Vectorial Complex Ray Model – from Geometrical Optics to Ray Theory of Wave

Kuan Fang REN[1,*], Claude ROZÉ[1], Yijia YUAN[2]

[1] UMR 6614/CORIA, CNRS - Université et INSA de Rouen, Saint-Etienne du Rouvray, 76801, France
[2] Shanghai Jiao Tong University - Paris Tech Elite Institute of Technology, 800 Dongchuan Road, Shanghai, 200240, China

*Corresponding author: fang.ren@coria.fr

Abstract

Numerical prediction of light interaction with large non-spherical particles is vital in many applications but no useful tool is presently able to reply this demand. The Vectorial Complex Ray Model (VCRM) we are developing permits to describe the scattering of large object of smooth surface and arbitrary shape. By introducing a new property – the curvature of the wave front in the ray model, VCRM predicts correctly the divergence or convergence of a wave at each interaction with the particle surface and the phase due to the focal line. Thanks to this new property, the wave effect near singularity regions such as the caustics, the critical angles as well as the diffraction may be included directly. The fundamentals of VCRM and Ray Theory of Wave are presented in this communication.

1 Introduction

The interaction between light (or electromagnetic wave) and an object concerns many fields of fundamental and application research, such as metrology of particles in atmosphere, diagnostics of the atomization/spray in two-phase flow, trapping and manipulation of cells in life science, sorting nanoparticles in material, even the design of antenna or the radar detection. Many methods have been developed for the prediction of different properties of ? this interaction. However, they are either valid for objects of very simple form or seriously limited in the size of the objects. The approximate methods such as geometrical optics or Monte-Carlo ray tracing can deal with the scattering of large objects with complex form but their precision is not sufficient for the applications. The Vectorial Complex Ray Model (VCRM) has been recently developed [1] to reply this need. We will present in this communication this model, the Monte-Carlo Ray Tracing of Wave [2] as its variety and Ray Theory of Wave (RTW) as their extension.

2 Desctiption of the models

In Geometrical Optics or classical ray tracing, a wave is described by bundles of rays which possess four properties: amplitude, phase, propagation direction and polarization. The wave form is not an intrinsic property of the rays. So the divergence or convergence of a wave on the surface of the particle as well as the phase due to the focal lines cannot be counted directly. In the special cases of spherical particles and circular cylinders, these effects are counted separately to deal with the phenomena of rainbow and the scattering near the critical angle. The models we present in this section include the curvature of the wave front as an intrinsic property of rays and therefore permit to treat the wavelike behaviour of light directly for large arbitrary shape particles.

2.1 Vectorial Complex Ray Model

In Vectorial Complex Ray Model, a ray is characterized by the amplitude, the phase, the propagation direction, the polarization and the wave front curvatures. All these features evolve at each interaction of ray with the particle surface. The direction of a ray is described by its wave vector $\vec{k}$. The directions of reflected and refracted rays are determined by the continuity of the tangent components of the wave vectors on the particle surface:

$$k_\tau' = k_\tau \tag{1}$$

The wave front and the particle surface in the vicinity of the incident point are described by 2 × 2 matrices Q (before interaction), Q' (after interaction) and C (interface curvatures) (Figure 1). Their relation is given by the following wave front matrix equation.

$$(k'-k)\cdot nC = k'\Theta'^T Q'\Theta' - k\Theta^T Q\Theta \tag{2}$$

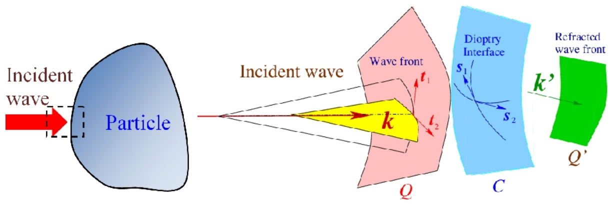

***Figure 1** Definition of the curvatures of wave fronts and dioptric surface.*

Eqs. (1) and (2) along with the Fresnel formulas permit to evaluate all five properties of the rays step by step. The wave divergence/convergence and the phase due to the focal lines are deduced directly from these values. The total scattered field is the superposition of the complex amplitude of all orders of the emergent rays. This model has been applied successfully to predict 2D (in the plane of symmetry) of an ellipsoid [1, 2, 3] and an elliptic cylinder

[4, 5]. Various new physical phenomena in light scattering by non-spherical particles are revealed.

Software has also been developed for the ray tracing and the calculation of the scattering diagram of an elliptical particle with any incident angle.

2.2 Monte-Carlo-Ray Tracing of Wave

The Monte Carlo Ray Tracing (MCRT) is a very flexible method and can be easily adapted to the particles of complex shape. It has been widely applied for the simulation of single and multiple scattering by large non-spherical particles. But the wave form is not counted in MCRT so its precision is limited.

Similar as in VCRM, we introduce also the curvatures of the wave in MCRT. This extended version of MCRT, called Monte-Carlo Ray Tracing of Wave (MCRTW) improves considerably the precision of the MCRT by taking into account the divergence or convergence and the phase shift due to the focal lines [3]. By comparison with the Mie theory for the scattering by a sphere, we proved that the MCRTW can correctly predict the scattering diagram in almost all the directions except in the forward direction due to the diffraction and near the rainbow or critical angles because of caustics. The MCRTW has been applied to the 2D scattering of the plane wave by a large spheroid.

2.3 Ray Theory of Wave

Ray model is practically the only way to deal with the interaction of light with a big non-spherical particle. It is conventionally admitted that the models based on ray tracing are valid when the particle is much larger than the wavelength. But this is only true if we are interested in the global properties or in the regions far from singularity. Near singularity regions, the wave effect must be counted even for very big particle. Since the two models described above permit to calculate precisely the all five properties of rays, particularly the wave form and phase, they are very suitable to be extended to deal with these singularities.

We recognize three types of singularity and each one is linked to a kind of measurement technique (Table 1). Until now these phenomena have been used in the optical metrology exclusively for spherical particles and circular cylinders. The concept introduced in VCRM and MCRTW will be casted into a more general theory – Ray Theory of Wave – to deal with the interaction of any wave with an object of smooth surface.

Singularity	Physical phenomena	Relevant techniques
Discontinuity of intensity	Diffraction	Diffractometry
Discontinuity of the intensity derivative	Critical angle scattering [7,8]	Refractometry of bubble[9]
Infinity of the intensity	Rainbow	Refractometry of rainbow

Table 1 *Singularities in the interaction of light with a particle, their relevant phenomena and measurement techniques*

The Ray Theory of Wave (RTW) in development is based on four principles:

1). All waves are described by rays and each ray is characterized by its direction, amplitude, phase, polarization and wave front curvature;

2). At interaction on a dioptric surface, the properties of the rays are governed by the Snell law given in Eq. (1), the Fresnel formulae and the wave front matrix equation (Eq. (2));

3). The total field is the summation of the complex amplitude of all the rays in the region far from the singularity points.

4). Near the singular regions, such the border of the particle (corresponding to forward diffraction), the caustics (rainbow angles) and the semi-caustics (critical angles), rays are considered as secondary sources and the total field is the contributions of the secondary rays near the singular angles.

The Airy theory [6] is a good example to deal with the singularity with ray model. In this theory the phase is expressed approximately by a cubic function and the amplitude is supposed constant, while in VCRM and MCRMW we predict precisely the phase and the amplitude of all rays even for a non-spherical particle.

3 Some results and discussion

We give in this section two typical results obtained with VCRM and MCRTW to show the applicability of these models and their potentials in the development of RTW.

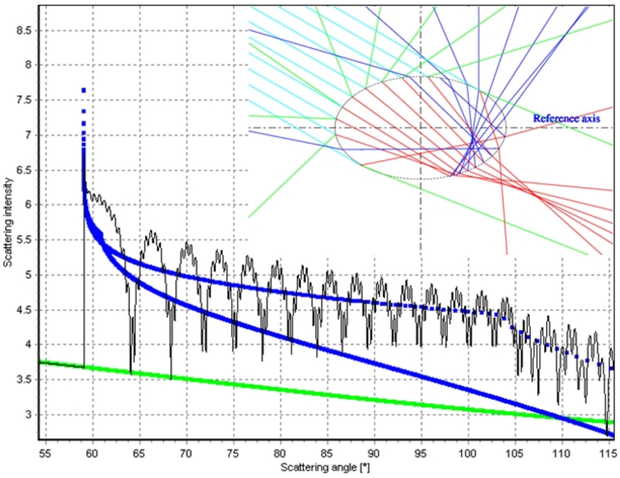

Figure 2 *Rainbow-like structure calculated by VCRM with the software VCRMEll2D for an ellipsoid of water droplet (m=1.33) with three semi-axis a=30 μm, b=40 μm and c=50 μm illuminated by a plane wave at 30° with long axis*

The first example is to show the behaviour of the scattering diagram near rainbow angle predicted by VCRM. Figure 2 shows the ray tracing (top right), the intensity of each emergent rays of the reflected (green curve) and refracted rays blue curves) and the total intensity (black curve) for an elliptical water droplet (m=1.33). The rainbow angle is located at 59° where the intensity tends to infinity but the diagram at larger angles has Airy-like structure. We have compared with Debye theory for the scattering by a spherical particle and found that the agreement is almost perfect. We find also in Figure 2 that the derivative of the intensity of the second order ray is not continuous at 104°; this is due to the total reflection of the first internal reflection. Therefore to predict precisely the scattering diagram in these regions (less than 59° and near 104°), the principle 4). of RTW given above should be applied.

The second example concerns the comparison of the MCRMW with VCRM (Figure 3). In this simulation, the total intensity of MCRMW is calculated by superposition of the complex amplitudes of the emergent rays arriving in the same direction. The agreement between the two models is satisfactory. Evidently, the precision of MCRTW depends on the total number of rays (called also photons). The computation time on a personal computer with 4 core 4X2.5 GHz and a memory of 4 Go for 10^8 photons is about 1 hour. The precision is always better for low order rays because of the number of rays.

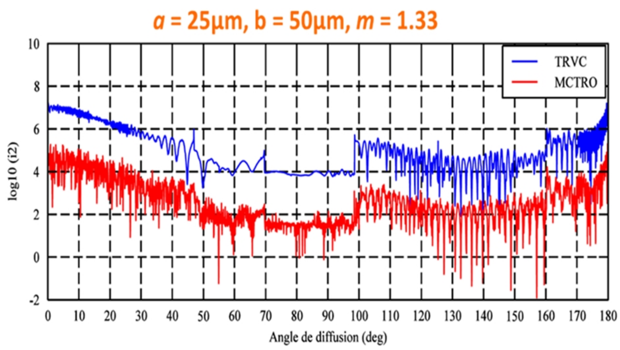

Figure 3 *Comparisons of the scattering patterns of a spheroidal droplet of transversal radius b=25 µm, symmetric radius a=50 µm and of refractive index m=1.33 illuminated by a polarized plane wave of wavelength λ = 0.6328 µm calculated by VCRM and MCRTW. The result of MCRTW is shifted by* 10^2 *for clarity.*

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