SCATTERING CALCULATIONS ON THE BASIS OF THE FREDHOLM INTEGRAL EQUATION METHOD

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ABSTRACT. The Fredholm integral equation method (FIM) is one of the solutions to the scattering of electromagnetic radiation by homogeneous and isotropic ellipsoidal particles. Some numerical calculations are performed with the FIM. The results for spherical particles are compared with those by the Mie theory. It is confirmed that the agreement between them is satisfactory for all the models calculated.

On the basis of the present method, we examine profiles of the absorption band around $\lambda = 10\ \mu m$ for spherical and ellipsoidal particles composed of crystalline olivine. It is found that the profile strongly depends on the shape of the particle. Even when the particle is moderately elongated (axial ratios are $2:\sqrt{2}:1$), the profile is significantly different from that for a sphere.

1. Fredholm Integral Equation Method (FIM)

The dyadic electric field E of the wave scattered by a particle with a refractive index m can be described by an integration equation

$$\mathbf{E}(\mathbf{r}) = \mathbf{I}_I \exp(i\mathbf{k}_I \cdot \mathbf{r}) + \int_{vol} \mathbf{G}(\mathbf{r}, \mathbf{r}')\gamma(\mathbf{r}')\mathbf{E}(\mathbf{r}')\,d\mathbf{r}', \tag{1}$$

where $\mathbf{k}_I$ is the wave number vector of the incident light and

$$\mathbf{I}_I = \mathbf{J} - \hat{\mathbf{k}}_I\hat{\mathbf{k}}_I, \tag{2}$$

$$\mathbf{G} = (\mathbf{J} + k^{-2}\nabla\nabla)\exp(ik\,|\mathbf{r} - \mathbf{r}'|)/(4\pi\,|\mathbf{r} - \mathbf{r}'|), \tag{3}$$

$$\gamma(\mathbf{r}) = k_0^2(m^2(\mathbf{r}) - 1), \tag{4}$$

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where J is a unit dyadic, $\hat{k}_I$ is a unit vector along k_I, and k (k_o) is the wave number within (without) the particle. When $r \to \infty$, the asymptotic form of equation (1) is

$$\mathbf{E}(\mathbf{r}) = \mathbf{I}_I \exp(i\mathbf{k}_I \cdot \mathbf{r}) + \mathbf{B}(\mathbf{k}_S, \mathbf{k}_I) \exp(ik_0 r)/r, \tag{5}$$

where k_s is the wave number vector of the scattered light, and B is the scattering amplitude given by

$$\mathbf{B}(\mathbf{k}_S, \mathbf{k}_I) = (4\pi)^{-1} \mathbf{I}_S \cdot \int_{\mathrm{vol}} \exp(-i\mathbf{k}_S \cdot \mathbf{r}) \gamma(\mathbf{r}) \mathbf{E}(\mathbf{r})\, d\mathbf{r}. \tag{6}$$

Equation (6) shows that we can evaluate numerically B provided that the field within the particle is known. The solution for E within the particle is, however, not obtained directly from equation (1), since it is an integral equation with a singular kernel. We perform a transformation such that the singularity is removed analytically. Following Holt et al (1978), we assume that the field within the particle is expressed as the spatial Fourier transform

$$\mathbf{E}(\mathbf{r}) = \int \mathbf{C}(\mathbf{k}_1) \exp(i\mathbf{k}_1 \cdot \mathbf{r})\, d\mathbf{k}_1. \tag{7}$$

Making use of Equation (7), we get a pair of the coupled Fredholm equations, which can be rewritten as matrix equations

$$\mathbf{B}(\mathbf{k}_S, \mathbf{k}_I) = (4\pi)^{-1} \mathbf{I}_S \cdot \sum_{l=1}^{n_{\max}} c_l C(\mathbf{k}_l) U(\mathbf{k}_S, \mathbf{k}_l), \tag{8}$$

and

$$\sum_{l=1}^{n_{\max}} \mathbf{K}(\mathbf{k}_j, \mathbf{k}_l) \cdot c_l \mathbf{C}(\mathbf{k}_l) = \mathbf{I}_I U(\mathbf{k}_j, \mathbf{k}_I), \tag{9}$$

where expressions of U and K are given elsewhere (Holt et al 1978, Matsumura and Seki 1990). Once B is obtained, the calculations of the optical cross-sections are straightforward as is described in classical textbooks.

In the practical calculation with the FIM, we must choose adequate pivots k_l ($l=1,\ldots,n_{max}$). In a spherical coordinate (θ_P, ϕ_P) which displays the directions of k_l, we first divide evenly the range of $0<\theta<\pi$ by $2n_\theta$, i.e., intervals $\Delta\theta_P$ are equal to each other. Next, for each θ_P, we divide the range of $0<\phi_P<2\pi$ evenly such that the intervals $\Delta\phi_P$ are nearly equal to $\Delta\theta_P$. Practically we get n_{max} = 2, 12, 30, and 56 for n_θ = 0, 1, 2, and 3 (when n_θ = 0, the pivots are poles only).

2. Application to silicate 10 μm band

We apply the FIM to the investigation of the band profile observed near λ =10 μm in many astronomical objects, which is attributed to silicate particles. The shape of the particle is assumed to be spherical or ellipsoidal (the axial ratios are $2:\sqrt{2}:1$).

Table 1 presents values of efficiency factor for absorption Q_{abs} as a function of n_θ. The equivalent radius a_{eq} is defined as $a_{eq}=(abc)^{1/3}$ where a, b, and c are three radii of the ellipsoid, and is set to be 1.0 μm in these calculations. We confirm that the convergence for n_θ is rapid, and that the obtained values are correct enough provided that $n_\theta = 1$.

TABLE 1. Examples of calculations: Q_{abs} for a_{eq}=1.0 μm

λ (μm)	9.8	10.0	11.0	11.6
Re(m)	0.5109	0.6682	0.8004	2.748
Im(m)	0.6344	1.061	1.379	2.291
x_{eq} ($=k_0a_{eq}$)	0.6410	0.6283	0.5713	0.5417
Sphere				
n_θ = 0	0.8397	1.807	2.366	0.8975
1	0.8943	1.902	2.415	0.8836
2	0.8943	1.902	2.415	0.8835
Mie	0.8943	1.902	2.415	0.8835
Ellipsoid ($2:\sqrt{2}:1$)				
n_θ = 0	0.8493	1.642	1.992	0.8934
1	0.9347	1.793	2.100	1.119
2	0.9347	1.793	2.100	1.119

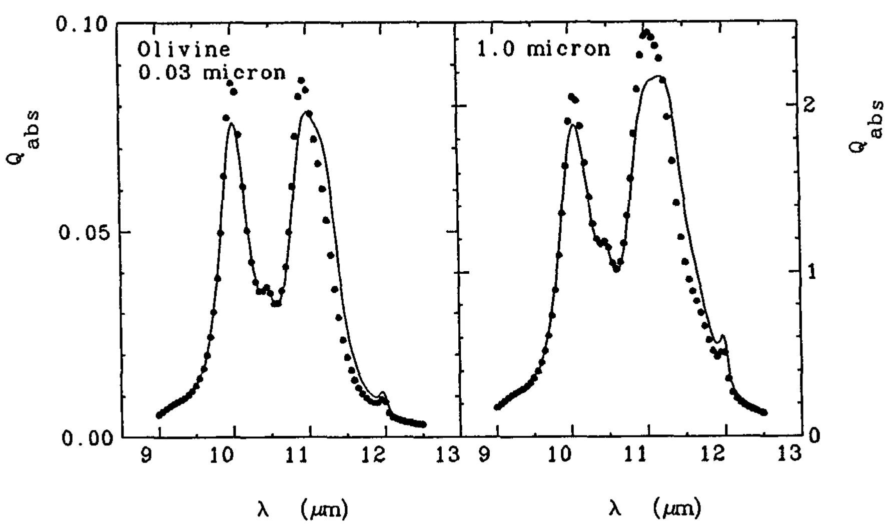

Figure 1. Band profiles for crystalline olivine. Solid lines are for ellipsoidal particles, while dots are for spherical ones. The left figure is for a_{eq} = 0.03 μm, and the right one is for a_{eq} = 1.0 μm.

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Figure 1 shows the results for crystalline olivine, where optical constants are cited from Mukai and Koike (1990). We find that the profile for the ellipsoidal particle (solid line) is significantly different from that for the spherical one (dots).

The results for amorphous silicate are demonstrated in figure 2 (m is from Day 1979). The behavior of the solid line (results for ellipsoid) is closely similar to that of the dashed line (results for sphere). Thus, the effect of the shape is less significant for amorphous silicate.

Recent observations of comets show a double peak structure in 10 μm-band, and this fact is interpreted as the presence of crystalline olivine in cometary grains. The present study suggests that the effect of the shape is important to the quantitative interpretation of such observations.

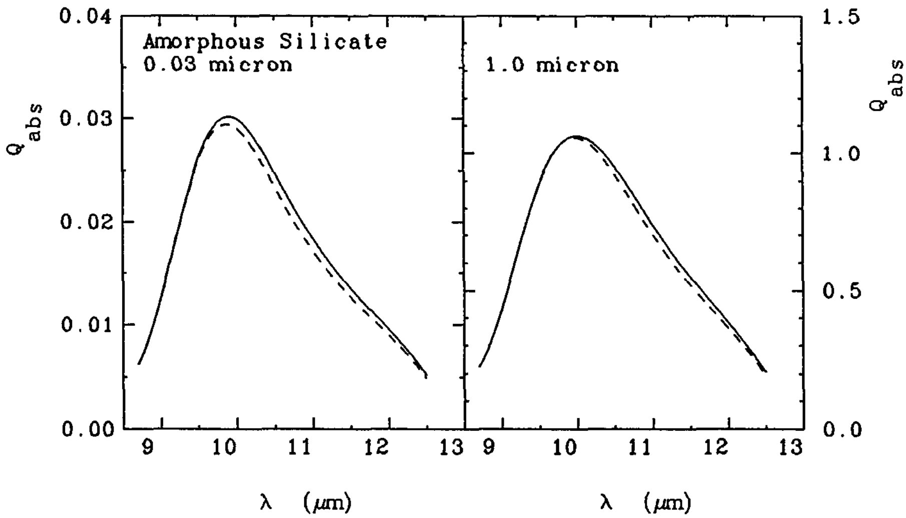

Figure 2. Same as figure 1 but for amorphous silicate. The results for sphere are shown by dashed line.

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