Particuology 24 (2016) 151–158

Contents lists available at ScienceDirect

Particuology

journal homepage: www.elsevier.com/locate/partic

Fraunhofer diffraction of irregular apertures by Heisenberg uncertainty Monte Carlo model

Yijia Yuan[a,b,*], Kuanfang Ren[b], Claude Rozé[b]

[a] Shanghai Jiao Tong University-Paris Tech Elite Institute of Technology, 800 Dongchuan Rd, Shanghai 200240, China
[b] CORIA-UMR 6614, Normandie Université, CNRS,Université & INSA de Rouen, Avenue de l'Université, BP 12, 76801 Saint Etienne du Rouvray, France

ARTICLE INFO

Article history:
Received 16 January 2015
Received in revised form 13 March 2015
Accepted 16 March 2015
Available online 27 June 2015

Keywords:
Diffraction of a ray/photon
Heisenberg uncertainty Monte Carlo model
Fraunhofer diffraction
Irregular aperture

ABSTRACT

Geometrical optics and the Monte Carlo method are very flexible in dealing with the interaction of light with non-spherical particles, but usually diffraction is not considered. To cover this gap, the Heisenberg Uncertainty Monte Carlo (HUMC) model is applied to calculate separately the diffraction of a ray or a photon. In this paper, we report an improvement of the HUMC model by specifying the phase of the photon subject to the Fraunhofer diffraction condition. After validating the model by comparing its results with analytical results for apertures of simple shapes, the HUMC model is then applied in simulations of Fraunhofer diffraction by apertures of complex shapes, such as those composed of one or two elliptical openings. We have shown that the diffracted intensity distributions of simple apertures obtained by the HUMC model are in good agreement with the results calculated from analytical expressions. The simulations of diffraction by apertures composed of two square or elliptical openings prove that the HUMC model is a powerful and flexible tool for predicting the Fraunhofer diffraction by a complex optical system.

Introduction

The precise and reliable prediction of the light scattering properties of particles is essential for optical metrology. Although the problem of light scattering by particles of simple shapes (sphere, infinite cylinder, for example) has been solved, there are still much to do for the particles of complex shapes, especially when their sizes are much larger than the wavelength. The particles encountered in multiphase flows are always of complex shape and of large size, but there are no theoretical or numerical methods to simulate with precision the interaction of light with such particles. Rigorous theories are limited to particles of very simple shapes whereas numerical methods can only be applied to particles of size less than some tens of wavelengths. We are therefore interested in ray tracing (RT), which is simple and intuitive for dealing with the scattering of light by a large particle of any shape.

Geometrical optics (GO) based on RT has been used in the scattering from large particles of regular shapes, such as sphere, cylinder, and spheroid (Van de Hulst, 1981; Glantschnig & Chen, 1981; Wait, 1955; Hovenac, 1991). However, in classical GO, the effect of interference is often not taken into account (Roosen & Imbert, 1976; Yang & Liou, 2009; Yang et al., 2005). For a homogeneous spherical particle, Xu, Cai, and Ren (2004); Xu, Ren, and Cai (2006a) have shown that, by taking into account the interference between rays of different orders and forward diffraction, GO can predict the scattered light correctly in all directions except the regions near the rainbow angles and critical angles where the wave effect should be considered. Nevertheless, when we attempted to extend GO to a particle of complex shape, the calculations of the divergence factor and the phase shift due to the focal lines become difficult, and even impossible (Xu, Ren, Cai, & Shen, 2006b; Yuan, 2012). To resolve this problem, Ren, Onofri, Rozé, and Girasole (2011); Ren, Rozé, and Girasole (2012) have developed the vectorial complex ray model (VCRM) which is capable of describing the scattering by a smooth object of arbitrary shape. By introducing the wave front curvature as one of the intrinsic properties of rays, VCRM enables the scattering of a wave by a large particle of any shape to be predicted with precision. It is especially suitable

---

* Corresponding author at: Shanghai Jiao Tong University-Paris Tech Elite Institute of Technology, 800 Dongchuan Rd, Shanghai 200240, China. Tel.: +0086 13774310452.
E-mail address: yj.yuan@sjtu.edu.cn (Y. Yuan).

http://dx.doi.org/10.1016/j.partic.2015.03.006

for an individual particle with a surface described by an analytical function, such as spheres, spheroids, ellipsoids, and circular and elliptical infinite cylinders.

In treating the scattering of a particle obtained using numerical simulations, such as a synthetic jet described by level sets in fluid mechanics, or in handling multiple scatterings, the Monte Carlo ray tracing (MCRT) is preferred (Tanguy, Ménard, & Berlemont, 2007). It is very flexible and can be easily applied to particles of complex shapes. Many researchers have contributed to this model (Takano & Liou, 1995; Grynko & Shkuratov, 2003; Shkuratov & Grynko, 2005). Nevertheless, the wave properties such as interference and diffraction have not been considered.

Diffraction plays an important role in the phenomenon of light scattering. In particular, when dealing with scattering problems using models based on ray tracing such as GO, VCRM, and MCRT, the diffraction must be taken into account separately. This phenomenon can be described by the Huygens–Fresnel principle. Much work has been performed by many researchers, although almost all studies were performed using integrals or the Fourier transform applied to apertures of simple shapes (Southwell, 1981; Kim, Grebel, & Jaggard, 1991; Urcid & Padilla, 2005; Sillitto, 1979; Wendling, Wendling, & Weickmann, 1979; Borovoi, Naats, Oppel, & Grishin, 2000). To apply the models in which the light waves scattered by objects of any shape are described by rays or photons, the diffraction of each ray or photon must be analyzed.

The geometrical theory of diffraction (GTD) is an extension of geometrical optics that introduces diffracted rays (Kelly, 1962; James, 1980). However, the theory is valid only for a few very simple and specific forms, called canonical problems, such as edges, corners, or vertices of boundary surfaces. We therefore turn our attention to the Heisenberg uncertainty Monte Carlo (HUMC) model which treats diffraction by an aperture of arbitrary shape in the framework of Monte Carlo (MC) techniques. It is based on the GTD hypothesis; that is, for high frequencies, the diffraction can be regarded as a local phenomenon and it depends only on the shape of the diffracted object near the diffraction point. This hypothesis of a local phenomenon can greatly simplify the calculations of the diffracted field.

Carlin (1964) proposed to deal with the minimum diffraction spot size by exploiting the uncertainty relation. Similar to the treatment of the reflection or refraction by the MC technique, Heinish and Chou (1971) applied a novel statistical analysis of MC based on the Heisenberg uncertainty principle to study the diffraction by an opening. By predicting the angle at which an approaching ray or photon is diffracted, the intensity distribution of diffracted field is deduced. Freniere, Gregory, and Hassler (1999) simplified the part of the diffracted photon tracing in the model of Heinish and Chou (1971). However, the oscillations of the diffracted field could not be reproduced because the interference between photons had not been taken into account. Serikov and Kawamoto (2001) suggested that each photon possesses a phase which is used to calculate the interference between the diffracted photons. They have validated the model by comparing the diffracted intensity simulated by the HUMC model with the results of analytical expressions for apertures of simple shapes. However, the model of Serikov and Kawamoto (2001) encountered a numerical problem in the calculation of the phase when the observation distance became very large compared with the particle size. This instance is often encountered in optical metrology, so we are especially interested in it and propose an improvement of the HUMC model by specifying the phase of Fraunhofer diffraction. The model is applied to estimates of the diffraction of light by openings of complex shapes.

The paper is organized as follows. A detailed description of the model is presented in Section 2. Section 3 is devoted to the validation of the model and our algorithm by comparing the results with analytical expressions for apertures of simple shapes. The simulation by the HUMC model for the diffraction from more complex shapes, such as a single elliptical opening or apertures composed of two square or elliptical openings is also presented in Section 3. Conclusions are given in Section 4.

Description of the HUMC model

We consider a plane wave of wavelength λ propagating along the z axis. An aperture of any shape is located in the plane $(x_1, y_1, z = 0)$ (see Fig. 1). The center of the aperture O_1 is located at the origin of the coordinate system (x_1, y_1). The point $P_1\,(x_1, y_1)$ is taken to be the incident position of a photon and $P_0\,(x_0, y_0)$ is an observation point situated in the observation plane $z = R$.

Direction of a diffracted photon

The photons are evenly incident over the aperture plane. Because diffraction is an edge phenomenon, its effect depends on the distance the photon is from the edge of the aperture. In passing through an aperture, the shortest distance $\Delta x'$ from the incident point P_1 to the edge of the aperture can be regarded as the position uncertainty of the photon. The momentum uncertainty $\Delta p_{x'}$ in the corresponding direction x' can be calculated by the Heisenberg uncertainty relation,

$$\Delta x' \Delta p_{x'} \geq \frac{\hbar}{2} \qquad (1)$$

where $\hbar = h/2\pi$ with h Planck's constant. The momentum uncertainty can be interpreted as an uncertainty in the propagation direction. Hence the uncertainty relation can be applied to predict the deviation of the photon from its original propagation direction. Since the momentum of a photon is defined by $\vec{p} = \hbar\vec{k}$ (here $\vec{k}$ is the wave vector and its module is the wave number defined by $k = 2\pi/\lambda$), the angle of deviation of the diffracted photon is deduced from the Heisenberg uncertainty relation (1). According to Freniere et al. (1999), the variance $\sigma_{x'}$ of the direction deviation is related to the shortest distance from the edge $\Delta x'$ and can be deduced by (see Fig. 2):

$$\tan\sigma_{x'} = \frac{\Delta p_{x'}}{p_z} \geq \frac{1}{2\Delta x' k} \qquad (2)$$

The deviation of the photon in the orthogonal direction y' can also be deduced in the same manner as the function of the shortest

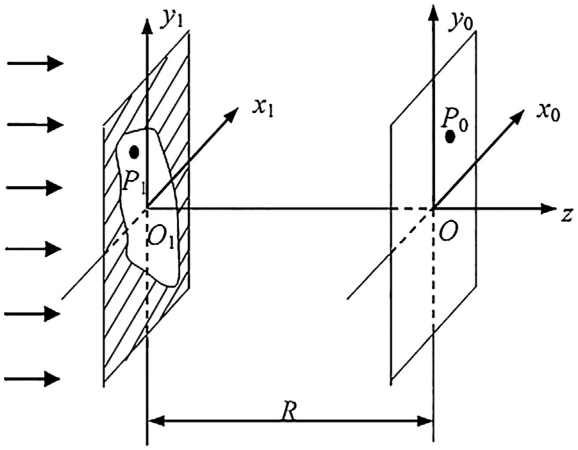

Fig. 1. Schema illustrating the diffraction of a plane wave from an aperture.