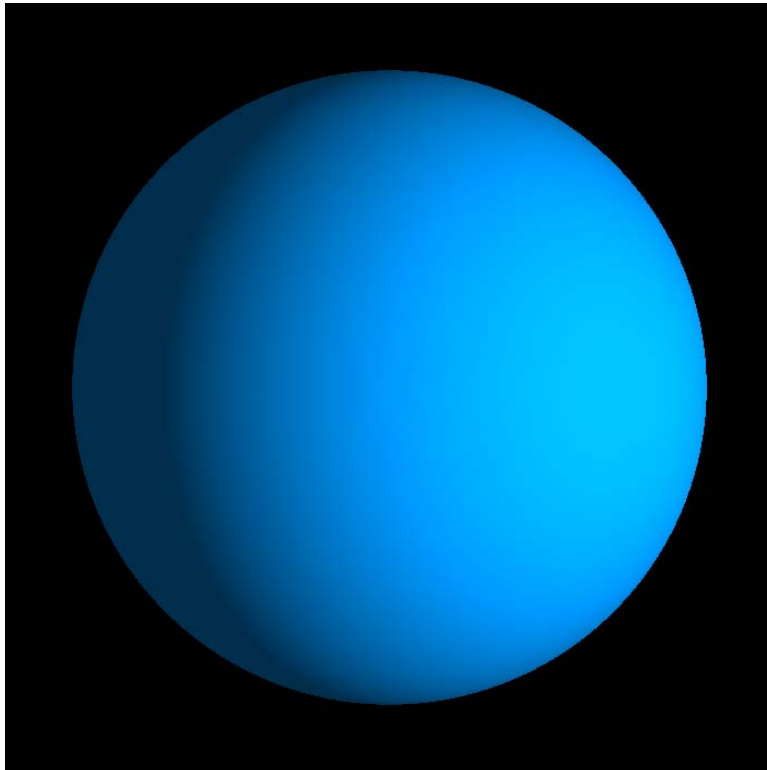


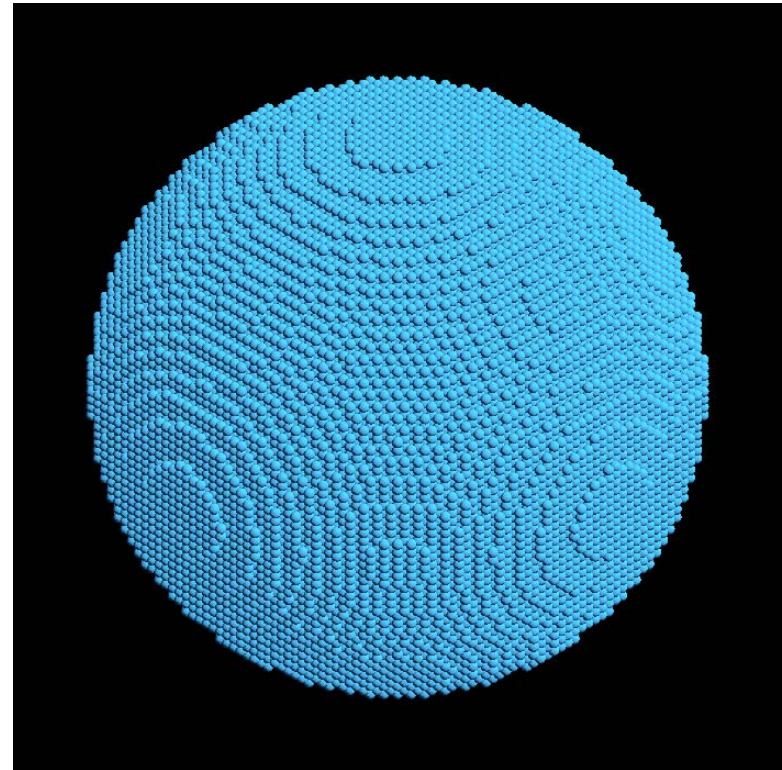
Interaction of light with cometary dust particles (2)

The main idea of DDA is to replace a target particle with a set of small volumes which reproduce its shape and internal structure.

initial perfect sphere



137,376 small volumes



Q1: What does this replacement give us?

A1: The light scattering by small particles has been studied very well and it has quite simple analytical expression.

Therefore, instead of problem of light scattering by a solid particle with complex shape and internal structure, we consider the scattering by array of coupled dipoles.

Within this approach, electric field induced on each dipole is result of a superposition of the incident field and fields induced by all other dipoles:

$$\mathbf{E}_i = \mathbf{E}_i^{\text{inc}} + \sum_{j \neq i}^N \mathbf{N}_{ji} \mathbf{E}_j$$

here α_i – polarizability of i -th dipole; \mathbf{E}_i – the total field induced on i -th dipole; $\mathbf{E}_i^{\text{inc}}$ – field of the incident wave at i -th dipole; \mathbf{N}_{ij} – operator describing scattering from j -th to i -th dipoles.

Q2: What does “small volume” mean?

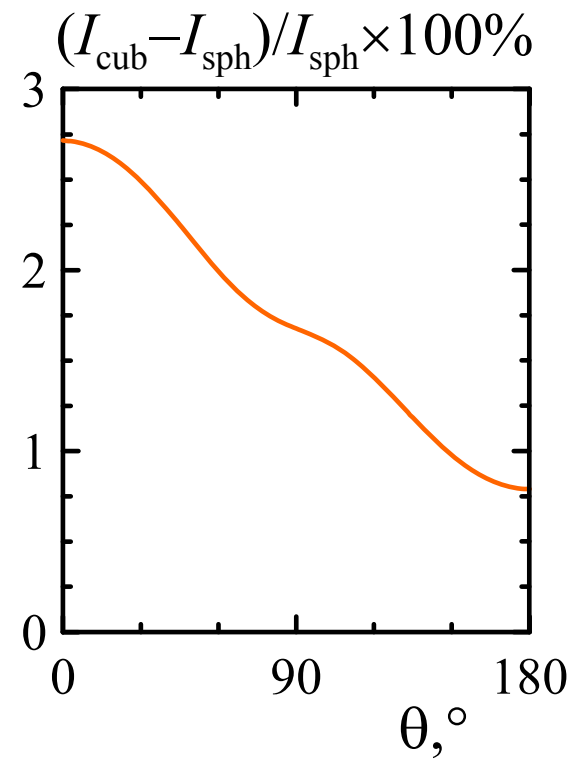
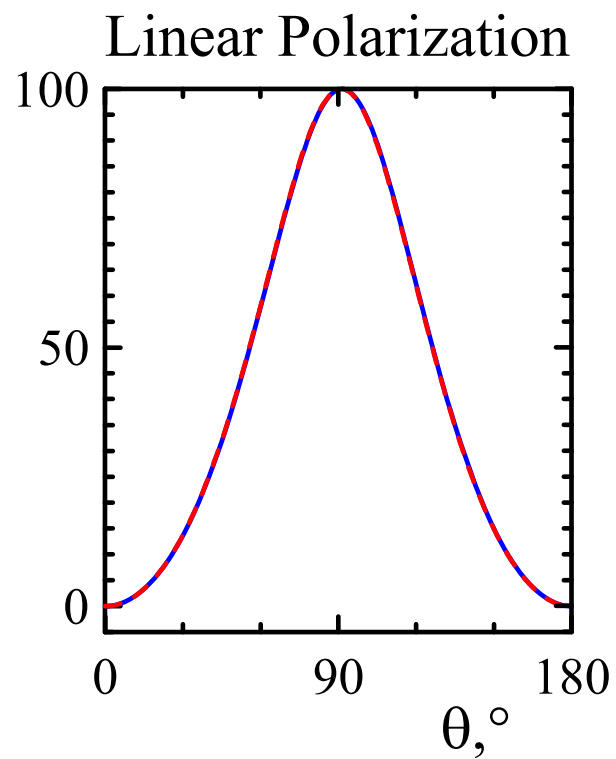
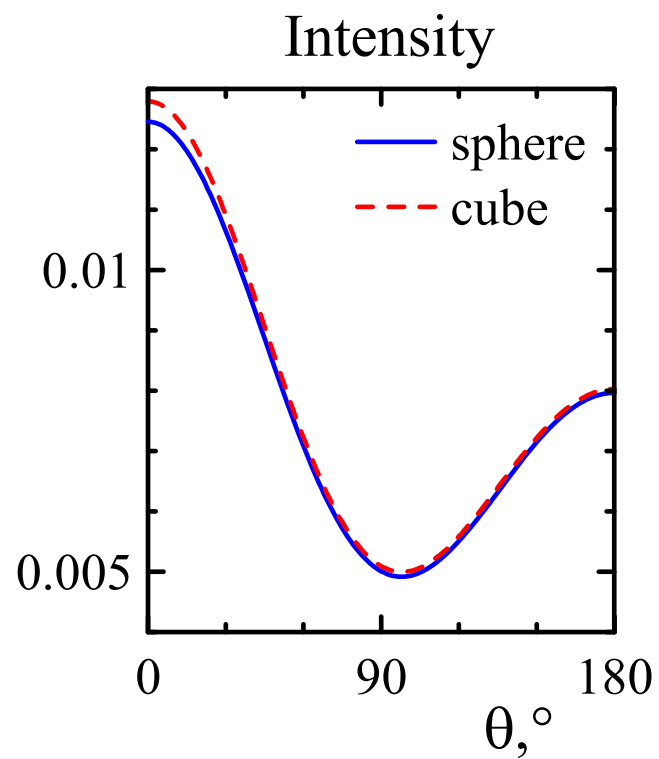
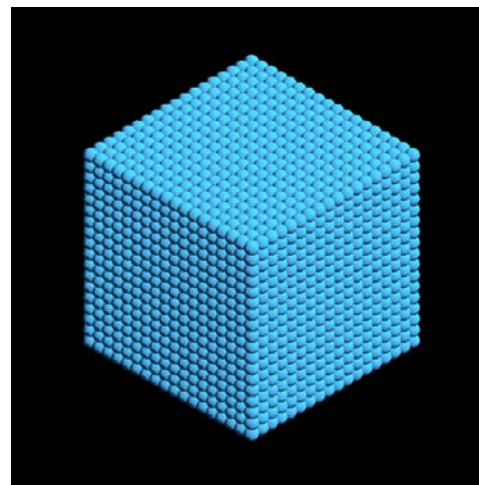
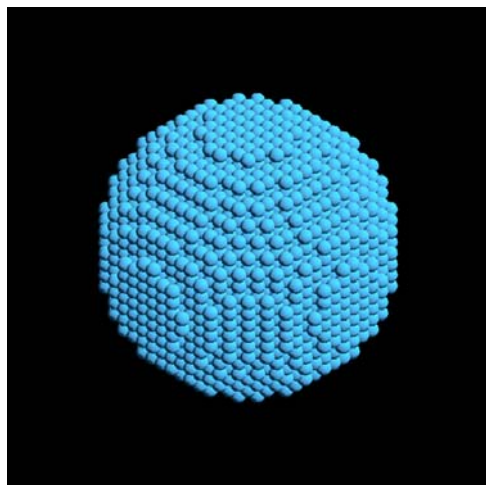
A2: In light scattering, all sizes are being measured in comparison with wavelength of radiation. Thus, “small volume” mean that size of volume is significantly smaller than wavelength. In terms of size parameter x , this condition is $x < 1$.

Q3: What is the shape of small volume?

A3: Any kind of shape. There is only one restriction – the small volume should be a rather compact and has approximately the same size in all directions (i.e., being equidimensional).

We will prove this statement. In order to do that, we compare light-scattering properties of small spherical and cubical grains.

We assume that grains consist of the same volume of a material (in case of sphere $x=0.7$) with refractive index $m=1.5+0.01i$.



We have to find out the operator \mathbf{N}_{ji} describing the dipole-dipole interaction. We will do that from Mie theory.

Full electric field scattered by a single sphere is defined as follows (Lecture 5, page 43):

$$E_r^{\text{sc}} = \frac{\cos \phi}{(kr)^2} E_0 \sum_{n=1}^{\infty} i^{(n+1)} (2n+1) a_n \xi_n(kr) P_n^1(\cos \theta)$$

$$E_{\theta}^{\text{sc}} = \frac{\cos \phi}{kr} E_0 \sum_{n=1}^{\infty} i^{(n+1)} \frac{2n+1}{n(n+1)} \left(a_n \frac{d\xi_n(kr)}{d(kr)} \frac{dP_n^1(\cos \theta)}{d\theta} + ib_n \xi_n(kr) \frac{P_n^1(\cos \theta)}{\sin \theta} \right)$$

$$E_{\phi}^{\text{sc}} = -\frac{\sin \phi}{kr} E_0 \sum_{n=1}^{\infty} i^{(n+1)} \frac{2n+1}{n(n+1)} \left(a_n \frac{d\xi_n(kr)}{d(kr)} \frac{P_n^1(\cos \theta)}{\sin \theta} + ib_n \xi_n(kr) \frac{dP_n^1(\cos \theta)}{d\theta} \right)$$

r , θ and ϕ – spherical polar coordinates; k – wavenumber;

$P_n^1(\cos \theta)$ – the associated Legendre functions;

$\xi_n(kr) = (kr) \cdot h_n^{(1)}(kr)$, here $h_l^{(1)}(kr)$ – spherical Hankel function;

a_n and b_n – coefficients of scattering.

Coefficients a_n and b_n are being decreased while the index n increases; it happens faster for smaller x . At $x < 1$, only a_1 is enough to describe light-scattering properties.

$$E_r^{\text{sc}} = -\frac{\cos \phi}{(kr)^2} E_0 3a_1 \xi_1(kr) P_1^1(\cos \theta)$$

$$E_\theta^{\text{sc}} = -\frac{\cos \phi}{kr} E_0 \frac{3}{2} a_1 \frac{d\xi_1(kr)}{d(kr)} \frac{dP_1^1(\cos \theta)}{d\theta}$$

$$E_\phi^{\text{sc}} = \frac{\sin \phi}{kr} E_0 \frac{3}{2} a_1 \frac{d\xi_1(kr)}{d(kr)} \frac{P_1^1(\cos \theta)}{\sin \theta}$$

Here

$$P_1^1(\cos \theta) = \sin \theta \quad \xi_1(kr) = -\exp(ikr) - \frac{i}{kr} \exp(ikr)$$

$$\frac{dP_1^1(\cos \theta)}{d\theta} = \cos \theta \quad \frac{d\xi_1(kr)}{d(kr)} = -i \exp(ikr) + \frac{\exp(ikr)}{kr} + \frac{i}{(kr)^2} \exp(ikr)$$

One can simplify the expressions for component of the scattered field as follows:

$$E_r^{sc} = \frac{\exp(ikr)}{kr} E_0 \frac{3}{2} a_1 2 \cos \phi \sin \theta \left(\frac{1}{kr} + \frac{i}{(kr)^2} \right)$$

$$E_\theta^{sc} = \frac{\exp(ikr)}{kr} E_0 \frac{3}{2} a_1 \cos \phi \cos \theta \left(i - \frac{1}{kr} - \frac{i}{(kr)^2} \right)$$

$$E_\phi^{sc} = -\frac{\exp(ikr)}{kr} E_0 \frac{3}{2} a_1 \sin \phi \left(i - \frac{1}{kr} - \frac{i}{(kr)^2} \right)$$

Or

$$\mathbf{E}^{sc} = \begin{pmatrix} E_r^{sc} \\ E_\theta^{sc} \\ E_\phi^{sc} \end{pmatrix} = \frac{\exp(ikr)}{kr} E_0 \frac{3}{2} a_1 \left[2 \left(\frac{1}{kr} + \frac{i}{(kr)^2} \right) \begin{pmatrix} \cos \phi \sin \theta \\ 0 \\ 0 \end{pmatrix} + \left(i - \frac{1}{kr} - \frac{i}{(kr)^2} \right) \begin{pmatrix} 0 \\ \cos \phi \cos \theta \\ -\sin \phi \end{pmatrix} \right]$$

The scattered field is expressed in spherical polar coordinates which are not convenient on practice. We have to transform these formulae to Cartesian system of coordinates as follows:

$$\begin{pmatrix} E_x^{sc} \\ E_y^{sc} \\ E_z^{sc} \end{pmatrix} = \begin{pmatrix} \sin \theta \cos \phi & \cos \theta \cos \phi & -\sin \phi \\ \sin \theta \sin \phi & \cos \theta \sin \phi & \cos \phi \\ \cos \theta & -\sin \theta & 0 \end{pmatrix} \cdot \begin{pmatrix} E_r^{sc} \\ E_\theta^{sc} \\ E_\phi^{sc} \end{pmatrix}$$

Result is:

$$\mathbf{E}^{sc} = \begin{pmatrix} E_r^{sc} \\ E_\theta^{sc} \\ E_\phi^{sc} \end{pmatrix} = \frac{\exp(ikr)}{kr} E_0 \frac{3}{2} a_1 \left(2 \left(\frac{1}{kr} + \frac{i}{(kr)^2} \right) \begin{pmatrix} (\sin \theta)^2 (\cos \phi)^2 \\ (\sin \theta)^2 \cos \phi \sin \phi \\ \sin \theta \cos \theta \cos \phi \end{pmatrix} - \left(i - \frac{1}{kr} - \frac{i}{(kr)^2} \right) \begin{pmatrix} -(\cos \theta)^2 (\cos \phi)^2 - (\sin \phi)^2 \\ (\sin \theta)^2 \cos \phi \sin \phi \\ \sin \theta \cos \theta \cos \phi \end{pmatrix} \right)$$

To interpret this result we use two unit vectors:

$$\mathbf{E}_0^{\text{inc}} = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \quad \text{and} \quad \mathbf{r}_0 = \begin{pmatrix} \cos \phi \sin \theta \\ \sin \phi \sin \theta \\ \cos \theta \end{pmatrix}; \quad \text{where, } \mathbf{E}^{\text{inc}} = E_0 \cdot \mathbf{E}_0^{\text{inc}}, \quad \mathbf{r} = r \cdot \mathbf{r}_0$$

It is easy to show that:

$$[\mathbf{r}_0 \times [\mathbf{r}_0 \times \mathbf{E}_0^{\text{inc}}]] = \begin{pmatrix} -(\cos \theta)^2 - (\sin \theta)^2 (\sin \phi)^2 \\ (\sin \theta)^2 \cos \phi \sin \phi \\ \sin \theta \cos \theta \cos \phi \end{pmatrix} \equiv \begin{pmatrix} -(\cos \theta)^2 (\cos \phi)^2 - (\sin \phi)^2 \\ (\sin \theta)^2 \cos \phi \sin \phi \\ \sin \theta \cos \theta \cos \phi \end{pmatrix}$$

and

$$(\mathbf{r}_0 \cdot \mathbf{E}_0^{\text{inc}}) \mathbf{r}_0 = \begin{pmatrix} (\sin \theta)^2 (\cos \phi)^2 \\ (\sin \theta)^2 \cos \phi \sin \phi \\ \sin \theta \cos \theta \cos \phi \end{pmatrix}$$

The simplified expression for the scattered electric field is:

$$\mathbf{E}^{\text{sc}} = \frac{\exp(ikr)}{kr} \frac{3}{2} a_1 \left(2 \left(\frac{1}{kr} + \frac{i}{(kr)^2} \right) (\mathbf{r}_0 \cdot \mathbf{E}^{\text{inc}}) \mathbf{r}_0 + \left(\frac{1}{kr} + \frac{i}{(kr)^2} - i \right) [\mathbf{r}_0 \times [\mathbf{r}_0 \times \mathbf{E}^{\text{inc}}]] \right)$$

One can introduce a polarizability α as follows: $\alpha = \frac{3}{2} \frac{i}{k^3} a_1$

Taking into account the expression for polarizability α , one can obtain:

$$\mathbf{E}^{\text{sc}} = \frac{\exp(ikr)}{r} \alpha \left(2 \frac{1-ikr}{r^2} (\mathbf{r}_0 \cdot \mathbf{E}^{\text{inc}}) \mathbf{r}_0 + \left(\frac{1-ikr}{r^2} - k^2 \right) [\mathbf{r}_0 \times [\mathbf{r}_0 \times \mathbf{E}^{\text{inc}}]] \right)$$

Finally, the electric field scattered by an electric dipole can be expressed as follows:

$$\mathbf{E}^{\text{sc}} = -\frac{\exp(ikr)}{r^3} \alpha \left(k^2 [\mathbf{r} \times [\mathbf{r} \times \mathbf{E}^{\text{inc}}]] - \frac{1-ikr}{r^2} \left(3(\mathbf{r} \cdot \mathbf{E}^{\text{inc}}) \mathbf{r} - r^2 \mathbf{E}^{\text{inc}} \right) \right)$$

Now, one can express the system of linear equations describing light scattering by array of dipoles:

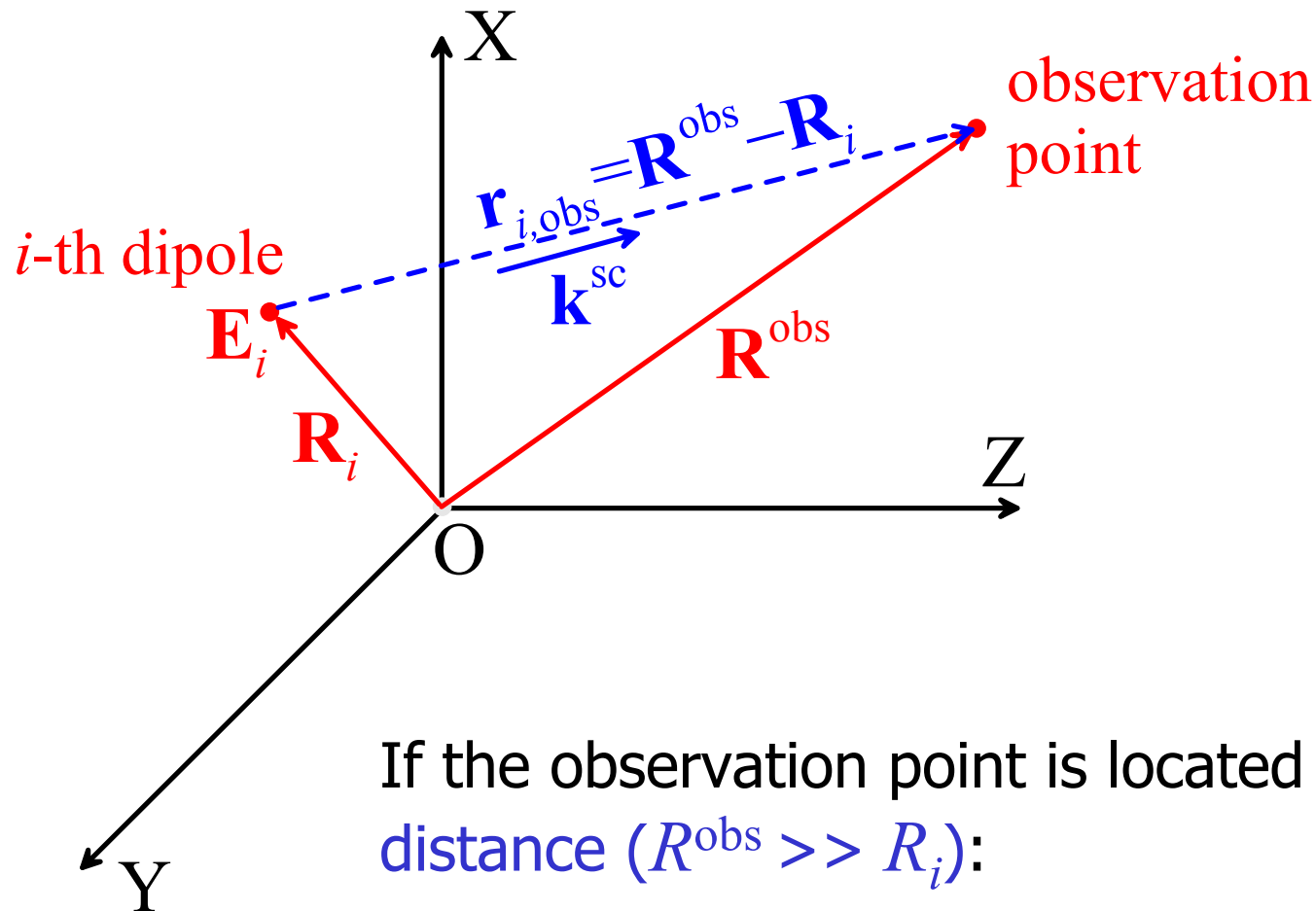
$$\mathbf{E}_i = \mathbf{E}_i^{\text{inc}} + \sum_{j \neq i}^N \mathbf{N}_{ji} \mathbf{E}_j = \mathbf{E}_i^{\text{inc}} - \sum_{j \neq i}^N \frac{\exp(ikr_{ji})}{r_{ji}^3} \alpha_j \left[\mathbf{k}^2 [\mathbf{r}_{ji} \times [\mathbf{r}_{ji} \times \mathbf{E}_j]] - \frac{1 - ikr_{ji}}{r_{ji}^2} \left(3(\mathbf{r}_{ji} \cdot \mathbf{E}_j) \mathbf{r}_{ji} - r_{ji}^2 \mathbf{E}_j \right) \right]$$

Solution of this system gives a set of electric fields induced on each dipole in the array.

Then, using the induced fields, one can compute amplitude of the scattered field \mathbf{E}^{sc} in far zone:

$$\mathbf{E}^{\text{sc}} = \sum_{i=0}^N \mathbf{F}_{i,\text{obs}} \mathbf{E}_i = -\mathbf{k}^2 \sum_{i=0}^N \frac{\exp(ikr_{i,\text{obs}})}{r_{i,\text{obs}}^3} \alpha_i [\mathbf{r}_{i,\text{obs}} \times [\mathbf{r}_{i,\text{obs}} \times \mathbf{E}_i]]$$

Formula for the scattered field can be further simplified:



If the observation point is located at very large distance ($R^{\text{obs}} \gg R_i$):

$$r_{i,\text{obs}} \approx R^{\text{obs}} \quad k r_{i,\text{obs}} = (\mathbf{k}^{\text{sc}} \cdot \mathbf{r}_{i,\text{obs}}) = (\mathbf{k}^{\text{sc}} \cdot (\mathbf{R}^{\text{obs}} - \mathbf{R}_i))$$

$$\exp(i k r_{i,\text{obs}}) = \exp(i(\mathbf{k}^{\text{sc}} \cdot \mathbf{R}^{\text{obs}})) \times \exp(-i(\mathbf{k}^{\text{sc}} \cdot \mathbf{R}_i))$$

Taking into account the aforesaid, **one can simplify the expression for the scattered field** in far zone as follows:

$$\mathbf{E}^{\text{sc}} = -\frac{\exp(i(\mathbf{k}^{\text{sc}} \cdot \mathbf{R}^{\text{obs}}))}{R^{\text{obs}}} \sum_{i=0}^N \exp(-i(\mathbf{k}^{\text{sc}} \cdot \mathbf{R}_i)) [\mathbf{k}^{\text{sc}} \times [\mathbf{k}^{\text{sc}} \times (\alpha_i \mathbf{E}_i)]]$$

That's all about formulation of DDA!

Computing light scattering for two incident waves with mutually perpendicular polarizations, one can derive the amplitude matrix and, then, Mueller matrix.

In what follows, we will discuss a few tricks significantly accelerating and improving accuracy of DDA computations

1. Acceleration of computations with fast Fourier transform (FFT)

Computation of light scattering with DDA means a finding of solution of the system of linear algebraic equations. It is being done with some iterative scheme.

In each iteration, at least, one matrix-vector product has to be computed, which takes of about N^2 operations (N – number of unknowns).

However, DDA can be reformulated into the form that the matrix-vector product will be a convolution. Computation of this convolution can be substantially accelerated with FFT: only $N \log N$ operations instead of N^2 .

In order to apply FFT, we have suppose that all the dipoles are located in regular cubic lattice. Then, one can reformulate the system of equations as follows:

$$\mathbf{E}_i = \mathbf{E}_i^{\text{inc}} + \sum_{j \neq i}^N \mathbf{N}_{ji} \mathbf{E}_j \quad \longrightarrow \quad \mathbf{E}_{i,j,l} = \mathbf{E}_{i,j,l}^{\text{inc}} + \sum_{m=0}^N \sum_{n=0}^N \sum_{o=0}^N \mathbf{N}_{i,j,l;m,n,o}^{3D} \mathbf{E}_{m,n,o}$$

Operator \mathbf{N}^{3D} depends on three integer numbers: $(m - i)$, $(n - j)$, and $(o - l)$. Therefore, matrix-vector product takes form of a convolution.

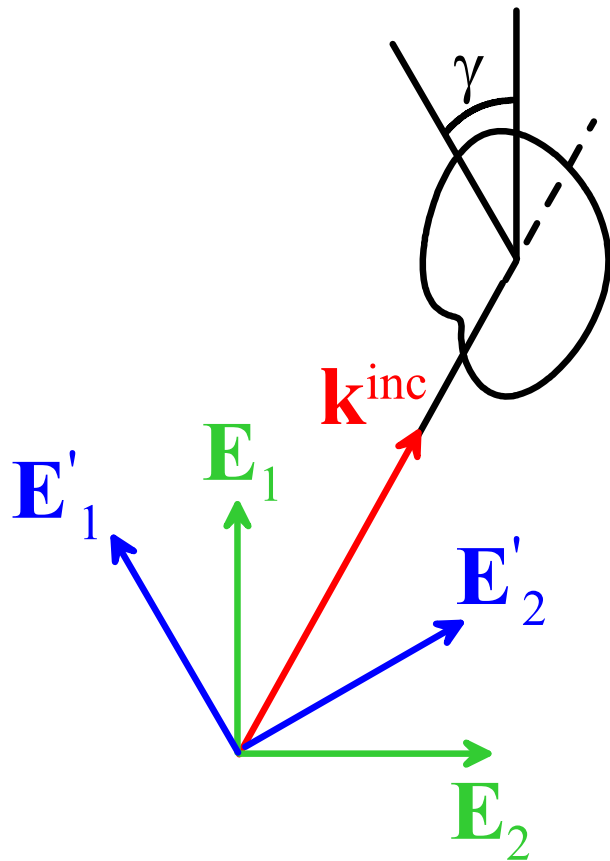
Fourier transform is being computed separately for operator \mathbf{N}^{3D} and vector \mathbf{E} . Then, corresponding elements of these two Fourier transforms are multiplied to each other and, the result is being reconstructed with Fourier inversion.

Though the DDA is dramatically speeded up with FFT, **there are also some penalties:**

- (1) cells have to be located in regular cubic lattice;
- (2) all the sites in the grid have to be treated (even those are empty).

2. Azimuthal averaging

In many applications to cosmic dust, light-scattering properties have to be averaged over orientations of sample particles. At that azimuthal averaging can be done without additional computations of the induced fields.



If we have already two solutions corresponding to incident waves with polarizations \mathbf{E}_1 and \mathbf{E}_2 . Using the fundamental feature (linearity) of a solution of Maxwell equations, we can construct solutions corresponding to incident fields with polarizations \mathbf{E}'_1 and \mathbf{E}'_2 .

3. Polarizability

So far, we were assuming that the polarizability of dipoles is derived directly from a_1 scattering coefficient in Mie theory.

Taking into account small size of sphere, one can also simplify expression for coefficient a_1 . It leads us to an extremely simple formula which is also referred to Clausius-Mossotti formula:

$$\alpha = \frac{3d}{4\pi} \frac{m^2 - 1}{m^2 + 2}, \text{ where } d = \sqrt[3]{\frac{V}{N}}$$

V is volume of the target, N – number of cells, m – refractive index.

It is obvious that the practical use of Clausius-Mossotti formula is limited by condition: $kd \rightarrow 0$. **However, it is not only option!**

At present, the most frequently used and famous relation is, so-called, the Lattice Dispersion Relation (LDR):

$$\alpha = \frac{\alpha^{CM}}{1 + (\alpha^{CM}/d^3)[b_1 + m^2 b_2 + m^2 b_3 S](kd)^2}$$

$$S = (k_x^{inc} E_x^{inc})^2 + (k_y^{inc} E_y^{inc})^2 + (k_z^{inc} E_z^{inc})^2$$

$b_1 = -1.8915316$, $b_2 = 0.1648469$, $b_3 = -1.7700004$,
 α^{CM} – polarizability given by Clausius-Mossotti formula.

As was experimentally found, the LDR provides reasonably good accuracy at $kd|m| \leq 1$.

Draine & Goodman, ApJ, **405**, 685 (1993).

Validity criterion for DDA

In general, the restriction on dipole size is as follows:

$$kd|m| \leq A.$$

At present, it is widely accepted that when

A = 1: DDA provides quite reasonable accuracy in the cross-sections of absorption and scattering; whereas, the angular profile of the intensity may reveal fractional errors exceeding 30%.

A = 0.5: DDA provides accurate results for the angular profile of intensity.

Though it is not clearly stated, one can suppose that, for accurate computations of polarization, it is required **A < 0.5**.

Draine & Flatau, JOSAA, 11, 1491 (1994)

Draine & Flatau, User Guide for the DDA Code DDSCAT 6.1 (2004)

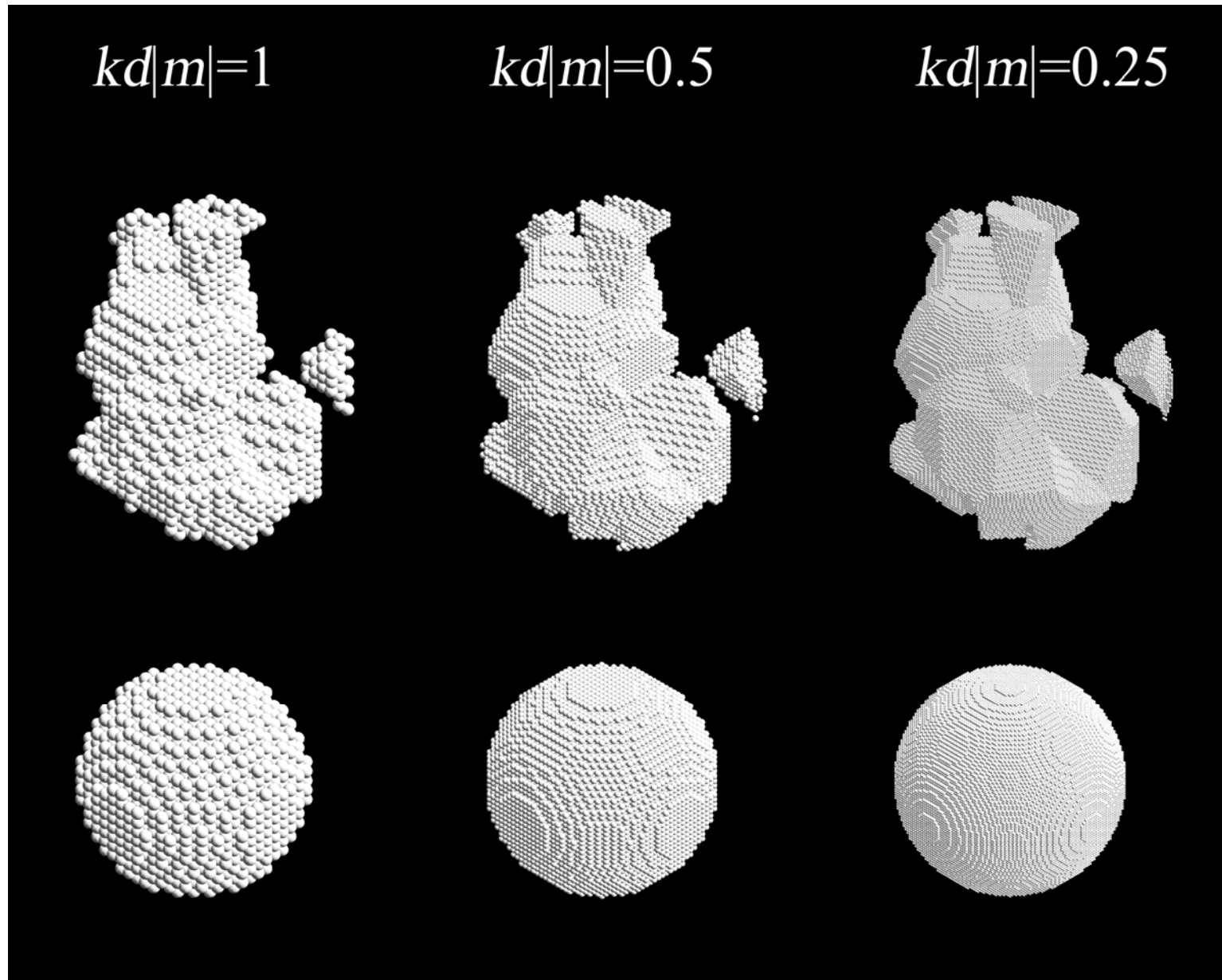
Generally, there are three sources of errors in DDA computation:

- (1) violation of Maxwell equations;
- (2) surface roughness caused by discrete presentation;
- (3) parasitic interference coming from regular grid.

If Maxwell equations are satisfied, there are only two types of errors caused by surface roughness and parasitic interference.

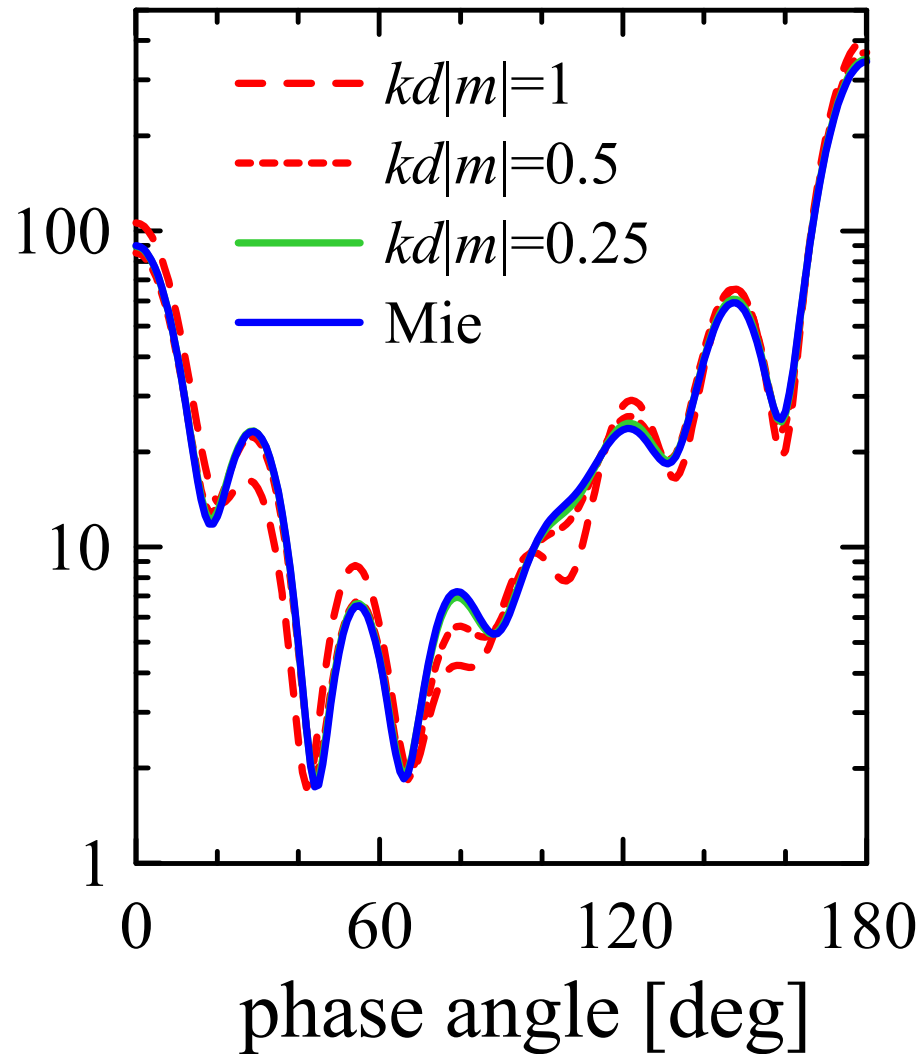
However, the averaging over particle orientations (and/or shapes) can efficiently reduce the impact of the parasitic interference. Thus, one can estimate the true impact of surface roughnesses on accuracy of DDA.

Sample particles at different degree of discretization

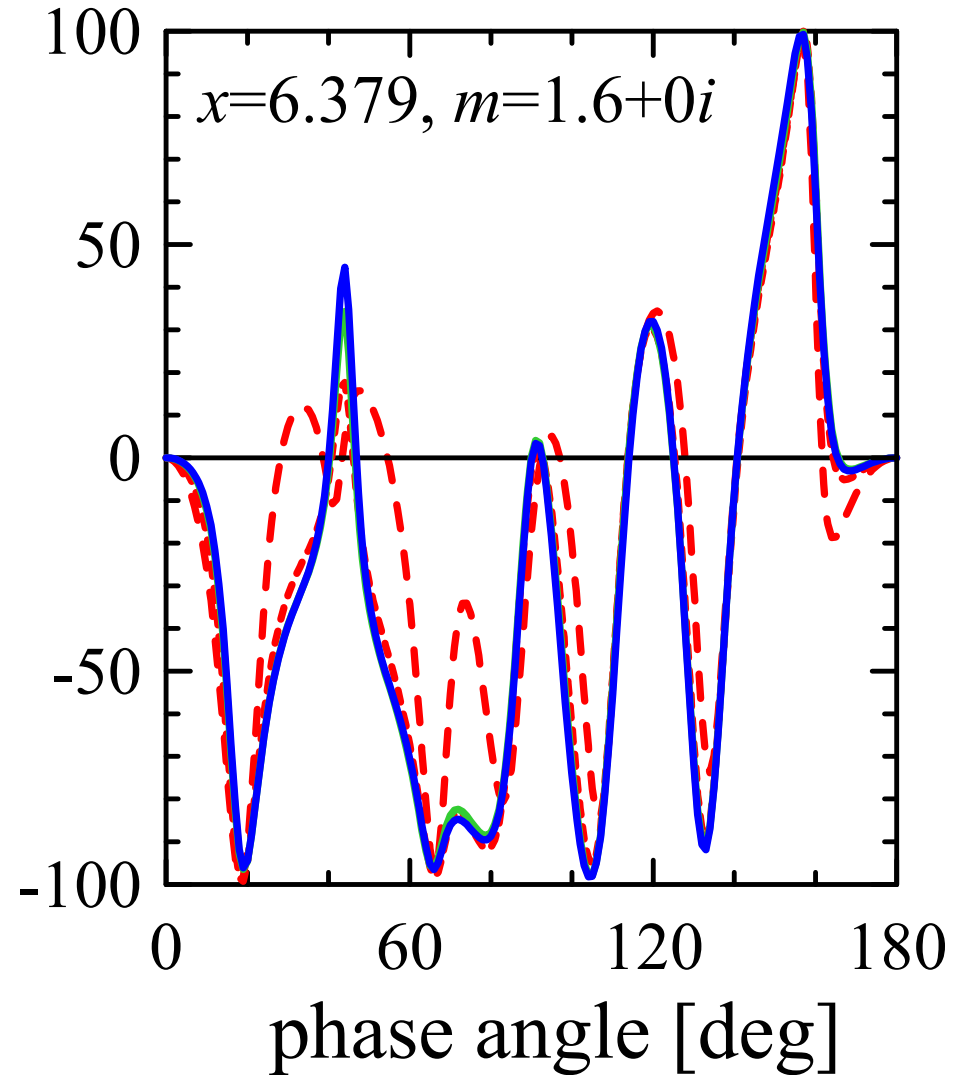


Single sphere at fixed orientation

Intensity

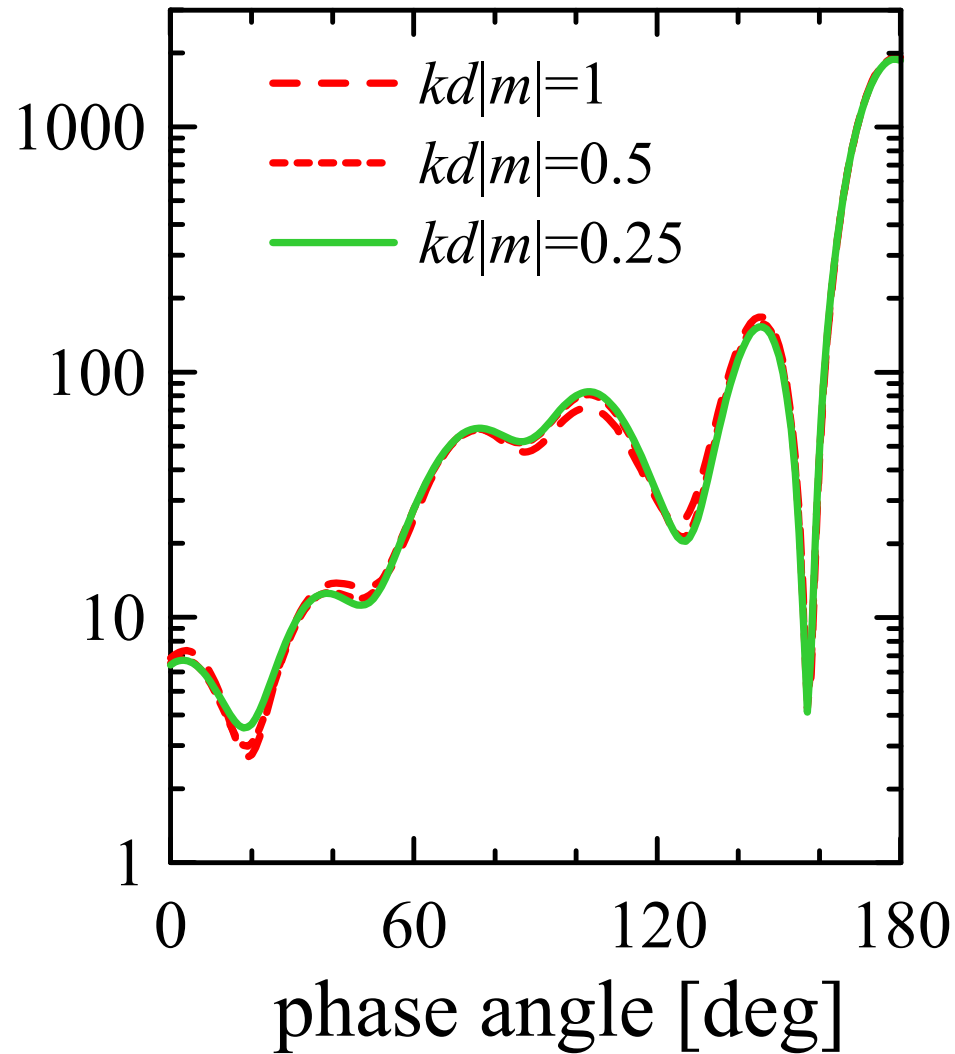


Linear Polarization

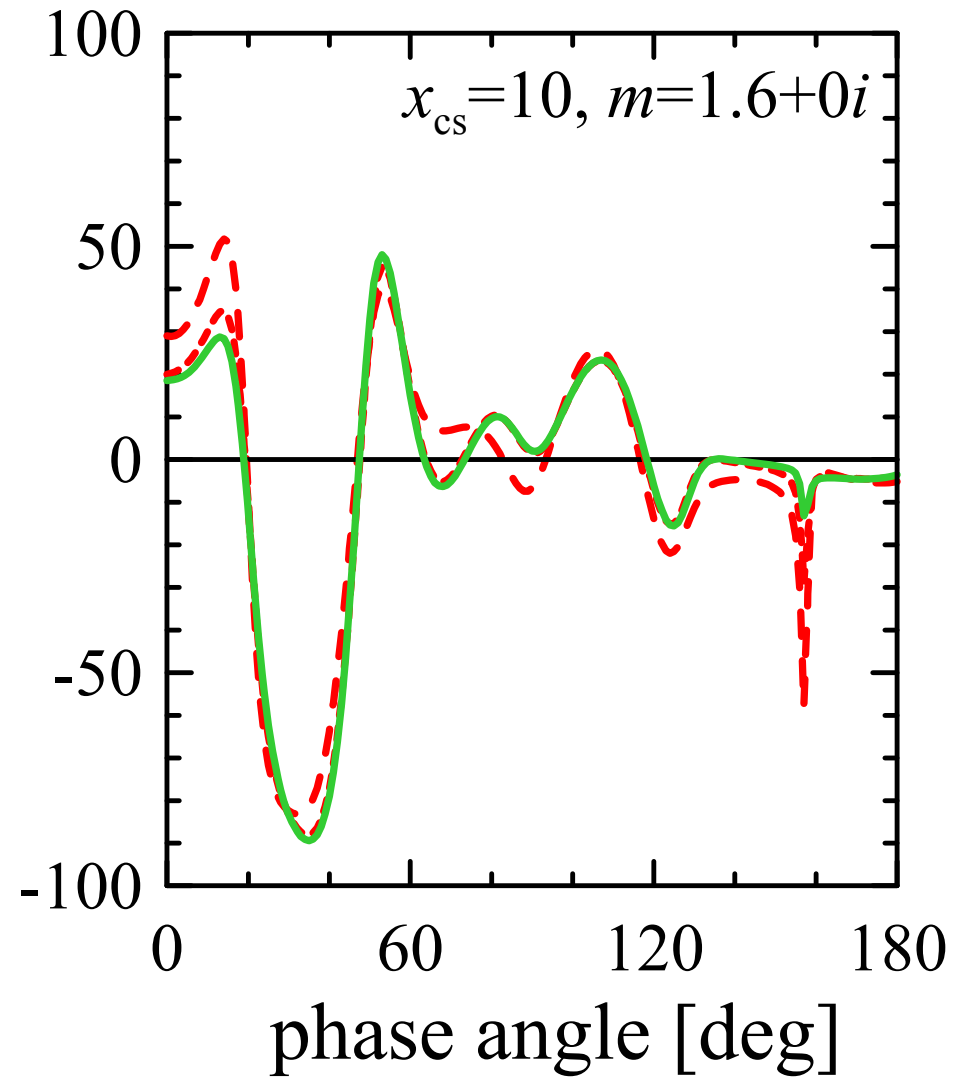


Irregular particle at fixed orientation

Intensity

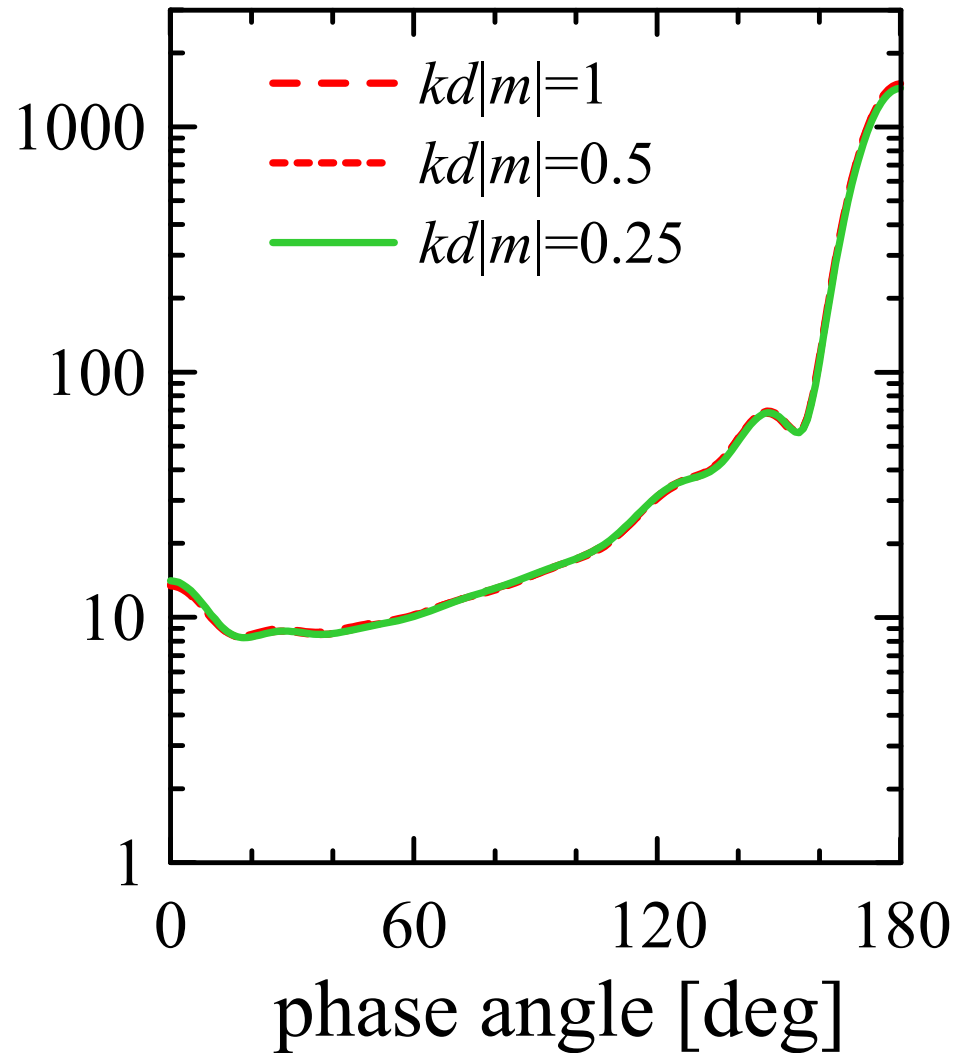


Linear Polarization

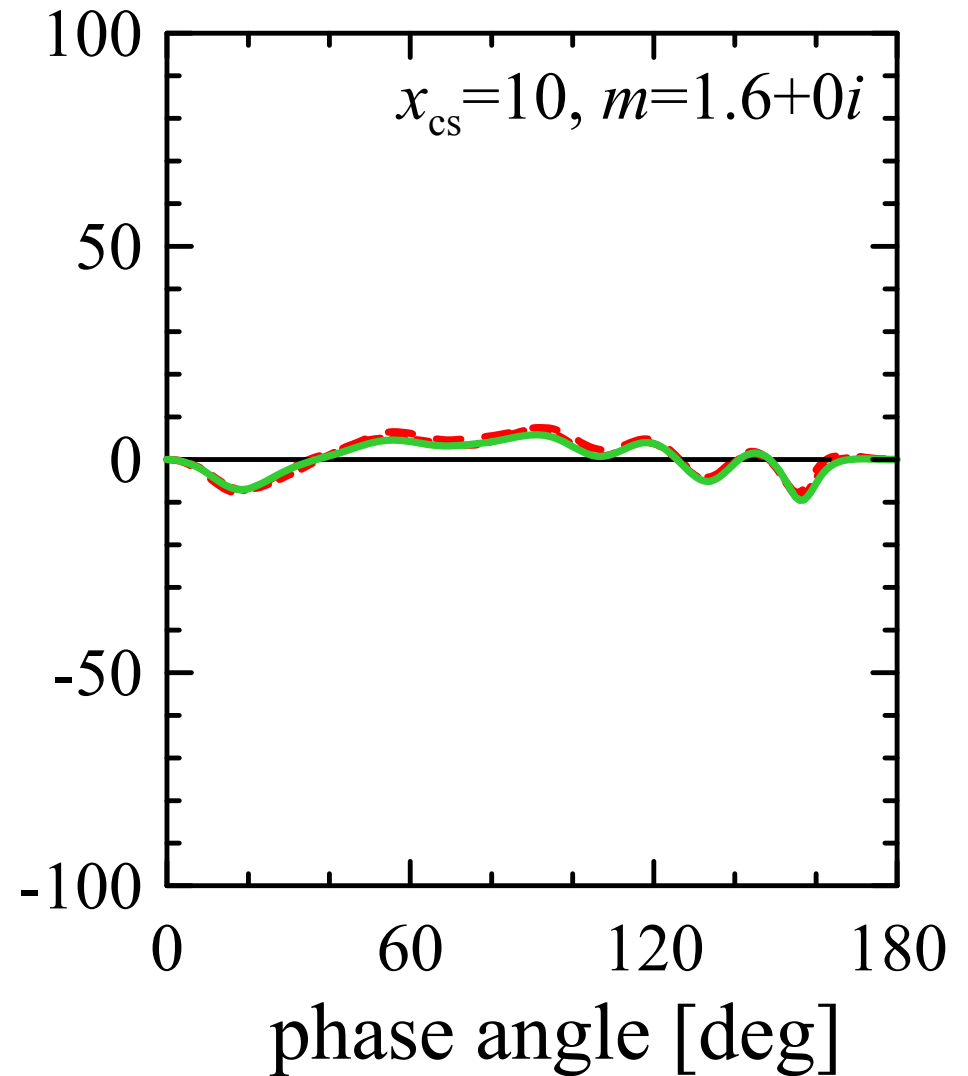


Irregular particle averaged over 600×100 orientations

Intensity



Linear Polarization



One can quantify the errors in intensity as follows:

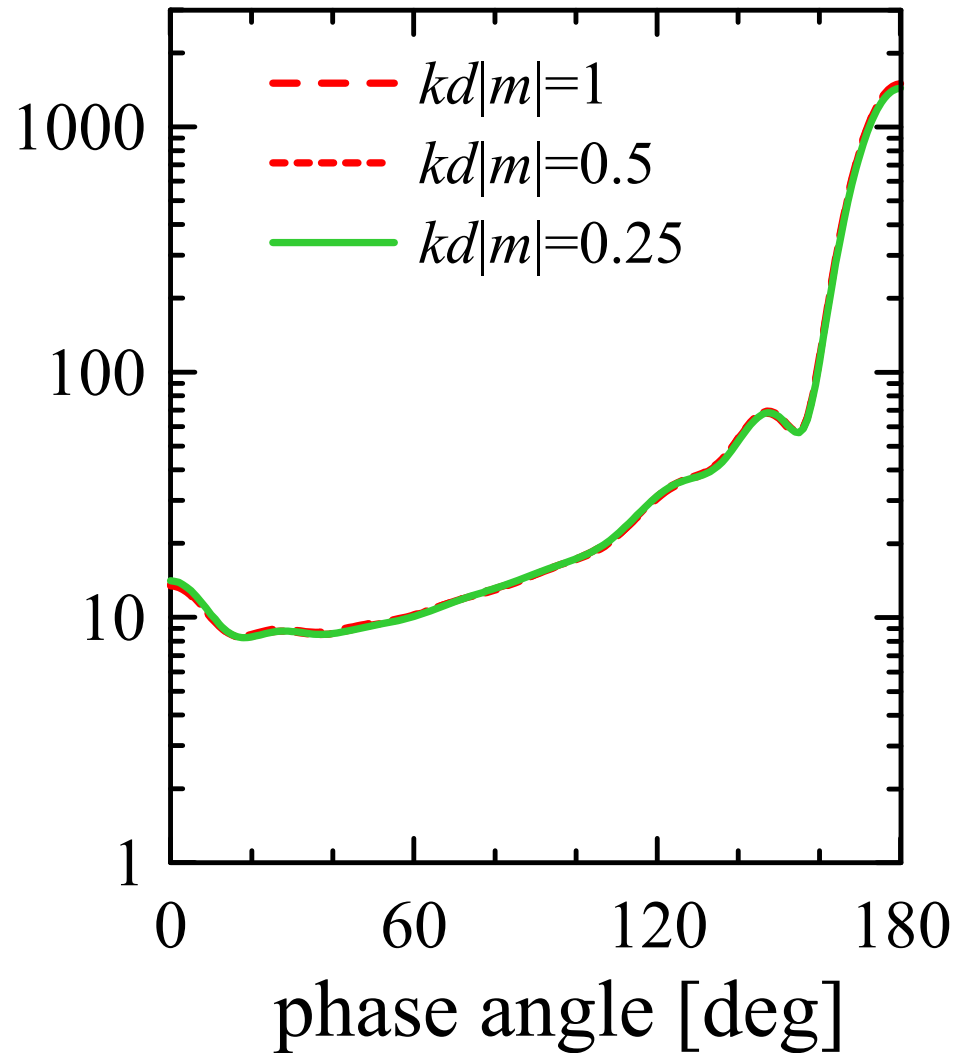
$$\text{Error} = \frac{|I_{\text{DDA}} - I_{\text{exact}}|}{I_{\text{exact}}} \cdot 100\%$$

In the case of sphere, I_{exact} obviously corresponds to result of Mie theory; whereas, in the case of irregular particle, I_{exact} can be associated with result obtained at the finest discretization.

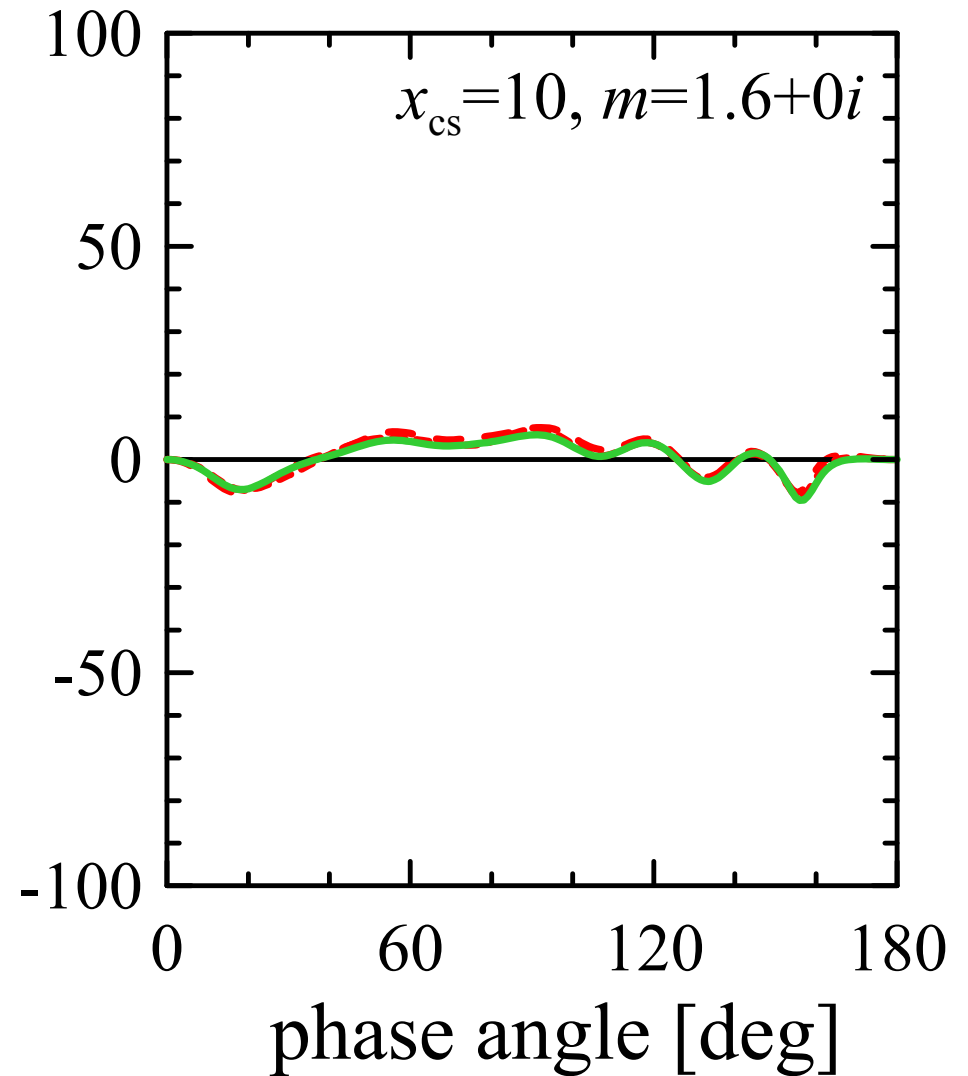
| | | $kd m $ | $\langle \text{Error} \rangle$ | max(Error) | $\sigma(\text{Error})$ |
|--------------------|-------|---------|--------------------------------|------------|------------------------|
| sphere | fixed | 1 | 23.74 | 73.00 | 15.06 |
| | | 0.5 | 7.50 | 23.36 | 5.21 |
| | | 0.25 | 1.99 | 4.90 | 1.27 |
| irregular particle | fixed | 1 | 5.04 | 30.42 | 6.13 |
| | | 0.5 | 1.75 | 16.57 | 2.70 |
| | aver | 1 | 2.05 | 6.20 | 1.55 |
| | | 0.5 | 1.43 | 3.65 | 1.16 |

Irregular particle averaged over 600×100 orientations

Intensity

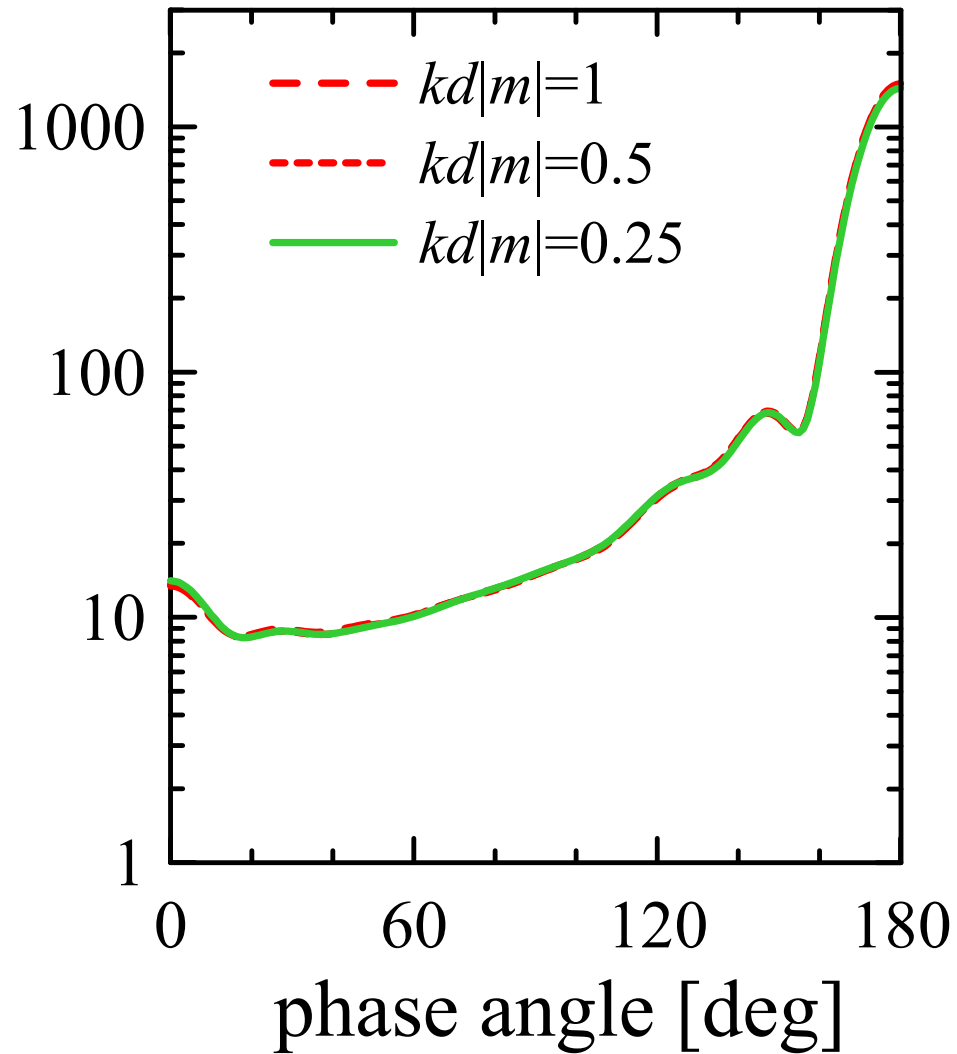


Linear Polarization

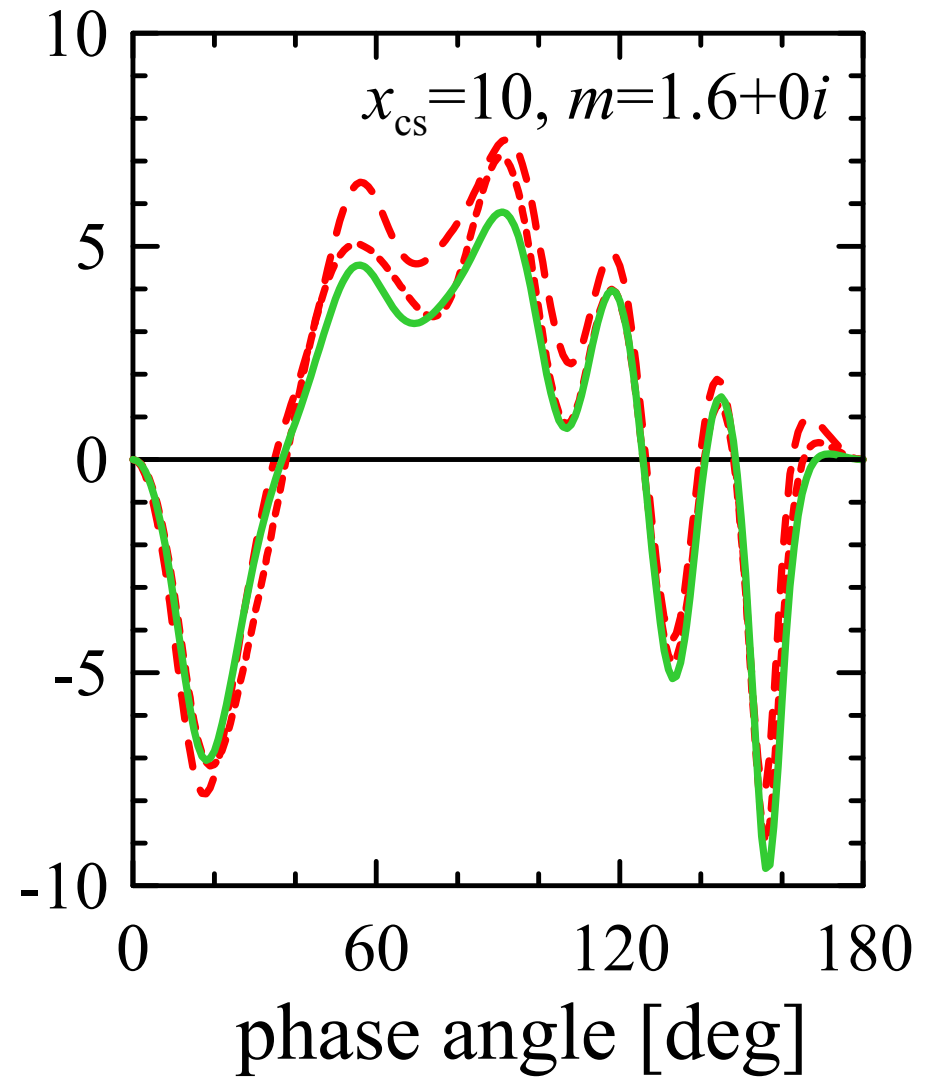


Irregular particle averaged over 600×100 orientations

Intensity

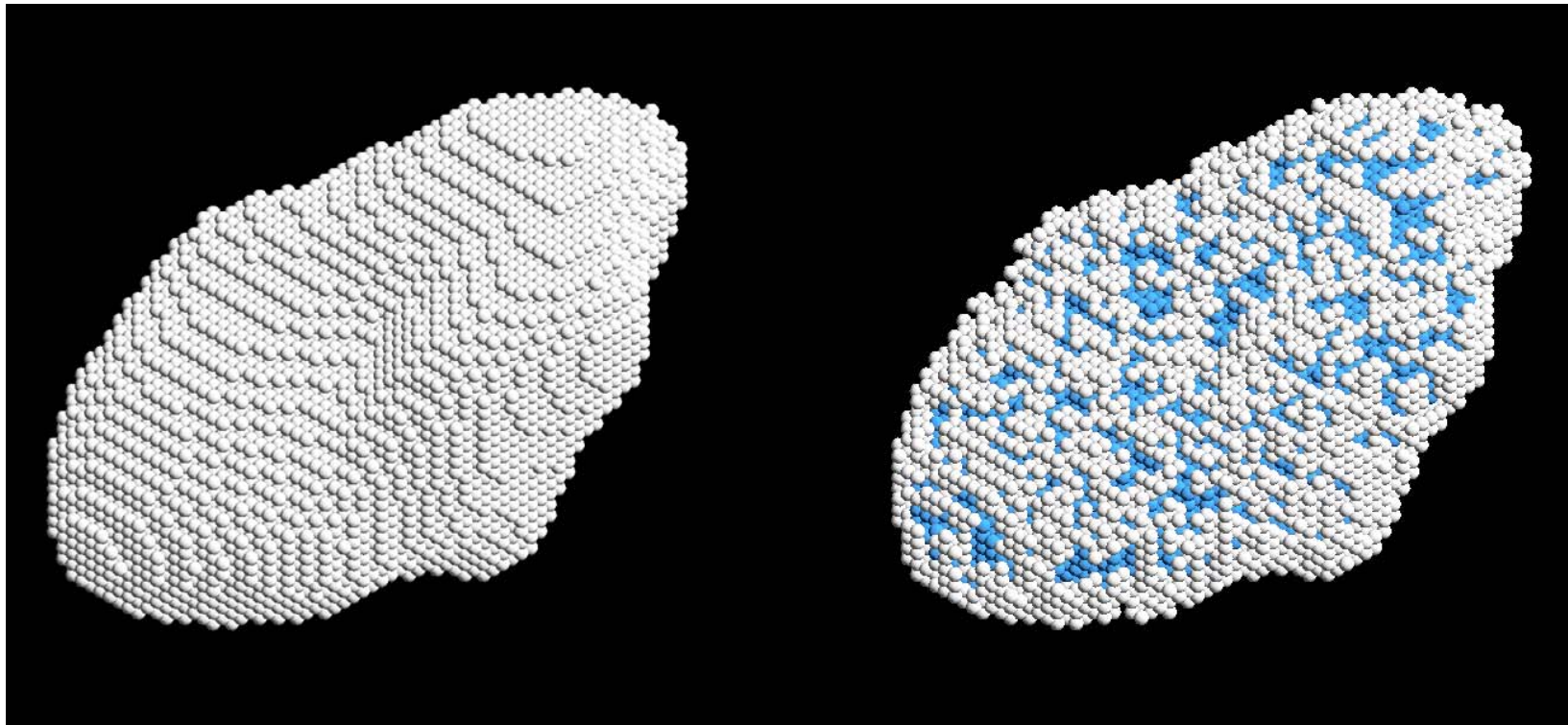


Linear Polarization

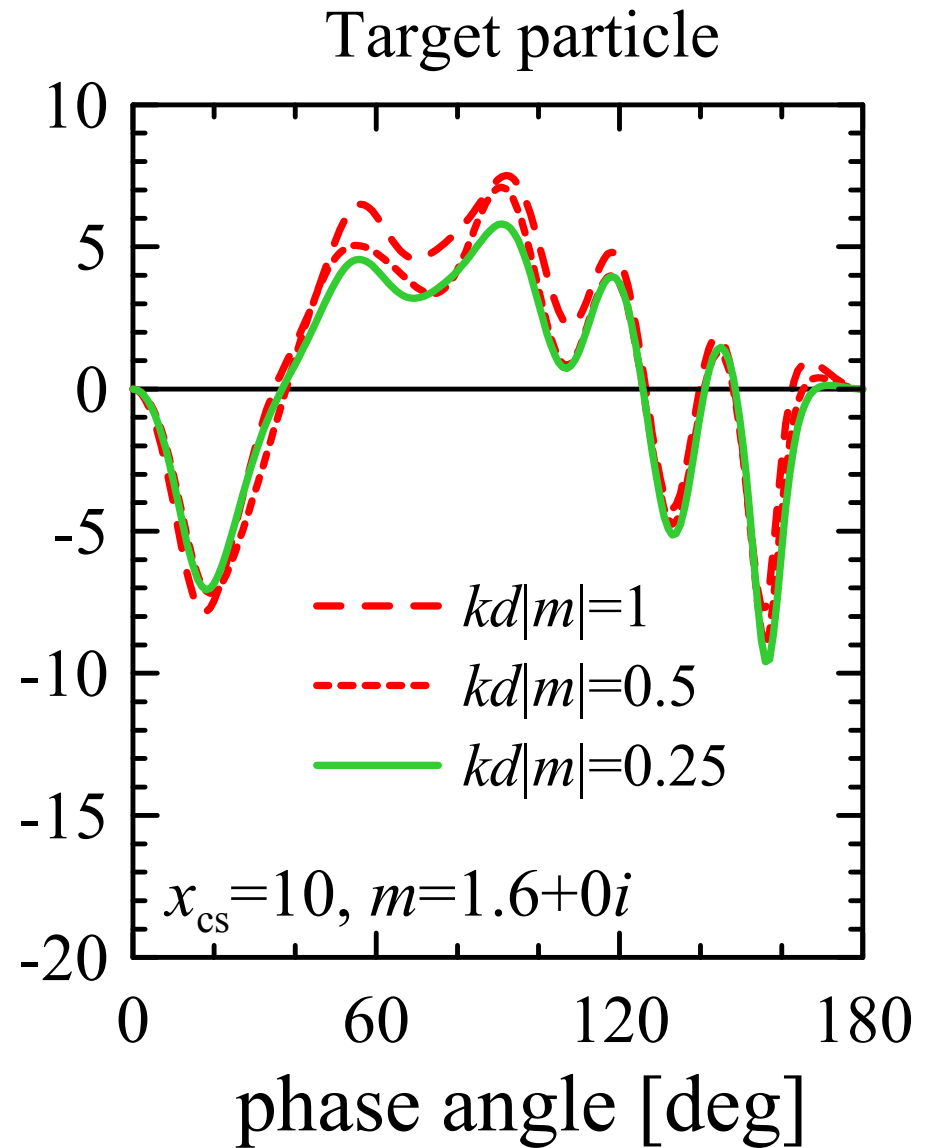
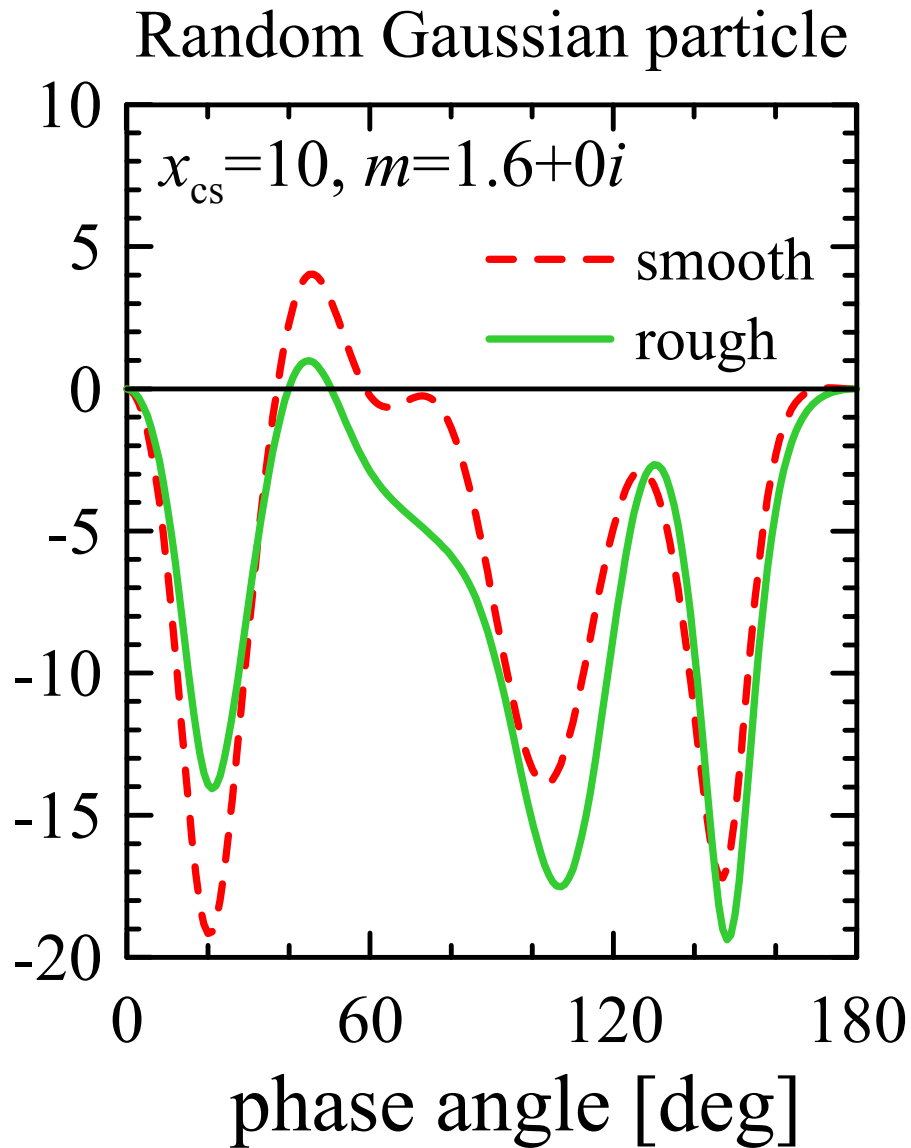


An important question: is the difference between the polarization profiles corresponding to coarse and fine representations of the target particle, really caused by surface roughness?

The answer on this question can be found from the study of impact of roughnesses on light scattering.



Comparison with impact of surface roughness on light scattering



Summary

When studying realistic irregularly-shaped particles which are averaged over orientations, DDA provides highly accurate result even under condition $kd|m| \leq 1$. While this parameter is approaching unit, the impact of surface roughness caused by discrete cells is getting visible in the angular profile of the degree of linear polarization. Nevertheless, in many practical applications, that roughness could be even desirable making a target more realistic.

References on DDA:

E. M. Purcell and C. R. Pennypacker, "Scattering and absorption of light by nonspherical dielectric grains," *Astrophys. J.* 186, 705–714 (1973).

B.T. Draine "The discrete-dipole approximation and its application to the interstellar graphite grains," *Astrophys. J.* 333, 848–872 (1988).

J.J. Goodman, B.T. Draine and P.J. Flatau, "Application of fast-Fourier-transform techniques to the discrete-dipole approximation," *Opt. Lett.* 16, 1198–1200 (1991).

B.T. Draine and J. Goodman, "Beyond Clausius-Mossotti: wave propagation on a polarizable point lattice and the discrete-dipole approximation," *Astrophys. J.* 405, 685–697 (1993).

E. Zubko, D. Petrov, Ye. Grynko, et al. "Validity criteria of the discrete dipole approximation," *Appl. Opt.*, 49, pp. 1267–1279 (2010).

Modeling cometary dust particles

Within DDA, there are no restrictions on shape and internal structure of a target particles. Therefore, you can build up any kind of shape. However, there are two requirements:

- (a) dust particles have to be essentially irregular (non-spherical, non-cubical, etc.)
- (b) dust particles have agglomerate structure. Packing density have to be chosen in order provide range of the measured density (from 0.3 to 3 g/cm³).

Refractive indices for cometary spices in visible:

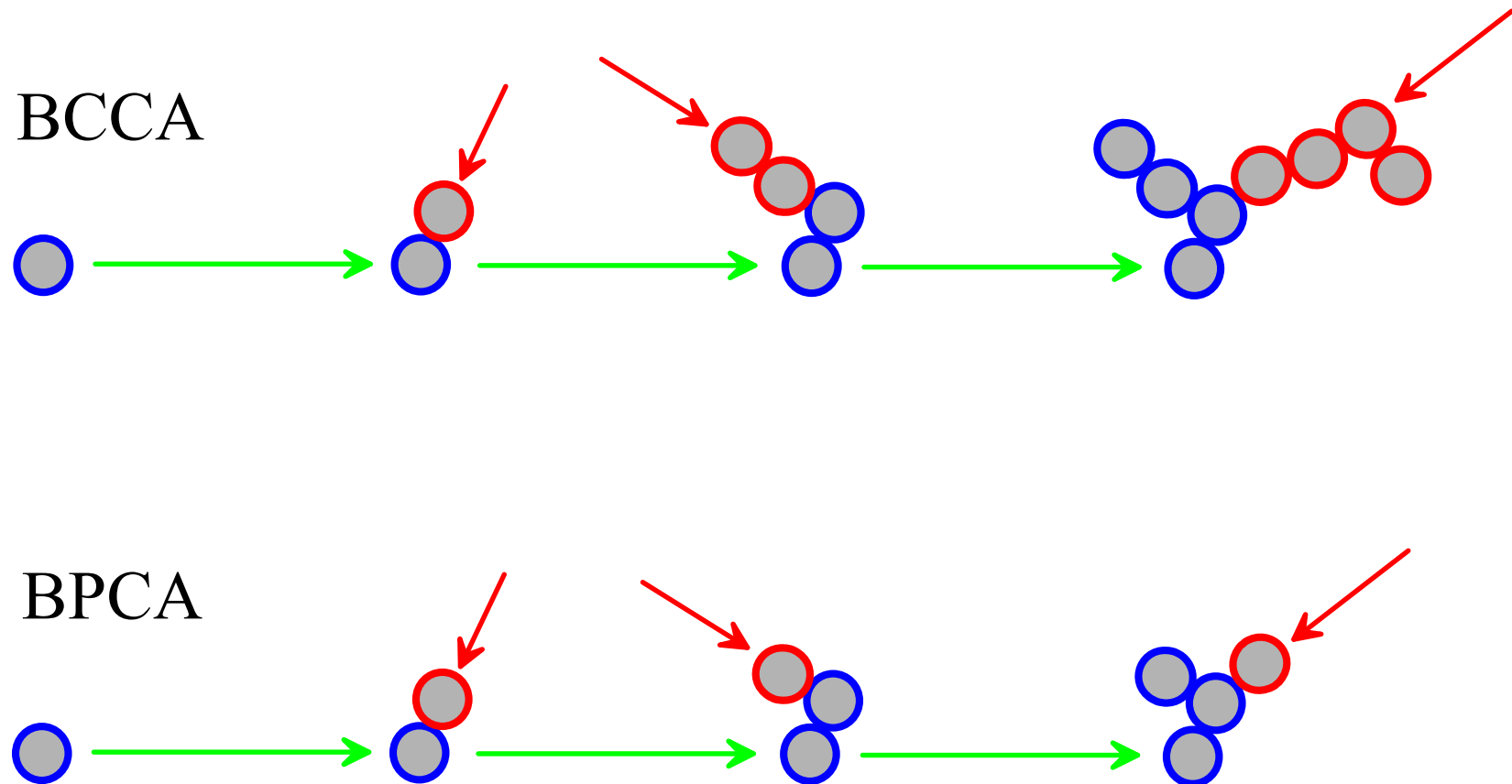
Mg-rich silicate: $\text{Re}(m) = 1.5 - 1.6$ $\text{Im}(m) = 0.00001 - 0.01$

Water ice: $\text{Re}(m) = 1.31$ $\text{Im}(m) = 0$

Organic material $\text{Re}(m) = 1.4 - 1.6$ $\text{Im}(m) = 0.002 - 0.5$

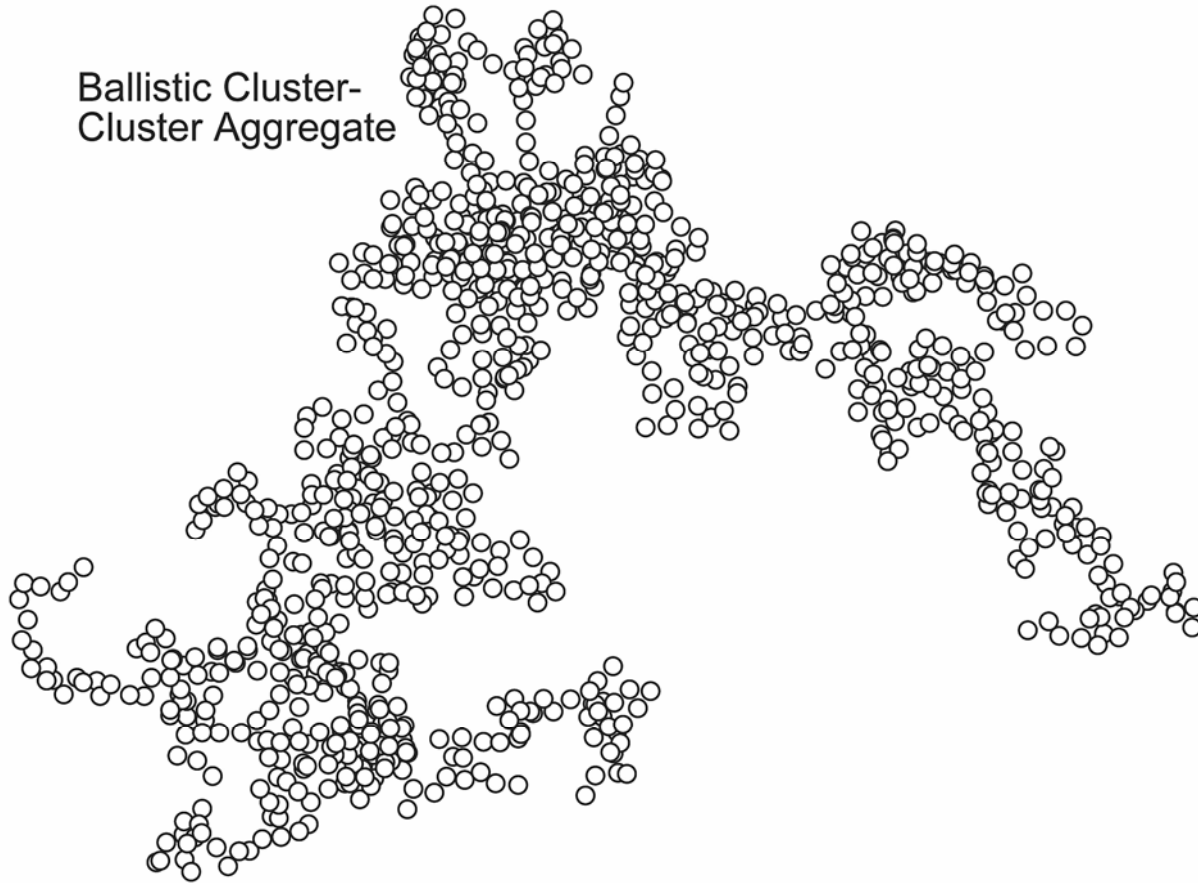
Popular shapes for cometary dust particles

Two models popular models are ballistic cluster-cluster aggregates (BCCA) and ballistic particle-cluster aggregates (BPCA). The fractal dimension of BCCA is about 2; whereas, for BPCA, it is about 3. The size of constituent sphere is of $0.2 \mu\text{m}$.

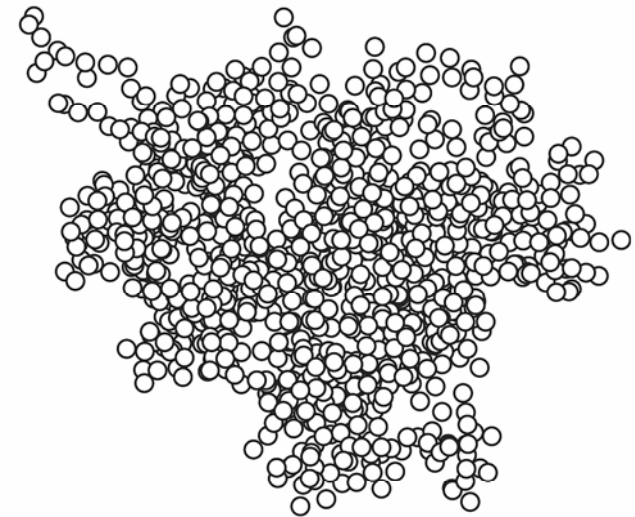


Examples of BCCA and BPCA

Ballistic Cluster-Cluster Aggregate

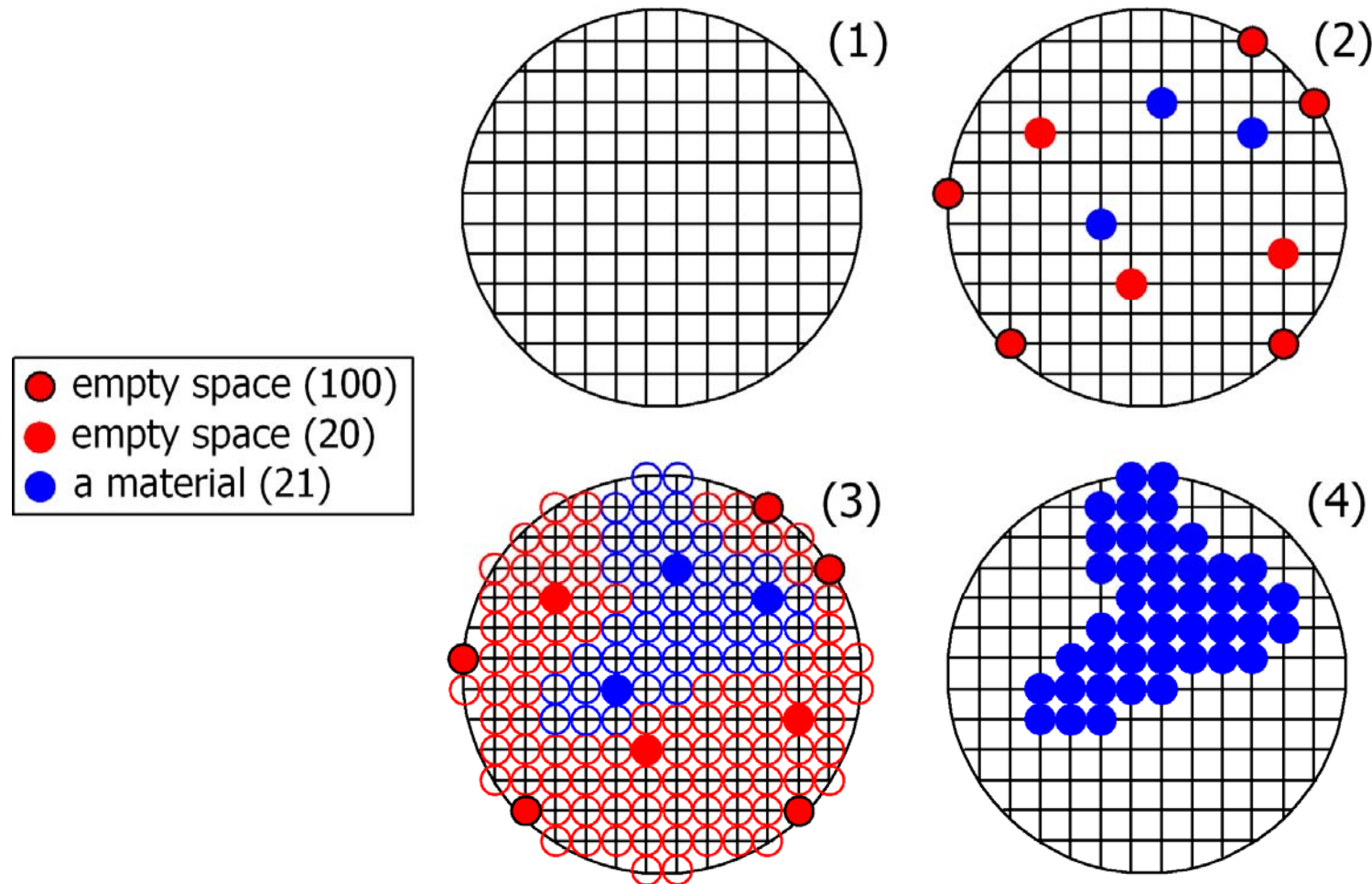


Ballistic Particle-Cluster Aggregate



An example for other models of cometary dust particles is agglomerated debris.

Algorithm for generation of agglomerated debris is as follows:



However, there must be alternative models!

Examples of agglomerated debris particles

