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Cross-sectional shape evaluation of a particle by scatterometry

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ABSTRACT

Reconstructing an image from the scattering pattern of particles with several wavelengths is difficult. This is because precise calculation in such cases is difficult, and because there is no proper procedure to evaluate shapes from the scattering pattern. We use rigorous coupled-wave analysis (RCWA), which we previously developed and applied to an isolated scatterer, and rotate the particle to reconstruct the image. We find that it is possible to discriminate between rectangles, triangles, and squares. The precision of length can be less than 0.2 of the wavelength, provided that the refractive index of the scatterer is known.

1. Introduction

Size and shape determination of particles is useful for blood cell counting [1] and soil analysis [2]. Particle counters [3], flow cytometry [1] and holography [4] are used for this purpose. One measurement method is scatterometry, which analyzes the diffraction pattern directly and has the advantage that lens focusing is not necessary when the particle is moving. Because the precision of the lens image is not guaranteed when the particle is smaller than 30 wavelengths [5], scatterometry is preferred for the finer measurement.

Scatterometry can calculate the scattering pattern and estimate the correct outline. Furthermore, it obtains a result for a wide region of the size. Although scatterometry is promising for an accurate analysis, few systems can calculate the scattering pattern of a particle with a certain shape of the cross section. One reason is that there is no simple and rigorous calculation method of scattering patterns [6].

Mie theory gives a rigorous solution for a sphere. However, it is not valid to approximate nonspherical shapes as spheres [7].

The T-matrix method, Fraunhofer approximation, or the discrete-dipole approximation has been used to calculate scattering patterns and has given a good prospect, but they do not have sufficient precision for a scatterer with a length of several wavelengths [8–10]. The boundary element method (BEM), finite-difference time-domain (FDTD) method, and rigorous coupled-wave analysis (RCWA) enable us to rigorously calculate the scattering characteristics of a particle [11–13]. BEM takes considerable time for programming and is not valid for unknown shape [14]. FDTD is not necessarily valid for far field calculations [15]. RCWA is preferred because it is simpler to program and requires less calculation time to determine a scattering pattern. Although RCWA has only been applied to periodic structures, it was recently applied to isolated structures [15].

The determination of the shape and size of a particle from its scattering pattern is an inverse problem [16]. Here, we consider a rectangular beam spot that crosses the rod-like particle. We divide the particle into many layers along the long side for calculation. We try to calculate shape of a cross section of the particle. The scattering pattern of the particle consists of a main peak with several side band peaks, corresponding to diffraction. The angular separation of these peaks contains information about the size and shape of the particle [17]. However, to the best of our knowledge, no one has succeeded in reconstructing an image of the cross section of a particle a few wavelengths in size, from the diffraction pattern when the shape is unknown. Some use the auxiliary lines of the diffraction pattern [18]. They usually use incident light with same direction for the diffraction pattern analysis and to clarify the shape is difficult in the condition [18,19]. In the present paper, we present the reconstruction method of a two-dimensional image using RCWA.

2. Theory

Scattering intensity was calculated by RCWA [13], using the program DiffractMOD^{TM} 1.5 (RSoft Design Group, Ossining, NY, USA). The periodic diffraction pattern produced by rectangular object is very similar to the diffraction pattern produced by a rectangular aperture of the same size. According to Fraunhofer

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diffraction theory, in *PQ* coordinate, the diffraction pattern of a rectangular aperture of sides $2a$ and $2b$ is given by the following Eq. (1) [20,21]

$$I(P, Q) = I_0\left(\frac{\sin(kpa)}{kpa}\right)^2\left(\frac{\sin(kqb)}{kqb}\right)^2 \tag{1}$$

where, I_0 is constant, k is $2\pi/\lambda$, and p and q are direction cosine of diffracted light. λ is wavelength. p and q are independent, and we consider only a and p as parameters here.

To analyze the diffraction pattern, we used the high-order peak in the pattern. The order of the peak may be the first, second, third etc. The angle of the peak is theoretically related to the size of the particle [17]. Light goes through the rectangular aperture, while on the other hand light is scattered by the rectangular scatterer. The scatterer works as a mask and its effect is opposite to the aperture. By easy calculation we know that the local maximum of the pattern of the rectangle has the same angle with the local minimum of that of the rectangular aperture in the angular distribution. The local maxima of the scatterer are expected to be also periodic, because the local minima of that of the rectangular aperture are periodic against $\sin(\theta_d)$. We utilized this relationship of rectangle to calculate the size of the scatterer. For the diffraction angle of the local maximum θ_{dm}, refractive index of air n_0, diffraction order m, and wavelength λ, the width w of the particle is given by

$$w = m\lambda/[n_0 \sin(\theta_{dm})] \tag{2}$$

3. Computational method

The diffraction pattern changes roughly periodically against sin(θ_d), where θ_d is diffraction angle. The diffraction pattern of a particle is Fourier transformed after leveling the peak heights of the pattern. The resulting spectrum has several peaks. The value of the transverse axis of the peak is candidate of side length. Here ‘spectrum’ is a Fourier transformed diffraction pattern.

Actually, there are several peaks in the spectrum and the proper peak should be assigned. The complexity of the spectrum decreases by several pre-treatments for changing the diffraction pattern into pure sinusoidal one. The first is removal of non-diffracted light. Almost all light is not diffracted by the particle, because the calculation area is much longer than the particle size. It does not contribute to the sinusoidal curve. The second is normalization of the local maxima of the diffraction pattern. Eq. (1) has coefficient $1/kpa$, which modifies the pure sinusoidal curve. If we Fourier transform it directly, the peak of the spectrum is too complex to assign. After we perform such pretreatments, the spectrum is still complex. Therefore, before selecting the proper peak, shape should be identified. The information of the shape reduces the number of the sides to calculate and it is also useful in actual measurement. Here, the process is divided into two steps. The first step is Fourier transformation and shape calculation. The second is to read the local maxima of the diffraction pattern and calculate the length of sides as mentioned later. We draw the calculation scheme in Fig. 1.

At first, we calculate the product sum of the intensity and its value of transverse axis of the spectrum, and averaged over the intensity to get the side length. The radar chart of the length and the incidence angle suggests the real shape as shown in the later. Now, we know the number of the sides of the shape and the corresponding angles. The spectrum has many peaks and needs peak assignment. By calculating product sum of intensity and length of transverse axis, we escape from this problem. We can judge the shape from the results. Though the product sum gives us the value of the side's length, the precision of it is not good. We

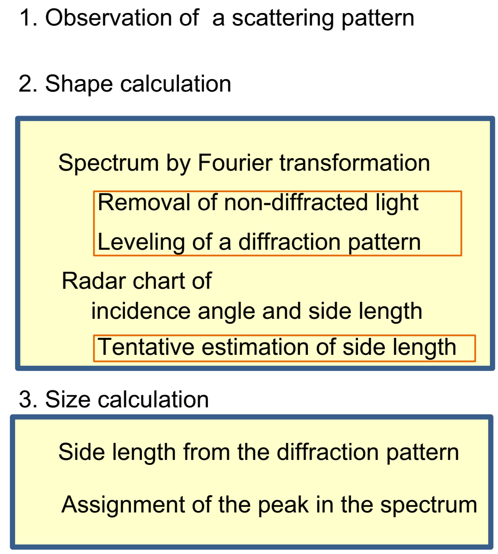

Fig. 1. Scheme of the calculation for shape and size of a particle.

can get much more precise value, when we calculate it directly from the diffraction pattern. However, the process is not simple and automatic. We used the value of the product sum for the shape calculation as the first step and assigned the peak of the spectrum for length measurements as the second step. The process of calculating the side's length becomes easy owing to information of the shape.

We then check the spectrum again. We select the incidence angles which produce sharp and strong single peaks. If the incidence angle is vertical to the side, the diffracted pattern should oscillate according to the side length and the oscillation may be relatively simple. Therefore, the incident light gives distinct peak in the spectrum. Considering the side length derived directly from the diffraction pattern, we select the proper peak. There are several peaks in the pattern. We read the value of the transverse axis of the peaks and used Eq. (2). If diffraction order m is more than one, we averaged w derived from the peaks.

4. Results and discussion

We examine the shapes in Fig. 2. The square has a width $v=3\lambda$, the isosceles triangle has a depth $d=\lambda$ and a width $v=3\lambda$, the rectangle has a width $v=3\lambda$ and a depth $d=2\lambda$, and the scalene triangle has a depth $d=\lambda$ with $a=1.9\lambda$ and $b=1.1\lambda$. All of these units are measured in wavelengths. The refractive index n of the scatterer is set to 1.5, if there is no mention about it. The incidence

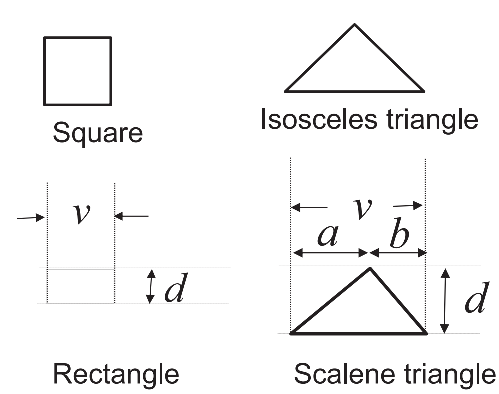

Fig. 2. The shapes identified by calculations, $v=3.0$ and $d=2.0$ for the rectangle; $v=3.0$, $d=1.0$, $a=1.1$, and $b=1.9$ for the triangle.