Spectroscopic Polarimetry of Light scattered by Surface Roughness and Textured Films in Nanotechnologies
Spectroscopic Polarimetry of Light scattered By...

A way to establish the linear polarization of reflected, scattered, and transmitting light from natural objects, such as moon, stars, sky, clouds, etc...

Much more polarization information is available in the detected light:

- Wavelength or dependent?
- Circular or elliptic polarization?
- Is the light source (Sun) itself polarized?

Polarization of light experiments in the laboratory are much different; few measurements are needed to completely characterize the polarization of any light beam.

**Use of the Stokes vector-Mueller matrix approach**

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As the Mueller matrix of a perfect reflector is given by

\[
M = \begin{bmatrix}
1 & -\cos 2\psi & 0 & 0 \\
-\cos 2\psi & 1 & 0 & 0 \\
0 & 0 & \sin 2\psi \cos \Delta & \sin 2\psi \sin \Delta \\
0 & 0 & -\sin 2\psi \sin \Delta & \sin 2\psi \cos \Delta
\end{bmatrix}
\]

The Ellipsometric measurements \(\Psi, \Delta\) are limited when the reflector surface roughness becomes significant or in case of backside incoherent reflecting samples. Non diagonal null matrix elements are detected, i.e.

\[
M_{rf} = \begin{bmatrix}
1.028 & -0.015 & 0.004 & 0.078 \\
-0.013 & 0.603 & -0.157 & -0.111 \\
0.004 & -0.156 & 0.637 & 0.044 \\
0.077 & -0.112 & 0.043 & 0.685
\end{bmatrix}
\]

The Mueller decomposition has to be performed for different Mueller matrix classes.

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The Mueller matrix Decomposition: How to present experimental Data?

We adopted the classical representation of the state of polarized light, through the Poincaré sphere. Sample are studied such as one desire to know, the specific behaviour of the surface reflecting sample, or effect of the transmitted light coming from the samples. The Mueller matrix $M$ will give this information through the analysis comparing the Stokes vectors of the light $S,S'$ respectively before and after interaction with the sample, will be modified such as

$$
S' = [M] S
$$

$$
S = S_0 [1, \cos 2\epsilon \cos 2\theta, \cos 2\epsilon \sin 2\theta, \sin 2\epsilon]^T
$$

$$
M = \begin{bmatrix}
1/4 & 0 & 0 & 0 \\
0 & 1/4 & 0 & 0 \\
0 & 0 & 1/4 & 0 \\
0 & 0 & 0 & 1/4
\end{bmatrix}
$$

$$
M_{rf} = \begin{bmatrix}
1.028 & -0.015 & 0.004 & 0.078 \\
-0.013 & 0.603 & -0.157 & -0.111 \\
0.004 & -0.156 & 0.637 & 0.044 \\
0.077 & -0.112 & 0.043 & 0.685
\end{bmatrix}
$$

Normalized and $P<1$ (the dimmed sphere) and **Physically realizable** Mueller matrix

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**Mueller Matrix- F.Ferrieu**
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The pattern of polarization of light scattered by a silicon surface, shown in red, is a signature of the light scattering mechanism, in this case, microroughness.

<table>
<thead>
<tr>
<th>Polarization</th>
<th>Jones $u_{(xy)}$</th>
<th>Stokes $g$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Horizontal (H)</td>
<td>$[1 \ 0]^{T}$</td>
<td>$[1 \ 1 \ 0 \ 0]^{T}$</td>
</tr>
<tr>
<td>Vertical (V)</td>
<td>$[0 \ 1]^{T}$</td>
<td>$[1 \ -1 \ 0 \ 0]^{T}$</td>
</tr>
<tr>
<td>Linear $+45^\circ$</td>
<td>$1/\sqrt{2}[1 \ 1]^{T}$</td>
<td>$[1 \ 0 \ 1 \ 0]^{T}$</td>
</tr>
<tr>
<td>Linear $-45^\circ$</td>
<td>$1/\sqrt{2}[-1 \ 1]^{T}$</td>
<td>$[1 \ 0 \ -1 \ 0]^{T}$</td>
</tr>
<tr>
<td>Left circular</td>
<td>$1/\sqrt{2}[1 \ j]^{T}$</td>
<td>$[1 \ 0 \ 0 \ 1]^{T}$</td>
</tr>
<tr>
<td>Right circular</td>
<td>$1/\sqrt{2}[1 \ -j]^{T}$</td>
<td>$[1 \ 0 \ 0 \ -1]^{T}$</td>
</tr>
</tbody>
</table>

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\[ M = \begin{bmatrix}
    m_{00} & m_{01} & m_{02} & m_{03} \\
    m_{10} & m_{11} & m_{12} & m_{13} \\
    m_{20} & m_{21} & m_{22} & m_{23} \\
    m_{30} & m_{31} & m_{32} & m_{33}
\end{bmatrix} \]

✓ First problem: The Mueller Matrix physical realizability !!

\[ m_{00} \geq 0 \]
\[ m_{00} + m_{11} + m_{22} + m_{33} \geq 0 \]
\[ m_{00} + m_{11} - m_{22} - m_{33} \geq 0 \]
\[ m_{00} - m_{11} + m_{22} - m_{33} \geq 0 \]
\[ m_{00} - m_{11} - m_{22} + m_{33} \geq 0 \]
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The Mueller matrix \([M]\), can be analyzed and decomposed within targets. But there exists only one and only one decomposition scheme following:

\[
[M] = \gamma_1[M_1] + \gamma_2[M_2] + \gamma_3[M_3] +
\]

**QUESTIONS:**

- What are the weighting \(\gamma\) ?
- How many matrices \(M\) are necessary to represent the most general matrix \(M\)?
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The physical entities

- Jones Vectors
  \[ \mathbf{\varepsilon} = \begin{pmatrix} A_x \\ A_y e^{i\delta_y} \end{pmatrix} \]
  \[ \phi = \langle \mathbf{\varepsilon}(t) \otimes \mathbf{\varepsilon}^*(t) \rangle \]
  \[ \phi = \begin{bmatrix} (\varepsilon_1(t)\varepsilon_1^*(t)) & (\varepsilon_1(t)\varepsilon_2^*(t)) \\ (\varepsilon_2(t)\varepsilon_1^*(t)) & (\varepsilon_2(t)\varepsilon_2^*(t)) \end{bmatrix} = \begin{bmatrix} \sigma_0^2 & \mu \sigma_0 \sigma_1 \\ \mu^* \sigma_0 \sigma_1 & \sigma_1^2 \end{bmatrix} \]

- Correlation function

- Coherency matrix

- Coherency matrix for Stokes vector \( L \)
  \[ L = \begin{bmatrix} \langle t_0 t_0^* \rangle & \langle t_0 t_1^* \rangle & \langle t_1 t_0^* \rangle & \langle t_1 t_1^* \rangle \\ \langle t_0 t_2^* \rangle & \langle t_0 t_3^* \rangle & \langle t_1 t_2^* \rangle & \langle t_1 t_3^* \rangle \\ \langle t_2 t_0^* \rangle & \langle t_2 t_1^* \rangle & \langle t_3 t_0^* \rangle & \langle t_3 t_1^* \rangle \\ \langle t_2 t_2^* \rangle & \langle t_2 t_3^* \rangle & \langle t_3 t_2^* \rangle & \langle t_3 t_3^* \rangle \end{bmatrix} \]
where are two angles characterizing the polarization state

Considering two orthogonal base states the electric field will be written as

where \([u_2]\) is a 2x2 unitary matrix

we can generate a 3x3 real matrix \([O_3]\) as

\[
O_3 = \frac{1}{2} \text{Tr}([U_2]^T \cdot \sigma_p \cdot [U_2] \cdot \sigma_p)
\]

The real matrix \([O3]\) can operate on a real vector \(r\) and produce a rotated vector \(r'\) obtained by a rotation. In a real space, this equation is equivalent to:

\[
r' = [O_3] r
\]

Homomorphism \(S[U]2-> [O3]\)

Homomorphism \(S[U]4-> [O6]\) enable to relate the Mueller matrix to the coherence matrix
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By

Mueller/coherence matrix relation?

\[ [M] = \begin{bmatrix}
A_0 + B_0 & C + N & H + L & I + F \\
C - N & A + B & E + J & K + G \\
H - L & E - J & A - B & M + D \\
I - F & K - G & M - D & A_0 - B_0 \\
\end{bmatrix} = [m_{ij}] \]

Then

\[ H \equiv T \]

\[ \begin{bmatrix}
A_0 + A & C - iD & H + iG & I - iJ \\
C + iD & B_0 + B & E + iF & K - iL \\
H - iG & E - iF & B_0 - B & M + iN \\
I + iJ & K + iL & M - iN & A_0 - A \\
\end{bmatrix} = [h_{ij}] \]

Hermitian coherency matrix must real positive eigen values

\[ T = H = T^\dagger \text{ is fullfilled} \]

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Answer to our Problem

\[ H \equiv [T_c] = \lambda_0 [T_{c0}] + \lambda_1 [T_{c1}] + \lambda_2 [T_{c2}] + \lambda_3 [T_{c3}] + \]

✓ The weights are the eigen values of the Hermitian coherency matrix positive and real.

✓ There will be 4 targets given by the orthogonal eigen vectors from matrix linked to the general Mueller matrix.

✓ The constraint is that each one has only one associated Jones Matrix. In such a case the matrix has only positive and real Eigen values.
Matrix Filtering

Analysis of the experimental data following the coherence matrix

\[ H \equiv [T_c] = \lambda_0 [T_{c0}] + \lambda_1 [T_{c1}] + \lambda_2 [T_{c2}] + \lambda_3 [T_{c3}] \]

Example: If \( \lambda_3 \) turns to be a negative value:

- Reasonable to subtract the eigen vector contribution and

- Take the resulting filtered Matrix as the best estimate
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Filtering data $[M]$ always inside the Poincaré unit sphere

Experimental data
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PROCEDURE

- Physical Interpretation of the EigenValues
- Example: free space propagation

\[
M = \begin{bmatrix}
1.0000 & 0.000 & 0.000 & 0.000 \\
0.000 & 1.000 & 0.000 & 0.016 \\
0.0010 & 0.011 & 0.990 & 0.008 \\
-0.005 & -0.003 & -0.003 & 1.006
\end{bmatrix}
\]

Corresponding Coherency Matrix

\[\rho, \theta (\text{degrees}) \text{ arguments}\]

<table>
<thead>
<tr>
<th>Column1</th>
<th>Column2</th>
<th>Column3</th>
<th>Column4</th>
</tr>
</thead>
<tbody>
<tr>
<td>1998.000(0.00)</td>
<td>5.500(-90.00)</td>
<td>10.735(62.24)</td>
<td>6.042(114.44)</td>
</tr>
<tr>
<td>5.500(90.00)</td>
<td>2.000(0.00)</td>
<td>6.042(24.44)</td>
<td>8.201(37.57)</td>
</tr>
<tr>
<td>10.735(-62.2)</td>
<td>6.042(-24.44)</td>
<td>8.000(180.00)</td>
<td>2.500(0.00)</td>
</tr>
<tr>
<td>6.042(-114.4)</td>
<td>8.201(-37.57)</td>
<td>2.500(0.00)</td>
<td>8.000(0.00)</td>
</tr>
</tbody>
</table>

Eigen values: modules versus (dB) Instrument Fidelity

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Requested Procedure (followed)

Eigen Vectors:

\[ \lambda_0 \geq \lambda_1 \geq \lambda_2 \geq \lambda_3 \]

Scattering Matrix (Jones-Mueller)

\[
S = \begin{bmatrix} S_{xx} & S_{xy} \\ S_{yx} & S_{yy} \end{bmatrix} \begin{bmatrix} [S] = \begin{bmatrix} 1.000(0^\circ) & 0.003(-92^\circ) \\ 0.004(-92^\circ) & 1.0000(0^\circ) \end{bmatrix} \end{bmatrix}
\]

As published

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Depolarization- Surface analysis

✓ The Physical Interpretation of Eigen value Problems in optical scattering Polarimetry can be given evaluating the k Stocke vector.

For a stochastic system, as a 4 symbols Bernouilli process:
✓ the eigen vectors representing the possible states

\[ p_i = \frac{\lambda_i}{\sum_{j} \lambda_j} \]

✓ the normalized eigen values, the probabilities Pi, of the system being found in this state.

\[ \bar{\alpha} = \sum_{i} P_i \alpha_i \]

\[ = P_1 \alpha_1 + P_2 \alpha_2 + P_3 \alpha_3 + P_4 \alpha_4 \]
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- The randomness of the system is then characterized, defining the entropy $H$, in between 0 and 1

$$H = - \sum_{i=1}^{N} p_i \log_N p_i$$

Example: Isotropic Depolarizer one has $H=1$
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\[ depol = [M]_{00} - \frac{1}{3} \sqrt{\text{trace}[M][M]^T - [M]_{00}} \]

\[ \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & m & 0 & 0 \\ 0 & 0 & m & 0 \\ 0 & 0 & 0 & m \end{bmatrix} \quad m = \lambda_1 = \lambda_2 = \lambda_3 = \frac{d}{2} \]

\[ H = - \sum_{i=1}^{N} p_i \log_N p_i \quad p_D = \frac{1}{3} \sqrt{4 \sum_{i=0}^{3} p_i^2 - 1} = 1 - depol \]

Entropy limit: total depolarizer

\[ H = - \frac{(3p_D + 1)}{4} \log_4 \left( \frac{3p_D + 1}{4} \right) - 3(1 - p_D) \frac{1}{4} \log_4 \left( \frac{(1 - p_D)}{4} \right) \]
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Surfaces Analysis with different roughness from literature data

Experimental data:
(empty triangle and circles)
Leroy – Brehonnet (1997)

<table>
<thead>
<tr>
<th>Samples</th>
<th>Entropy</th>
<th>depolarization</th>
</tr>
</thead>
<tbody>
<tr>
<td>Dielectric C</td>
<td>0.9902</td>
<td>0.0935523</td>
</tr>
<tr>
<td>Nylon</td>
<td>0.9842</td>
<td>0.125090</td>
</tr>
<tr>
<td>Dielectric S</td>
<td>0.0381</td>
<td>0.990365</td>
</tr>
<tr>
<td>polished Al 0.3microns 500 nm</td>
<td>0.5941</td>
<td>0.658</td>
</tr>
<tr>
<td>(exp errors correc)</td>
<td>0.6183</td>
<td>0.64199690</td>
</tr>
</tbody>
</table>

\[ E = -\frac{(3p_D + 1)}{4}\log_4 \left( \frac{3p_D + 1}{4} \right) - 3(1 - p_D)/4\log_4((1 - p_D)/4) \]
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(a)

(b)

Entropy/pixel mapping

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Entropy/dePolarization index

Wavelengths(nm)

Depolarization

Polarimeter Fidelity

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free space

Diffuse reflector

Al mirror

Be scatter 20°,0
The distribution of the depolarized energy among the smaller eigenvalues contains important information about the structure of the surface such as roughness.

<table>
<thead>
<tr>
<th>Key information required for spectral analysis an/or surface mapping</th>
<th>Depolarization, Anisotropy index and surface scattering Entropy, Coherency</th>
<th>Comparison between Polarimeters can be performed</th>
</tr>
</thead>
</table>

Experimental data to be checked Physical realisability

Matrix filtering

Decomposition algorithm established

predominant Scattering: non depolarizing Mueller Jones Matrix

Polarimetric coherence can be introduced in term of the eigenvalue

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Spectroscopic Polarimetry of Light scattered By...

Rough Si wafer Bck side

Smooth wafer side

Entropy/Depolarization space

AOI=70°  Ψ unchanged  Δ shifts

2 sides Si Wafer data analysis

Mueller Matrix - F. Ferrieu

Analysis
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Surface Roughness and diffuse scattered light: The Si wafer example

Two approaches
• SPM (small perturbation model)
• Second order description of surface scatterers

Figure 3 Diagram for determining the phase difference between two parallel waves scattered from different points on a rough surface (SCHANDA 1980).
The first order SPM estimate. The Small Perturbation Model (SPM): 

\[ R_{sp} = R_{ps} \]

The scattering matrix \([S]\) for a Bragg surface is of the form:

\[
[S] = \begin{bmatrix} S_{HH} & S_{HV} \\ S_{VH} & S_{VV} \end{bmatrix} = [SS & SP] = m_s \begin{bmatrix} R_s(\theta, \varepsilon_s) & 0 \\ 0 & R_p(\theta, \varepsilon_s) \end{bmatrix}
\]

Second order perturbation model

(H is for s or TE polarized and V is p or TM polarized)

\[
[S_{ss} & S_{sp} \\ S_{ps} & S_{pp}] \Rightarrow k_p = Stokes_p = 1/\sqrt{2} [S_{HH} + S_{VV}, S_{HH} - S_{VV}, S_{HV} + S_{VH}, j(S_{HV} - S_{VH})]^T
\]

\[
T = (k_p, k_p^*) = 1/2 \begin{bmatrix} (|S_{HH} + S_{VV}|^2) & ((S_{HH} + S_{VV})(S_{HH} - S_{VV})^*) & 2((S_{HH} + S_{VV})S_{HV}^*) \\ ((S_{HH} - S_{VV})(S_{HH} + S_{VV})^*) & (|S_{HH} - S_{VV}|^2) & 2((S_{HH} - S_{VV})S_{HV}^*) \\ 2(S_{HV}(S_{HH} + S_{VV})^*) & 2(S_{HV}(S_{HH} - S_{VV})^*) & 4(|S_{HV}|^2) \end{bmatrix}
\]
with all the $R_{sp}$ values are zeroed. The corresponding normalized correlation

$$\gamma(HH + VV)(HH - VV) = \frac{[< (S_{HH} + S_{VV})(S_{HH} - S_{VV})^* >]}{\sqrt{[< |S_{HH} + S_{VV}|^2 >](< |S_{HH} - S_{VV}|^2 >)^*}}$$

$$= \frac{[< (R_s + R_p)(R_s - R_p)^* >]}{\sqrt{[< |R_s + R_p|^2 >](< |R_s - R_p|^2 >)^*}} = 1$$

coefficient is one, as a consequence the SPM cannot describe a depolarization effects.

The Polarimetric Surface scattering model.
The Polarimetric Surface scattering model.

Which surface is smoother? Each has the same roughness value...obviously a transverse parameter is needed.

Surface slope, $m$ seems a logical choice

Then Coherency Matrix appears as

$P(\beta) = \begin{cases} 1/2\beta_1 & |\beta| \leq \beta_1 \\ 0 & \text{otherwise} \end{cases}$

$[T] = \int_0^{2\pi} [T(\beta)]P(\beta)d\beta$

Configuration averaging over a uniform distribution of slopes

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\[
T(\beta) = \begin{bmatrix}
1 & 0 & 0 \\
0 & \cos 2\beta & \sin 2\beta \\
0 & -\sin 2\beta & \cos 2\beta \\
\end{bmatrix}
\begin{bmatrix}
\langle |R_s + R_p|^2 \rangle & \langle (R_s + R_p)(R_s - R_p)^* \rangle & 0 \\
\langle (R_s - R_p)(R_s + R_p)^* \rangle & \langle |R_s - R_p|^2 \rangle & 0 \\
0 & 0 & 0 \\
\end{bmatrix}
\begin{bmatrix}
1 & 0 & 0 \\
0 & \cos 2\beta & -\sin 2\beta \\
0 & \sin 2\beta & \cos 2\beta \\
\end{bmatrix}
\]

\[
T = \begin{bmatrix}
A & B \text{sinc}(2\beta_1) & 0 & 0 \\
B^* \text{sinc}(2\beta_1) & C(1 + \text{sinc}(4\beta_1)) & 0 & 0 \\
0 & 0 & 0 & 0 \\
0 & 0 & 0 & C(1 - \text{sinc}(4\beta_1)) \\
\end{bmatrix}
\]

- A, B, C are calculated from Fresnel-Bragg Rp, Rs i.e. \(A = |R_p + R_s|^2\),...
- \(\text{sinc}(2\beta_1) = \frac{\text{Sinc}(2\beta_1)}{2\beta_1}\),...are only roughness coefficients
- This Model intend to demonstrate that correlations coefficients can be only roughness dependant
- as other are pure smooth surface solution with \(\varepsilon\) of material
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\[
T = \langle k_p, k_p^* \rangle = \frac{1}{2} \begin{pmatrix}
|S_{HH} + S_{VV}|^2 & (S_{HH} + S_{VV})(S_{HH} - S_{VV})^* \\
(S_{HH} - S_{VV})(S_{HH} + S_{VV})^* & 2(S_{HH} - S_{VV}) S_{HV}^* \\
2(S_{HV}(S_{HH} + S_{VV})^*) & 2(S_{HV}(S_{HH} - S_{VV})^*)
\end{pmatrix}
\]

\[
\gamma(HH+VV)(HH-VV) = \frac{T_{12}}{\sqrt{T_{11} T_{22}}} = \text{sinc}(2\beta_1)/\sqrt{1 + \text{sinc}(4\beta_1)} \leq 1.
\]

Application: Si Wafer polished side and rough-back side

Figure 70° AOI measurement between 1.5 and 3 eV photon energies on both sides of a Silicon wafer (polished side with native oxide and rough backside of the wafer). The roughness and controls entirely the \(\gamma(HH+VV)(HH-VV)\) coherence.
Simulation literature: Examples

Monte Carlo techniques of surface roughness

For c-Si with different roughnesses (h,L)

Integral eq. Method (IEM)

Fig. 4. (b) degree of polarization, of bulk with different surface roughnesses simulated at different angles of incidence in the energy range of 1.5–3.5 eV. As in conventional ellipsometry, the output vector was collected at the specular reflected direction.
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- Si roughness references Surfaces
  - Metal surface modification and aging or under stress modification
  - Porous Silicon Bulk Scattering
  - Porous materials (low k) Diffuse

- Fibers Nanofilts,...
- Si Nano dots Mie scattering process
- Multistack diffuse roughness in optical filters

- Nanotechnology materials
Spectroscopic Polarimetry of Light scattered By...

The details of these oscillations are displayed by the general mathematical form of the Mueller matrices for polarizers and quarter wave plates.\(^3\) We have

for a linear polarizer

\[
\begin{bmatrix}
1 & 0 & 0 & 0 \\
0 & C_2 & C_2 S_2 & 0 \\
0 & -C_2 & C_2 S_2 & 0 \\
0 & 0 & 0 & 0
\end{bmatrix}
\]

for a quarter wave plate

\[
\begin{bmatrix}
1 & 0 & 0 & 0 \\
0 & C_2 & C_2 S_2 & - S_2 \\
0 & C_2 & C_2 S_2 & S_2^2 \\
0 & S_2 & -C_2 & 0
\end{bmatrix}
\]

where \(C_2 = \cos 2\phi, S_2 = \sin 2\phi, C_2^3 = \cos^2 2\phi,\) and \(S_2^3 = \sin^2 2\phi.\)

W. S. Bickel and W. M. Bailey

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Fig. 1. (Color online) Schematic of the polar nephelometer.