Determination of electric-field–gradient orientation and asymmetry with Mössbauer absorption of linearly polarized γ radiation

Y. S. Liu
Department of Physics, University of Brasília, 70 910, Brasília, Distrito Federal, Brazil
(Received 13 June 1983)

Zory's method of electric-field–gradient orientation determination by using the area ratio of a two-line spectrum in the Mössbauer absorption, by ^{57}Fe, using unpolarized γ radiation in a thin single-crystal absorber is extended to that of using linearly polarized γ radiation. The method is applied to FeS_2 pyrite and to marcasite, and some definite predictions on how the area ratio should vary with the directions of incidence as well as that of the plane of polarization are obtained.

I. INTRODUCTION

Zory's method for electric-field–gradient (EFG) determination by using the area ratio[1] of a two-line spectra in the Mössbauer absorption of nuclear γ radiation by ^{57}Fe in the thin-absorber limit, when applied to FeS_2 pyrite, does not give very useful information. The reason is that FeS_2 pyrite is a crystal of high symmetry and in each cell there are four equivalent but differently oriented sites, and so when summed over contributions from all these sites, the area ratio is unity for various directions of the incident γ radiation with respect to the crystal axes.[2] One may hope that, by using polarized γ radiation, it may be possible to observe variation of the area as the state of polarization is altered, and this will furnish additional information for the determination of the EFG parameters. Studies of polarization dependence of the Mössbauer absorption of γ radiation by nuclei in either thin or thick absorbers, in the presence of magnetic field and/or with quadrupole interaction, have been reported by many workers.[3,4] However, the area-ratio method is an easy way to verify a hypothesis or prediction on the EFG, which may be obtained based on consideration of symmetry in the crystalline structure. In this work we obtain a general expression for the area ratio as a function of the angle of the plane of polarization as well as the direction of the incident γ radiation considering only the electric quadrupole interaction of the excited ^{57}Fe with the EFG.

As usual, we denote the EFG principal axes as $\hat{x},\hat{y},\hat{z}$, with $|V_{zz}|\geq|V_{yy}|\geq|V_{xx}|$. The Hamiltonian for the quadrupole interaction, with nuclear spin I quantized with respect to the EFG z axis, is

$$H_Q=\frac{e^2qQ}{4I(2I-1)}[3I_z^2-I(I+1)+\tfrac{1}{2}\eta(I_+^2+I_-^2)]\ , \tag{1}$$

where eQ is the nuclear quadrupole moment, $eq=V_{zz}$ is the z component of the EFG, and $\eta=(V_{xx}-V_{yy})/V_{zz}$ denotes the asymmetry parameter.

For the ground state of ^{57}Fe, $I=\frac{1}{2}$; the eigenvalue is zero. Hence the separation of the two absorption lines is due to the quadrupole interaction of the first excited state of ^{57}Fe, which is $I=\frac{3}{2}$. The two energy eigenvalues are

$$\left.\begin{matrix}E_3\\E_1\end{matrix}\right\}=\pm\tfrac{1}{2}e^2qQ(1+\eta/3)^{1/2}\ . \tag{2}$$

The eigenstates associated with these eigenvalues, in terms of the angular momentum eigenstates $|I,m\rangle$, are[1]

$$\begin{aligned}E_3:\ &|\psi_3\rangle=\cos\rho\,|\tfrac{3}{2},\tfrac{3}{2}\rangle+\sin\rho\,|\tfrac{3}{2},-\tfrac{1}{2}\rangle\ ,\\&|\psi_{-3}\rangle=\cos\rho\,|\tfrac{3}{2},-\tfrac{3}{2}\rangle+\sin\rho\,|\tfrac{3}{2},\tfrac{1}{2}\rangle\ ,\\E_1:\ &|\psi_1\rangle=\sin\rho\,|\tfrac{3}{2},\tfrac{3}{2}\rangle-\cos\rho\,|\tfrac{3}{2},-\tfrac{1}{2}\rangle\ ,\\&|\psi_{-1}\rangle=\sin\rho\,|\tfrac{3}{2},-\tfrac{3}{2}\rangle-\cos\rho\,|\tfrac{3}{2},\tfrac{1}{2}\rangle\ ,\end{aligned} \tag{3}$$

where

$$\cos\rho=\{1+[3/(3+\eta^2)^{1/2}]^{1/2}\}/\sqrt{2}\ ,$$
$$\sin\rho=\{1-[3/(3+\eta^2)^{1/2}]^{1/2}\}/\sqrt{2}\ .$$

II. AREA RATIO

The probability that linearly polarized γ radiation in the direction $\hat{k}$ (Fig. 1), with polarization vector $\hat{\epsilon}$, is absorbed by a ^{57}Fe nuclei at site i in its ground state $|\frac{1}{2},m\rangle$, making a transition to the excited state $|\psi_j\rangle$, is proportional to $|\langle\frac{1}{2},m\,|\hat{\epsilon}\cdot\vec{M}\,|\psi_j\rangle|^2$, where $\vec{M}$ is assumed to be the nuclear magnetic dipole moment operation. With $f(\theta_i,\phi_i)$ being the recoiless absorption probability (the recoil-free fraction) of nuclei at sites i, the ratio of the areas of absorption lines is given by

$$\frac{a_3}{a_1}=\frac{\sum_i f(\theta_i,\phi_i)P_3}{\sum_i f(\theta_i,\phi_i)P_1}\ , \tag{4}$$

where

$$\begin{aligned}P_j=&|\langle\tfrac{1}{2},\tfrac{1}{2}\,|\hat{\epsilon}\cdot\vec{M}\,|\psi_j\rangle|^2+|\langle\tfrac{1}{2},\tfrac{1}{2}\,|\hat{\epsilon}\cdot\vec{M}\rangle\,|\psi_{-j}\rangle|^2\\&+|\langle\tfrac{1}{2},-\tfrac{1}{2}\,|\hat{\epsilon}\cdot\vec{M}\,|\psi_j\rangle|^2+|\langle\tfrac{1}{2},-\tfrac{1}{2}\,|\hat{\epsilon}\cdot\vec{M}\,|\psi_{-j}\rangle|^2\ .\end{aligned}$$

We consider the case in which the polarization vector $\hat{\epsilon}$ makes an angle with respect to the normal of the plane containing $\hat{k},\hat{z}$, i.e.,

$$\hat{\epsilon}=\hat{\theta}\sin\delta+\hat{\phi}\cos\delta\ , \tag{5}$$

where $\hat{\theta}$ and $\hat{\phi}$ are unit vectors along the directions of increasing θ and ϕ, respectively. In terms of the spherical unit vectors, $\hat{e}_1 = -(\hat{x}+i\hat{y})/\sqrt{2}$, $\hat{e}_2 = (\hat{x}-i\hat{y})/\sqrt{2}$, and $\hat{e}_0 = \hat{z}$, they are

$$\hat{\theta} = -\hat{e}_0 \sin\theta + (-\hat{e}_1 e^{-iy} + \hat{e}_{-1} e^{i\phi})\cos\theta/\sqrt{2} ,$$
$$\hat{\phi} = i(\hat{e}_1 e^{-i\phi} + \hat{e}_{-1} e^{i\phi})/\sqrt{2} . \tag{6}$$

Using the matrix elements given by Condon and Shortley,[5] we have, in terms of a constant R which is related to the reduced matrix element,

$$\langle \tfrac{1}{2}, \pm\tfrac{1}{2} \,|\, \vec{\mathrm{M}} \,|\, \tfrac{3}{2}, \pm\tfrac{3}{2} \rangle = \sqrt{3} R \hat{e}_{\pm 1} ,$$
$$\langle \tfrac{1}{2}, \pm\tfrac{1}{2} \,|\, \vec{\mathrm{M}} \,|\, \tfrac{3}{2}, \pm\tfrac{1}{2} \rangle = \sqrt{2} R \hat{e}_{0} ,$$
$$\langle \tfrac{1}{2}, \mp\tfrac{1}{2} \,|\, \vec{\mathrm{M}} \,|\, \tfrac{3}{2}, \pm\tfrac{1}{2} \rangle = R \hat{e}_{\mp 1} ,$$

and therefore,

$$| \langle \tfrac{1}{2}, \tfrac{1}{2} \,|\, \hat{\epsilon}\cdot\vec{\mathrm{M}} \,|\, \psi_3 \rangle |^2 = | \langle \tfrac{1}{2}, -\tfrac{1}{2} \,|\, \hat{\epsilon}\cdot M \,|\, \psi_{-3} \rangle |^2$$
$$= \frac{R^2}{4}(1+\cos^2\theta + \sin^2\theta \cos 2\delta)(3 - 2\sin^2\rho)$$
$$+ \frac{\sqrt{3}}{2} R^2 \{ [(1+\cos^2\theta)\cos 2\delta + \sin^2\theta] \cos 2\phi + 2\cos\theta \sin 2\delta \sin 2\phi \} \cos\rho \sin\rho$$

and

$$| \langle \tfrac{1}{2}, \tfrac{1}{2} \,|\, \hat{\epsilon}\cdot\vec{\mathrm{M}} \,|\, \psi_{-3} \rangle |^2 = | \langle \tfrac{1}{2}, -\tfrac{1}{2} \,|\, \hat{\epsilon}\cdot\vec{\mathrm{M}} \,|\, \psi_3 \rangle |^2$$
$$= 2R^2 \sin^2\theta \sin^2\delta \sin^2\rho . \tag{7a}$$

By changing $\cos\rho$ to $\sin\rho$, and $\sin\rho$ to $-\cos\rho$, we obtain

$$| \langle \tfrac{1}{2}, \tfrac{1}{2} \,|\, \hat{\epsilon}\cdot\vec{\mathrm{M}} \,|\, \psi_1 \rangle |^2 = | \langle \tfrac{1}{2}, -\tfrac{1}{2} \,|\, \hat{\epsilon}\cdot\vec{\mathrm{M}} \,|\, \psi_{-1} \rangle |^2$$
$$= \frac{R^2}{4}(1+\cos^2\theta + \sin^2\theta \cos 2\delta)(1 + 2\sin^2\rho)$$
$$- \frac{\sqrt{3}}{2} R^2 \{ \,|\, [(1+\cos^2\theta)\cos 2\delta + \sin^2\theta] \,|\, \cos 2\phi + 2\cos\theta \sin 2\delta \sin 2\phi \} \cos\rho \sin\rho ,$$

and

$$| \langle \tfrac{1}{2}, \tfrac{1}{2} \,|\, \hat{\epsilon}\cdot\vec{\mathrm{M}} \,|\, \psi_{-1} \rangle |^2 = | \langle \tfrac{1}{2}, -\tfrac{1}{2} \,|\, \hat{\epsilon}\cdot\vec{\mathrm{M}} \,|\, \psi_1 \rangle |^2$$
$$= 2R^2 \sin^2\theta \sin^2\delta \cos^2\rho . \tag{7b}$$

Therefore the area ratio for absorption of linearly polarized γ radiation is

$$\frac{a_3}{a_1} = \frac{\sum_i f(\theta_i,\phi_i) \,|\, A_i(3 - 2\sin^2\rho) + \sqrt{3} B_i \sin 2\rho + C_i \sin^2\rho \,|}{\sum_i f(\theta_i,\phi_i) \,|\, A_i(1 + 2\sin^2\rho) - \sqrt{3} B_i \sin 2\rho + C_i \cos^2\rho \,|} , \tag{8}$$

where

$$A_i = 1 + \cos^2\theta_i + \sin^2\theta_i \cos 2\delta_i ,$$
$$B_i = [\sin^2\theta_i + (1+\cos^2\theta_i)\cos 2\delta_i] \cos 2\phi_i + 2\cos\theta_i \sin 2\delta_i \sin 2\phi_i ,$$
$$C_i = 8\sin^2\theta_i \sin^2\delta_i .$$

In the case where $\eta = 0$, this reduces to

$$\frac{a_3}{a_1} = \frac{\sum_i f(\theta_i,\phi_i)[3(1+\cos^2\theta_i + \sin^2\theta_i \cos 2\delta_i)]}{\sum_i f(\theta_i,\phi_i)(5 - \cos^2\theta_i - \sin^2\theta_i \cos 2\delta_i)} \tag{9}$$

III. PYRITE

The are four equivalent Fe sites per unit cell, respectively, at (0,0,0), $(0,\frac{1}{2},\frac{1}{2})$, $(\frac{1}{2},0,\frac{1}{2})$, and $(\frac{1}{2},\frac{1}{2},0)$ and with EFG z axes along [111], [$\bar{1}$11], [1$\bar{1}$1], and [11$\bar{1}$], and $\eta = 0^2$. If a single crystal of pyrite is orientated such that the direction of the 14.4-keV γ radiation is along a crystallographic axis, for example, the a axis, then the polarization axis can be specified by

$$\hat{\epsilon} = \hat{b}\cos\beta + \hat{c}\sin\beta . \tag{10}$$

The values for $\cos 2\delta_i$ in Eq. (9) are $-\sin 2\beta$, $-\sin 2\beta$, $\sin 2\beta$, and $\sin 2\beta$, respectively, for the four sites, while $\cos^2\theta_i = \frac{1}{2}$, as given in Table I. Since the recoil-free fraction is given by

$$f_i = e^{-k^2\langle r^2 \rangle} , \tag{11}$$

where k is the propagation constant of the γ radiations. Since for pyrite $\langle x^2 \rangle = \langle y^2 \rangle$,

$$f_i = \exp[-k^2(\langle x^2 \rangle \sin^2\theta_i + \langle z^2 \rangle \cos^2\theta_i)] , \tag{12}$$

$\langle x^2 \rangle$, $\langle y^2 \rangle$, $\langle z^2 \rangle$ being the mean-square displacements

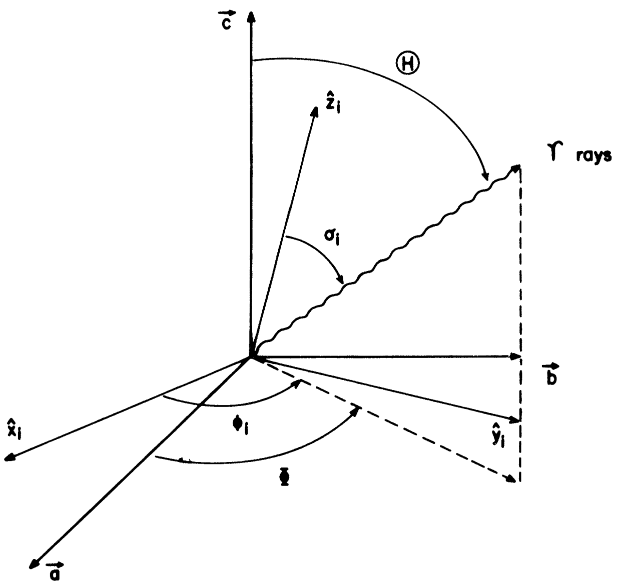

FIG. 1. Schematics of the absorption process of the 14.4-keV γ rays by ^{57}Fe, relative to the crystallographic axes $(\vec{a},\vec{b},\vec{c})$ and to the EFG axes $(\hat{x}_i,\hat{y}_i,\hat{z}_i)$ of the ith site.

(MSD) along the principal MSD axes. The recoil-free fraction is the same for all the four sites. Thus from Eq. (9) we conclude that $a_3/a_1=1$, independent of the polarization angle. Here we have taken the asymmetry parameter to be zero, which is a conclusion from the consideration of crystallographic symmetry. However, if experimental data show that indeed the area ratio is unity, we cannot conclude immediately that $\eta=0$, since the area ratio can still be unity even when the asymmetry parameter is not zero. The reason for this is that the asymmetry effects from the four equivalent sites may cancel out each other. As an example, we consider the same experimental arrangement as above, i.e., linearly polarized γ radiation along the a axis. When the asymmetry parameter is nonzero, the EFG x and y axes are no longer undetermined. We note that the EFG z axis of the ^{57}Fe nucleus at site (0,0,0) is [111], and all the others can be obtained by a rotation around the crystallographic c axis of angles $\pi/2$, π, and $3\pi/2$. Hence if the azimuthal angle of the γ radiation is ϕ with respect to the EFG axes the ^{57}Fe nucleus at the site (0,0,0). All the others should be as given in Table I. Thus, when summed over contributions from the four sites, we obtain

$$\sum_i A_i=\tfrac{16}{3}\;,$$

$$\sum_i B_i=0\;,$$

$$\sum_i C_i=\tfrac{16}{3}\sum_i(1-\cos2\theta_i)/2=\tfrac{32}{3}\;.$$

Hence, taking f to be isotropic, we obtain from Eq. (9), $a_3/a_1=1$ independent of η.

IV. MARCASITE

The crystal structure of marcasite is orthorhombic[6] with $a=4.436$ Å, $b=5.414$ Å, and $c=3.381$ Å. The iron atoms occupy two equivalent sites (0,0,0) and $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$, while the sulfur atoms at $(u,v,0)$ and $(\frac{1}{2}-u,v+\frac{1}{2},\frac{1}{2})$, with $u=0.200$, $v=0.378$. Thus each iron atom is surrounded by six sulfur atoms, two at a distance of 2.2305 Å and four at 2.2506 Å away, forming a distorted octahedron. (Fig. 2). On a point-charge model, this distorted octahedron would give rise to an EFG such that the y axis is along the crystallographic axis c, while the z axis is along $0.988\hat{a}-0.153\hat{b}$ for the EFG at the site (0,0,0), and along $0.988\hat{a}+0.153\hat{b}$ for the EFG at $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$, with the asymmetry parameter $\eta=0.575$. However, as the Fe—S bondings in marcasite are highly covalent,[7] one may expect that the EFG at a Fe nucleus is almost entirely due to its two nearest-neighboring sulfur atoms (S_5, S_6 in Fig. 2). If this is indeed the case, then $\eta=0$, and z axes are in the a-b plane. For Fe at (0,0,0), $\hat{z}_1=P\hat{a}+q\hat{b}$, and for Fe at $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$, $\hat{z}_2=P\hat{a}-q\hat{b}$, where

$$P=ua/[(ua)^2+(vb)^2]^{1/2}=0.3977\;,$$

$$q=vb/[(ua)^2+(vb)^2]^{1/2}=0.9175\;,$$

while the x and y axes are undetermined.

If the direction of the incident γ radiation is specified by the experimental angles θ and Φ with respect to the crystallographic axes a, b, and c, then the angles with respect to the EFG z axes are given by

$$\cos\theta_1=(P\cos\Phi+q\sin\Phi)\sin\theta\;,$$

$$\cos\theta_2=(P\cos\Phi-q\sin\Phi)\sin\theta\;.$$

Since we take η to be zero, we have, same as in the case of pyrite,

$$f_i=\exp[-k^2(\langle x^2\rangle\sin^2\theta_i+\langle z^2\rangle\cos^2\theta_i)]\;.$$

TABLE I. Propagation and polarization vectors with respect to EFG principal axes of each Fe site (θ_i, ϕ_i, and δ_i) when γ ray is along the crystallographic axis a; the azimuthal angle with respect to site 1 is arbitrarily taken to be ϕ.

Site	EFG 3 axes	$\cos\theta_i$	$\sin\theta_i$	ϕ_i	$\cos2\phi_i$	$\sin2\phi_i$	$\cos2\delta_i$	$\sin2\delta_i$
1	[111]	$1/\sqrt{2}$	$\sqrt{2/3}$	ϕ	$\cos2\phi$	$\sin2\phi$	$-\sin2\beta$	$\cos2\beta$
2	$[\bar{1}11]$	$-1/\sqrt{3}$	$\sqrt{2/3}$	$\phi+\pi/2$	$-\cos2\phi$	$-\sin2\phi$	$-\sin2\beta$	$-\cos2\beta$
3	[111]	$1/\sqrt{3}$	$\sqrt{2/3}$	$\phi+3\pi/2$	$-\cos2\phi$	$-\sin2\phi$	$\sin2\beta$	$\cos2\beta$
4	$[11\bar{1}]$	$1/\sqrt{3}$	$\sqrt{2/3}$	$\phi+\pi$	$\cos2\phi$	$\sin2\phi$	$\sin2\beta$	$\cos2\beta$

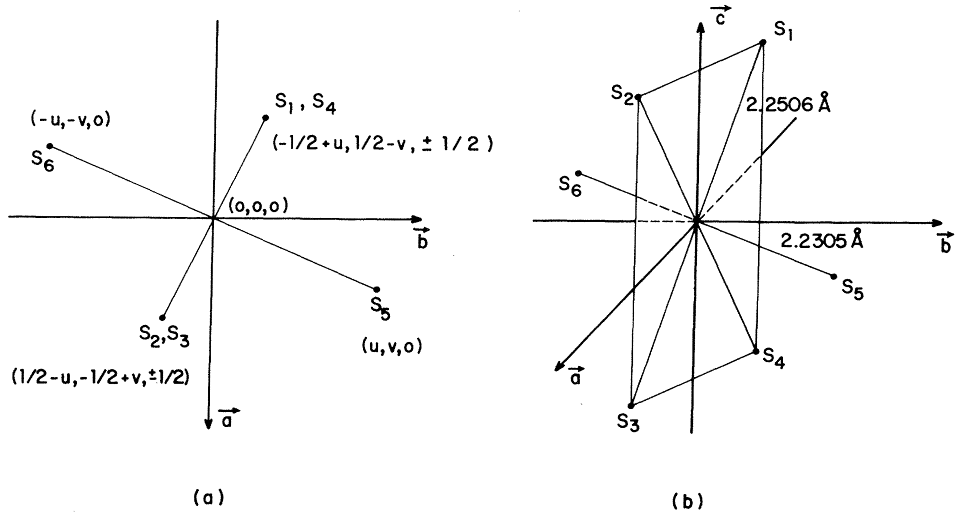

FIG. 2. Immediate sulfur atoms of the iron atom at (0,0,0): S_5, S_6 at $\pm(u,v,0)$, 2.2305 Å; S_1, S_2, S_3, S_4 at $\pm(\frac{1}{2}-u,-\frac{1}{2}+v,\frac{1}{2})$, 2.2506 Å. (a) Projected positions of the S atoms on *a*-*b* plane. (b) S atoms S_5, S_6 lie on *a*-*b* plane, almost perpendicular to the plane formal of S_1, S_2, S_3, and S_4.

For γ radiation along any of the crystallographic axes, $\cos^2\theta_1=\cos^2\theta_2$ and hence $f_1=f_2$. The area ratio of Eq. (9) becomes

$$\frac{a_3}{a_1}=\frac{\sum_i 3(1+\cos^2\theta_i+\sin^2\theta_i\cos2\delta_i)}{\sum_i (5-3\cos^2\theta_i-3\sin^2\theta_i\cos2\delta_i)} . \tag{13}$$

This gives very definite predictions for the dependence of the area ratios on the angles of the polarization vector of γ radiation. For example:

(1) γ radiation along $\hat{a}(\theta=\pi/2,\Phi=0)$, $\hat{\epsilon}=\hat{b}\cos\beta+\hat{c}\sin\beta$:

$$\cos2\delta_1=\cos2\delta_2=-\cos2\beta ,$$

$$\cos^2\theta_1=\cos^2\theta_2=P^2 ,$$

$$\frac{a_3}{a_1}=\frac{3(1+P^2-q^2\cos2\beta)}{5-3P^2+3q^2\cos2\beta}, \quad q^2=1-P^2 .$$

(2) γ radiation along $\hat{b}(\theta=\pi/2,\Phi=\pi/2)$, $\hat{\epsilon}=\hat{c}\cos\beta+\hat{a}\sin\beta$:

$$\cos2\delta_1=\cos2\delta_2=\cos2\beta ,$$

$$\cos^2\theta_1=\cos^2\theta_2=q^2 ,$$

$$\frac{a_3}{a_1}=\frac{3(1+2+P^2\cos2\beta)}{5-3q^2-3p^2\cos2\beta} .$$

(3) γ radiation along $\hat{c}(\theta=0)$, $\hat{\epsilon}=\hat{a}\cos\beta+\hat{b}\sin\beta$:

$$\cos^2\theta_1=\cos^2\theta_2=0 ,$$

$$\left.\begin{matrix}\cos2\delta_1\\ \cos2\delta_2\end{matrix}\right\}=(q^2-P^2)\cos2\beta\mp2Pq\sin2\beta ,$$

$$\frac{a_3}{a_1}=\frac{3+3(q^2-P^2)\cos2\beta}{5-3(q^2-P^2)\cos2\beta} .$$

If we make a further assumption that f is isotropic, then we obtain more interesting results. For example, for γ radiation in the *a*-*b* plane, $\theta=\pi/2$,

$$\left.\begin{matrix}\cos^2\theta_1\\ \cos^2\theta_2\end{matrix}\right\}=(P\cos\Phi\pm q\sin\theta)^2$$

for $\hat{\epsilon}||\hat{c}$,

$$\cos2\delta_1=\cos2\delta_1=1 ,$$

$$\frac{a_3}{a_1}=3 ,$$

for $\hat{\epsilon}\perp\hat{c}$,

$$\cos2\delta_1=\cos2\delta_2=-1 ,$$

$$\frac{a_3}{a_1}=\frac{3(P^2\cos^2\Phi+q^2\sin^2\Phi)}{4-3(P^2\cos^2\Phi+q^2\sin^2\Phi)} .$$

V. DISCUSSION

When circularly polarized γ radiation is used, the polarization vector is $\hat{\epsilon}=\hat{\theta}\pm i\hat{\phi}$, and A_i, B_i, C_i of Eq. (8) become

$$A_i=1+\cos^2\theta_i ,$$

$$B_i=\sin^2\theta_i\cos2\phi_i ,$$

$$C_i=4\sin^2\theta_i ,$$

so the area ratio is

$$\frac{a_3}{a_1}=\frac{\sum_i f_i(\theta_i,\phi_i)[3(1+\cos^2\theta_i)+2(1-3\cos^2\theta_i)\sin^2\rho+\sqrt{3}\sin^2\theta_i\cos^2\phi_i\sin2\rho]}{\sum_i f_i(\theta_i,\phi_i)[5-3\cos^2\theta_i-2(1-3\cos^2\theta_i)\sin^2\rho-\sqrt{3}\sin^2\theta_i\cos2\phi_i\sin2\rho]}\ ,$$

which is the same as the expression of Zory's for unpolarized γ radiation, i.e.,

$$\frac{a_3}{a_1}=\frac{\sum_i f_i(\theta_i,\phi_i)[4(3+\eta^2)/3\,|^{1/2}+(3\cos^2\theta_i-1+\eta\sin^2\theta_i\cos2\phi_i)]}{\sum_i f_i(\theta_i,\phi_i)[4(3+\eta^2)/3\,|^{1/2}-(3\cos^2\theta_i-1+\eta\sin^2\theta_i\cos2\phi_i)]}$$

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