity of scattering simulation results by using these two methods worked before when we investigated light scattering by oblate, flat Cassini-oval based particles [5].

2 Particle shape model

We look for a shape model to approximate two similar spheres that are sintered together. For this we use a two-dimensional concave Cassini-oval. The Cassini-oval is defined by

$$\left[(x-a)^2+\left(\frac{y}{c}\right)^2\right]\left[(x+a)^2+\left(\frac{y}{c}\right)^2\right]=\mathrm{b}^4 \quad\Rightarrow\quad y=\pm c\cdot\left(-a^2-x^2\pm\left(4x^2a^2+b^4\right)^{1/2}\right)^{1/2}$$

The shape of a Cassini-oval by definition depends on the two parameters *a* and *b*; by adding a third parameter *c* one can additionally manipulate the overall thickness of the form. Rotating this curve around its main axis delivers a three-dimensional, concave peanut-like shape. Carefully choosing these parameters enables to create a shape model that fits the two initial spheres; additionally we make sure that the volume of the peanut shape is equal to the volume of the two original spheres. Fig. 1 shows an example of such a shape.

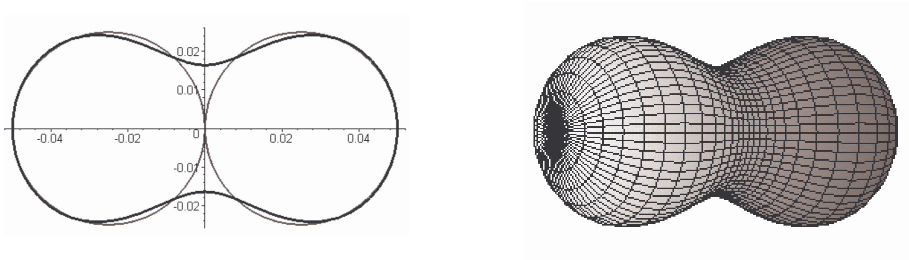

Figure 1: Cassini-oval based shape model; two-dimensional compared to two equi-volumed spheres (left) and the corresponding three-dimensional model (right). a = 0.0340625, b = 0.0365625, c = 1.236; the diameter of the spheres is 50nm. Overall particle size is 100nm.

3 Results

First we compare light scattering results for a peanut-like silver particle calculated by the NFM-DS with those we get from DSM to make sure, that both theories deliver the same scattering patterns. This helps to estimate the quality of the result; in case of accordance it is very likely that the result is correct. Fig. 2 shows the scattering patterns for a silver particle with shape and dimension as shown in Fig. 1.

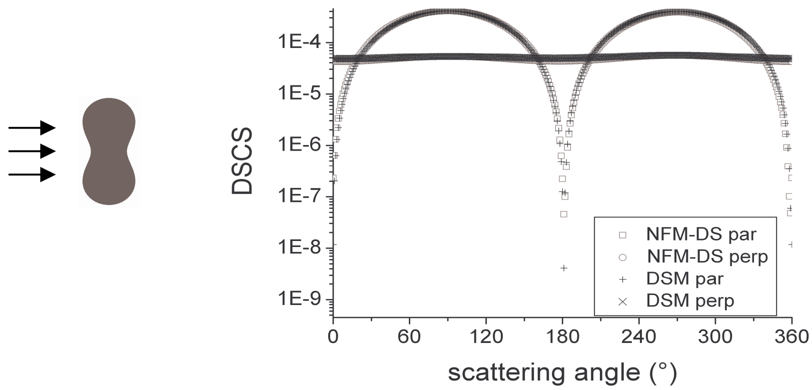

Figure 2: Comparison of light scattering patterns calculated by NFM-DS and DSM. Particle shape is a Cassini-oval based peanut as shown in Fig. 1, particle length is 100nm. Wavelength is 478nm, incident angle is 90° to rotational axis; therefore forward scattering can be observed at 90°. Refractive index is 0.13-2.729i.

As one can see there is a good congruence between both light scattering results.
In the next step we do a spectral analysis of the scattering behavior of the peanut-like silver particle as well as a corresponding two-sphere model as presented in Fig. 1. This spectral analysis will show if the shape model has influence on the scattering patterns and at which wavelengths this influence can be observed best. Fig. 3 shows exemplary scattering diagrams for both parallel and perpendicular polarization for a wavelength range between 250nm and 500nm. The refractive index follows the studies made by Johnson and Christy [5].

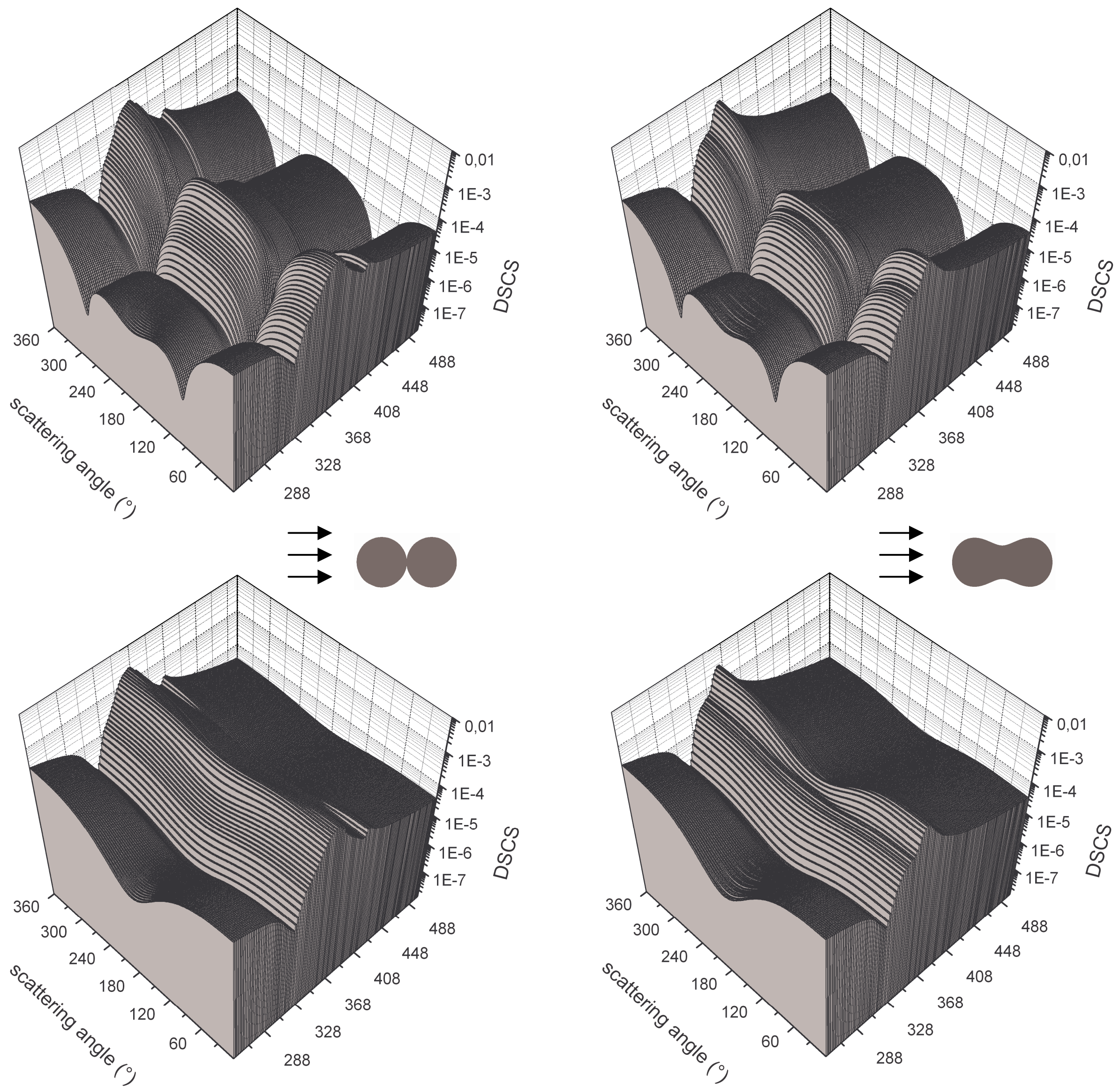

Figure 3: Spectral analysis of two spheres (left) and an equi-volume Cassini-oval based peanut (right) as shown in Fig. 1. Particle length is 100nm. Wavelength-range is from 250nm to 500nm; direction of incident light is along rotational axis. Upper diagrams show parallel, lower diagrams show perpendicular polarization.

Looking at Fig. 3 one can make several observations: comparing the diagrams for parallel polarization one sees, that for both shape models the highest intensity is reached for a wavelength about 366nm (for this particular particle size). But for the two-sphere model there is a small second peak at 404nm while this is not visible for the Cassini-oval model. On the other side this model shows a kind of small plateau before the main peak at 366nm is reached which can not be observed for the two-sphere model. For the perpendicular polarization there are also differences, mostly at the 180° scattering angle for the highest intensity. Here the diagram for the Cassini-oval model shows a significant indentation.

5 Conclusion

Fig. 3 demonstrates that there are different light scattering patterns for the different shape models, two identical spheres touching each other on one side and a single particle with a corresponding volume based on a Cassini-oval on the other side. While this is just one example for a specific particle size, shape and material, it is nevertheless reasonable that similar effects could be observed for other particle sizes as well. Further studies using light scattering simulations now can help to give a better understanding of the characteristics of such particle systems and clusters. One practical application could be to determine from measured scattering characteristics if the observed particles are sintered together or just slightly touch each other. Simulations results could also provide the information, which wavelengths and observation angles are most suitable for observations. Both light scattering theories used for this work are advantageous for this purpose: while the DSM is very fast and reliable, the NFM-DS offers all benefits of the T-matrix approach, for example fast post-processing calculations for incident angles different from the original one or orientation averaging.
To give a better impression on the topic, more detailed results will be presented at the ELS10 conference.

Acknowledgments

We would like to acknowledge support of this work by Deutsche Forschungsgemeinschaft DFG.

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