

Modeled Integrated Scattering Tool (MIST)

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The MIST program has been developed to provide users with a general application to model an integrated scattering system. The program performs an integration of the bidirectional reflectance distribution function (BRDF) over solid angles specified by the user and allows the dependence of these integrals on model parameters to be investigated. The models are provided by the SCATMECH library of scattering codes.

1. Introduction

Light scattering is widely used by scanning surface inspection tools to inspect materials, such as silicon wafers, flat panel display substrates, data storage media, and optics, for defects, particles, and surface roughness. These instruments often direct collimated or lightly-focused light at a sample and collect scattered light with one or more large optics. The optics collect light over significant solid angles in order to maximize sensitivity. When designing these instruments, it helps to be able to predict the signal for different geometric conditions and model parameters.

The BRDF characterizes the directional dependence of the scattering by a material. The BRDF is given by

$$f_r(\theta_i, \theta_s, \phi_s) = \lim_{\Omega \rightarrow 0} \frac{\Phi_s}{\Phi_i \Omega \cos \theta_s}, \quad (1)$$

where Φ_s is the power scattered into solid angle Ω , centered on polar angle θ_s and azimuth angle ϕ_s , and Φ_i is the power incident on the sample at an angle θ_i . The angles θ_i , θ_s , and ϕ_s are defined in Fig. 1. The function $f_r(\theta_i, \theta_s, \phi_s)$ also depends upon the polarization state of the incident light and the polarization sensitivity of the detection system. Any optic collecting light over a finite solid angle measures a reflectance given by

$$\rho(\Omega) = \int_{\Omega} f_r(\theta_i, \theta_s, \phi_s) \cos \theta_s d\Omega. \quad (2)$$

If we make a change of variables, $\xi = \theta_s \cos \phi_s$ and $\eta = \theta_s \sin \phi_s$, then Eq. 2 becomes

$$\rho(\Omega) = \int_{\Omega} f_r(\theta_i, \theta_s, \phi_s) \cos \theta_s \text{sinc} \theta_s d\xi d\eta \quad (3)$$

Eq. (3) is slightly easier to use than Eq. (2), since the differentials can be made more uniform over the collection aperture.

The MIST program uses theoretical models for the BRDF which are supplied by the SCATMECH library and calculates the quantity $\rho(\Omega)$ using Eq. (3) for geometries specified by the user. Furthermore, MIST allows the user to vary parameters in the model or in the definition of the solid angle, providing the user with the dependences on those parameters.

Besides using it as a design tool, one application of MIST is the development of calibration curves for an instrument. For example, the absolute response of an instrument to spherical particles can be accurately determined as a function of the particle size using the SCATMECH model **Bobbert_Vlieger_BRDF_Model**. If a set of reference particles are used to calibrate the instrument, then these calibration curves can be used to interpolate (or even extrapolate) to other particle sizes. The advantage of using a model-based calibration curve, over using non-physically-based interpolation techniques, is that it is more accurate and the calibration should not change if the set of reference particles changes. Furthermore, a smaller number of reference particles are needed for calibration, and over sampling of the calibration curve provides information about uncertainties in the measurement and can compensate for uncorrelated uncertainties in the reference particle diameters.

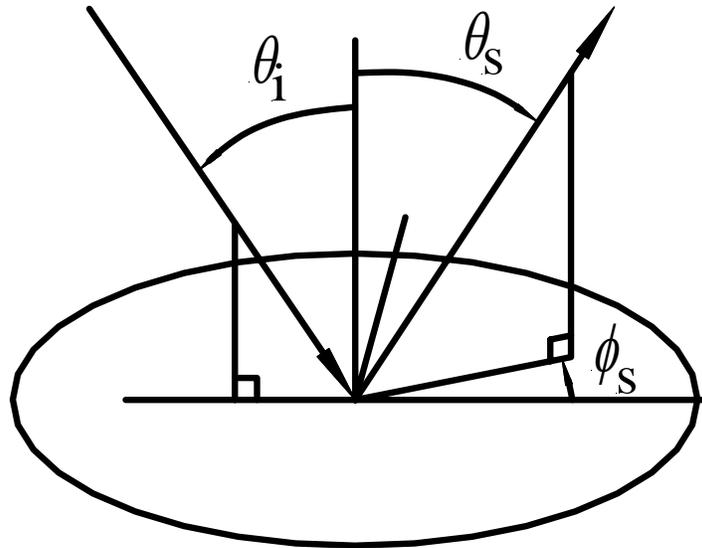


FIGURE 1 The scattering geometry and angle convention used by the calculations. The incident angle is θ_i . The scattering direction is defined by polar angle θ_s and azimuth angle ϕ_s .

2. Installing MIST

The MIST software package is supplied in a self-extracting executable file (**mistzip100.exe**). To install the software, the user should run the **mistzip100.exe** from a temporary directory. The program will create a directory (**C:\MIST** by default) and extract files into this directory.

3. Running MIST

MIST is a 32-bit Windows console application. To run MIST, open up a Command Prompt window and change to the MIST directory. From the command prompt, type

```
MIST inputfile.txt
```

where **inputfile.txt** is the name of a file containing program instructions, and press return. The program will follow the instructions given in **inputfile.txt** to calculate the reflectance into specified solid angles. The format of **inputfile.txt** is described in Section 4 of this documentation.

An alternate means for running MIST is provided by the WinMIST application. WinMIST is a simple program which allows the user to specify an input file, edit it using NOTEPAD, to run a simulation, and to copy the results to the clipboard. It has a simple interface providing five buttons:

Select Input File – Opens an open file dialog box enabling the user to select an input file.

Edit Input File – Opens the input file with NOTEPAD.

Run Simulation – Runs MIST using the selected file as input.

Results to Clipboard – Opens an open file dialog box enabling the user to select a file to copy to the Windows clipboard. The copied data can then be pasted into a spreadsheet.

Exit – Exits the WinMIST program.

4. Input File

The input file is an ASCII text file containing instructions necessary for MIST to determine the integrated reflectance. The file is divided into six sections as described and ordered below. Comments, which begin with a semicolon (;) and end at the end of a line, can be included anywhere in the file. The file is divided into tokens, which are strings of characters delimited by spaces. Tokens containing spaces

can be defined by surrounding them with pairs of double quotes ("*"*). All whitespace (e.g., spaces, tabs, and carriage returns) are otherwise ignored, allowing the file to be formatted as the user desires. The MIST program does not case-sensitively interpret its commands, but any SCATMECH model parameters must have the correct case.

4.1 MODEL Statement

The MODEL statement defines which SCATMECH BRDF model will be evaluated during integration. For example, the statement

```
MODEL = Bobbert_Vlieger_BRDF_Model
instructs MIST to use the SCATMECH model named Bobbert_Vlieger_BRDF_Model.
```

4.2 VARIABLES Section

The variables section contains declarations of any symbolic variables used by the program. It has the format

```
VARIABLES:
    variable1 = string1
    variable2 = string2
    ...
    variablen = stringn
END
```

Each *variable* is a unique name, and *string* is a string of characters having no spaces or other whitespace. The following are examples of declarations:

```
diameter = 0.1
pi = atan(1)*4
deg = pi/180
angle = 60*deg
q = sin(angle)
```

Each numeric variable is assigned its value in the order in which it was declared and before each integration step. The user may use formulas using common functions and operators.

Variables beginning with # (number sign) or \$ (dollar sign) have special meanings. Those that begin with # are evaluated to a numerical value, and sent to the SCATMECH model. Those that begin with \$ are left as a character string and sent to the SCATMECH model without interpretation. In both cases, the parameter name sent to the model has the preceding # or \$ removed. Since SCATMECH models are case-sensitive, the case of the variable must match that of the model parameter. Furthermore, the model parameter must be a valid parameter for the specified SCATMECH model. The following are examples of variables that are sent to the SCATMECH model:

```
#lambda = 0.488
#r = diameter/2
$substrate = (4.15,0.05)
```

Note that complex numbers (as for \$substrate above) must be transferred to the model as a string.

Four variables that must be declared are given in the following table:

Required Variables	
Variable	Description
DIFFERENTIAL	The approximate differential solid angle (in sr) used during the integration must be specified. The smaller this value, the longer the calculation will take, but the more accurate the results. A reasonable value for a fast calculation can be obtained by a value of 0.01.

MINSAMPLES	The minimum number of samples for any integration. If the solid angle of the integration is small compared to DIFFERENTIAL , then the program will use a smaller differential solid angle. It is best to set this value to about 10.
INCIDENTANGLE	The incident angle (in rad) of the incoming light.
INCIDENTPOL	The Stokes vector intensity for the incident light.

Stokes parameters are defined as for the SCATMECH library. In MIST, Stokes parameters consist of four comma-separated values between parentheses. For example, the following specifies *p*-polarized incident light:

```
INCIDENTPOL = (1,-1,0,0)
```

4.3 VARY Section

The MIST program will calculate the integrated reflectance as a function of any variable declared in the VARIABLES section. The VARY section declares which variables are varied from one integration to the next. Its format is

```
VARY:
  FOR variable1 FROM string1a TO string1b BY string1c
  ...
  FOR variable1 FROM stringna TO stringnb BY stringnc
END
```

where each string evaluates to a value. For example:

```
FOR #r FROM 0.01 TO 0.10 BY 0.01
```

The initial values for the variables given in the VARIABLES section are ignored. The first FOR statement specifies the slowest changing parameter (outer loop), while the last specifies the fastest (inner loop). All other variables are assigned their values after the varied parameters have their values assigned. Therefore, the following statements allow the program to vary diameter, even though the SCATMECH model requires a radius:

```
VARIABLES:
  diameter = 0      ; must declare variable
  #r = diameter/2   ; radius set to correspond to diameter
END

VARY:
  FOR diameter FROM 0.1 TO 1.0 BY 0.1 ; #r will vary, too.
END
```

4.4 INTEGRALS Section

The integrals section contains descriptions of each optical element in the system. Its format is

```
INTEGRALS:
  integral1 = shape1
    shape1parameter1 = string11
    shape1parameter2 = string12
    ...
    shape1parametern = string1n
  END
  ...
  integralm = shapem
    shapemparameter1 = stringm1
    shapemparameter2 = stringm2
    ...
    shapemparametern = stringmn
```

```

                END
    END

```

For example:

```

INTEGRALS:
Optic1 = CIRCLE
        CENTER = (0,0)
        ALPHA = 10*deg
        END
Optic2 = POLYGON
        VERTEX = (60*deg,45*deg)
        VERTEX = (60*deg,135*deg)
        VERTEX = (60*deg,-135*deg)
        VERTEX = (60*deg,-45*deg)
        END
    END

```

Each integral is given a name (**Optic1** and **Optic2** in the above example). The result of each integration is placed into a variable having the name of the integral. There are three different types of integration shapes: hemispheres, circles, and polygons.

Directions are specified as pairs of values, separated by a comma and surrounded by parentheses. The first value is interpreted as the polar angle and the second as the azimuth angle. For example, the direction

(45*deg, 0*deg)

specifies a direction with $\theta_s = 45^\circ$ and $\phi_s = 0^\circ$.

Evaluation of any expression on the right-hand side of an assignment occurs before each integration step and can use any of the variables defined in the VARIABLES section.

Specific arguments for each integration type are as follows:

4.4.1 The hemispherical collection element—A **HEMI** element collects light over the entire reflection hemisphere. There are no parameters.

4.4.2 The circular collection element—A **CIRCLE** element collects light over a right circular cone. The valid parameters, with their default values, are given in the following table:

CIRCLE Parameters		
Parameter	Default Value	Description
CENTER	(0,0)	Direction of the center of the circular cone
ALPHA	0	Half angle of the circular cone
POL	(1,0,0,0)	The Stokes sensitivity at the center of the circular cone

4.4.3 The polygonal collection element—A **POLYGON** element collects light over a cone having an arbitrary number of straight sides. The sides of the polygon are straight as viewed from the reflectance sphere projected onto the surface plane (see Appendix). The vertices are specified along the polygon through successive VERTEX commands. The valid arguments, with their default values, are given in the following table:

POLYGON Parameters		
Parameter	Default Value	Description
VERTEX	N/A	A direction defining a corner of the polygon.

POL	(1,0,0,0)	The Stokes sensitivity at the center of the circular cone
POLCENTER	(0,0)	The direction for which the polarization is defined

4.5 OUTPUTS Section

The OUTPUTS section provides an enumerated list of the algorithms used to compute the columns of the output data. Its format is

```

OUTPUTS:
  1 string1
  ...
  n stringn
END

```

Since one sometimes is interested in the sum of the signals from several elements, or the ratio of the signals from two elements, the OUTPUTS section allows one to define the specific combinations that the user may be interested in. Any of the variables defined in the VARIABLES or INTEGRALS sections may be used in the calculation of the final outputs. In the following example, where there were two integrals (call **Optic1** and **Optic2**, as above), each of the individual signals and their ratio will be output to the results file:

```

OUTPUTS:
  1 Optic1
  2 Optic2
  3 Optic1/Optic2
END

```

The first columns of the output file are always the parameters defined in the VARY section. The subsequent columns are the values specified in the OUTPUTS section.

4.6 FILES Section

The files section defines the names of the files that the results are stored in. Its format is:

```

FILES:
  RESULTS = filename1
  SAMPLES = filename2
  LISTING = filename3
  HEADER = string1
  ...
  HEADER = stringn
END

```

There are three different types of output files: the results file, the samples file, and the listing file. There may be as many header strings as desired, and the header strings are best surrounded by double quotes ("), since the user may want to include spaces in the header text. The results file contains tab-delimited columns of numbers giving the results of the calculation (defined in the OUTPUTS section). The results file begins with the header strings, followed by a line with strings defining each column. The samples file contains tab-delimited columns of numbers providing the directions sampled during the first integration step. The first line of the samples file contains column labels. The samples file can be used to check that the optics have been defined correctly. The listing file contains information about the calculation, including each time a parameter is set in the model.

5. Examples

A series of NISTMIST input files are available to aid users in writing specific input files for their applications. In particular, the distribution includes input files for each SCATMECH model, and parameters are defined specific to each model. The example files are given names which are the SCATMECH model name with the extension **.txt**. For example, the input file **Bobbert_Vlieger_BRDF_Model.txt** calculates scattering using the SCATMECH class

Bobbert_Vlieger_BRDF_Model. The example input files all calculate the reflectance into two different solid angles shown in Fig. 2 as a function of incident angle and for p-polarized light. The following table is a list of the example input files:

Example input files
Bobbert_Vlieger_BRDF_Model.txt
Correlated_Roughness_BRDF_Model.txt
Correlated_Roughness_Stack_BRDF_Model.txt
Diffuse_Subsurface_BRDF_Model.txt
Double_Interaction_BRDF_Model.txt
Facet_BRDF_Model.txt
First_Diffuse_BRDF_Model.txt
Lambertian_BRDF_Model.txt
Microroughness_BRDF_Model.txt
OneLayer_BRDF_Model.txt
Rayleigh_Defect_BRDF_Model.txt
Roughness_Stack_BRDF_Model.txt
Shadowed_Facet_BRDF_Model.txt
Subsurface_Facet_BRDF_Model.txt
Subsurface_Sphere_BRDF_Model.txt
Two_Face_BRDF_Model.txt
Uncorrelated_Roughness_Stack_BRDF_Model.txt

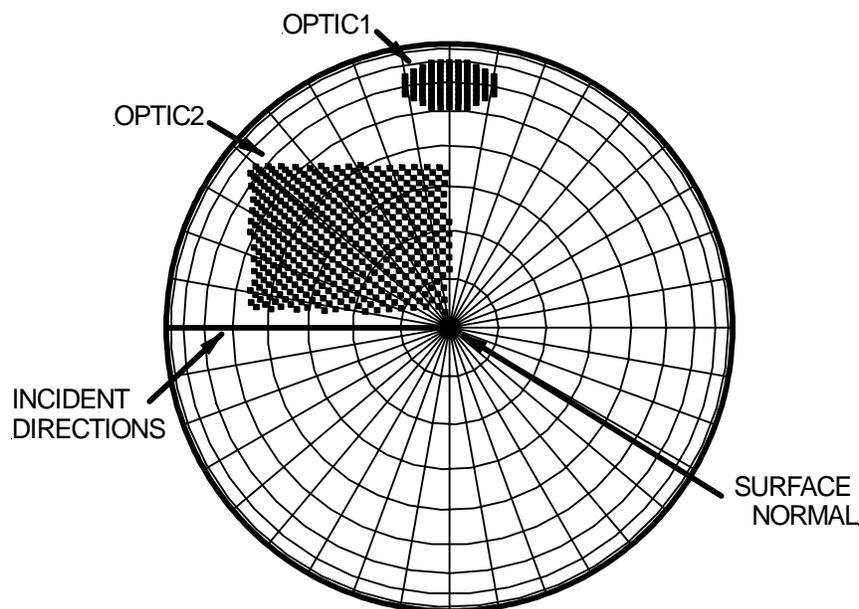


FIGURE 2 The sampled points used by the example programs. The incident directions are shown as the solid horizontal line. The scattered directions are shown as the points.

6. Accuracy

While most of the BRDF models contained in the SCATMECH library are based upon physical principles, most are approximations that have a limited range of accuracy. It is up to the user to assess the accuracy of each model to determine if the results he or she obtains are of quantitative value or are just qualitative guides to data trends.

Aside from the intrinsic accuracy of the particular model, the accuracy of the integration depends upon the values of the variables **SOLIDANGLE** and **MINSAMPLES**, any structure in the scattering within the integration solid angle, and the shape of the integration solid angle. The program chooses the number of sampled points by dividing the solid angle of a right circular cone that circumscribes the integration solid angle by the variable **SOLIDANGLE**, assuring that this value is above **MINSAMPLES**. It then samples directions on a square grid within this right circular cone. If the point is outside of the integration solid angle, it returns zero intensity for that direction. The results are adjusted by the ratio of the calculated projected solid angle (as determined by the sampled points) and the actual projected solid angle of the desired shape, as determined by a path integral around the perimeter.

7. Other Notes

7.1 Specifying material properties

In all of the examples, complex material indices of refraction are specified by constant values. The SCATMECH library, however, allows the use of external files which contain the optical constants as functions of wavelength. Such a file should be a text file containing three tab-delimited columns, in which the first column represents the wavelength, the second column the index of refraction, and the third column the absorption coefficient. The optical properties of the substrate, for example, can then be specified by the variable declaration

```
$substrate = silicon.txt
```

where **silicon.txt** is such a text file. In this manner, the VARY section statement

```
FOR #lambda FROM 0.2 TO 0.8 BY 0.02
```

will allow the reflectance to be calculated over a variety of wavelengths even though the optical properties of the substrate are wavelength dependent.

At this time, there is no way to vary the optical properties of a material numerically, unless that material has a negligible absorption coefficient.

7.2 Redirection of the input file

The input file can redirect its input at the beginning of any line by using a less-than character (<) followed by a filename:

```
<newfile.txt
```

MIST will then begin reading from newfile.txt until it reaches a line beginning with a greater-than character (>). For example, the file **newfile.txt** may contain a section of the MIST input that the user never intends to change:

```
FILES:  
  RESULTS = results.dat  
  SAMPLES = samples.dat  
  LISTING = listing.txt  
END  
>
```

Thus, the FILES section can be replaced by a simplified statement. Another application of redirection may include the specification of a specific instrument geometry. Then a file named instrument.txt may contain the INTEGRALS and OUTPUTS section appropriate for that instrument.

7.3 Use of Local BRDF Models

Any of the SCATMECH models which inherit the class **Local_BRDF_Model** (such as **Bobbert_Vlieger_BRDF_Model** or **Rayleigh_Defect_BRDF_Model**) calculate the differential scattering cross-section (DSC) rather than the BRDF. The class **Local_BRDF_Model** uses the parameter **density** to convert the DSC to BRDF. If one is interested in the integrated cross section for an isolated particle or defect, then one should set this parameter by

```
#density = cos(INCIDENTANGLE)
```

If, instead, one is interested in a net effective reflectance, when the effective beam radius is w , then one should set this parameter by

```
w = 12           ; beam radius in micrometers
area = pi*w^2
#density = cos(INCIDENTANGLE)/area
```

7.4 Using MIST to Calculate Integrated Scatter by Isolated Spheres

While MIST was not designed with isolated spheres in mind, with a little insight and knowledge of the SCATMECH models, it can effectively be used for such. If the incident angle is 90° , the transmission hemisphere will be symmetric with the reflection hemisphere. The subsurface sphere model effectively performs the scattering by a free space sphere embedded in a transparent substrate, but, the density must be set to a value close to, but not equal to 90° . The example file `mie.txt` is provided.

7.5 Using MIST to Calculate BRDF

MIST can be used to calculate BRDF by using Eq. (1). The following INTEGRALS and OUTPUTS sections will calculate the BRDF as a function of scattering angle (assuming a variable named `thetas`):

```
INTEGRALS:
    scatter = CIRCLE
            CENTER = (thetas,0)
            ALPHA = 0.1*deg
            END
END
OUTPUTS:
    1 scatter/(cos(incidentangle)*pi*(0.1*deg)^2)
END
```

8. Legal Disclaimer

The MIST and SCATMECH software packages were developed at the National Institute of Standards and Technology by employees of the Federal Government in the course of their official duties. Pursuant to Title 17 Section 105 of the United States Code this software is not subject to copyright protection and is in the public domain. NISTMIST and SCATMECH are experimental systems. NIST assumes no responsibility whatsoever for its use by other parties, and makes no guarantees, expressed or implied, about its quality, reliability, or any other characteristic. We would appreciate acknowledgment if the software is used. This software can be redistributed and/or modified freely provided that any derivative works bear some notice that they are derived from it, and any modified versions bear some notice that they have been modified.

9. Registering MIST

Registration of the NISTMIST program is voluntary and enables you to be notified when new versions are released. It also enables you to provide feedback that helps us improve the library and its documentation. To register, send an e-mail message to `thomas.germer@nist.gov`, indicating your interest in registering your copy of the software.

10. Source Code

MIST was written in C++. The source code is included in the software distribution. The code is intended to be linked with the SCATMECH library.

APPENDIX

Figure 3 provides a graph of the spherical coordinates of the reflectance hemisphere. This diagram is useful for planning calculations.

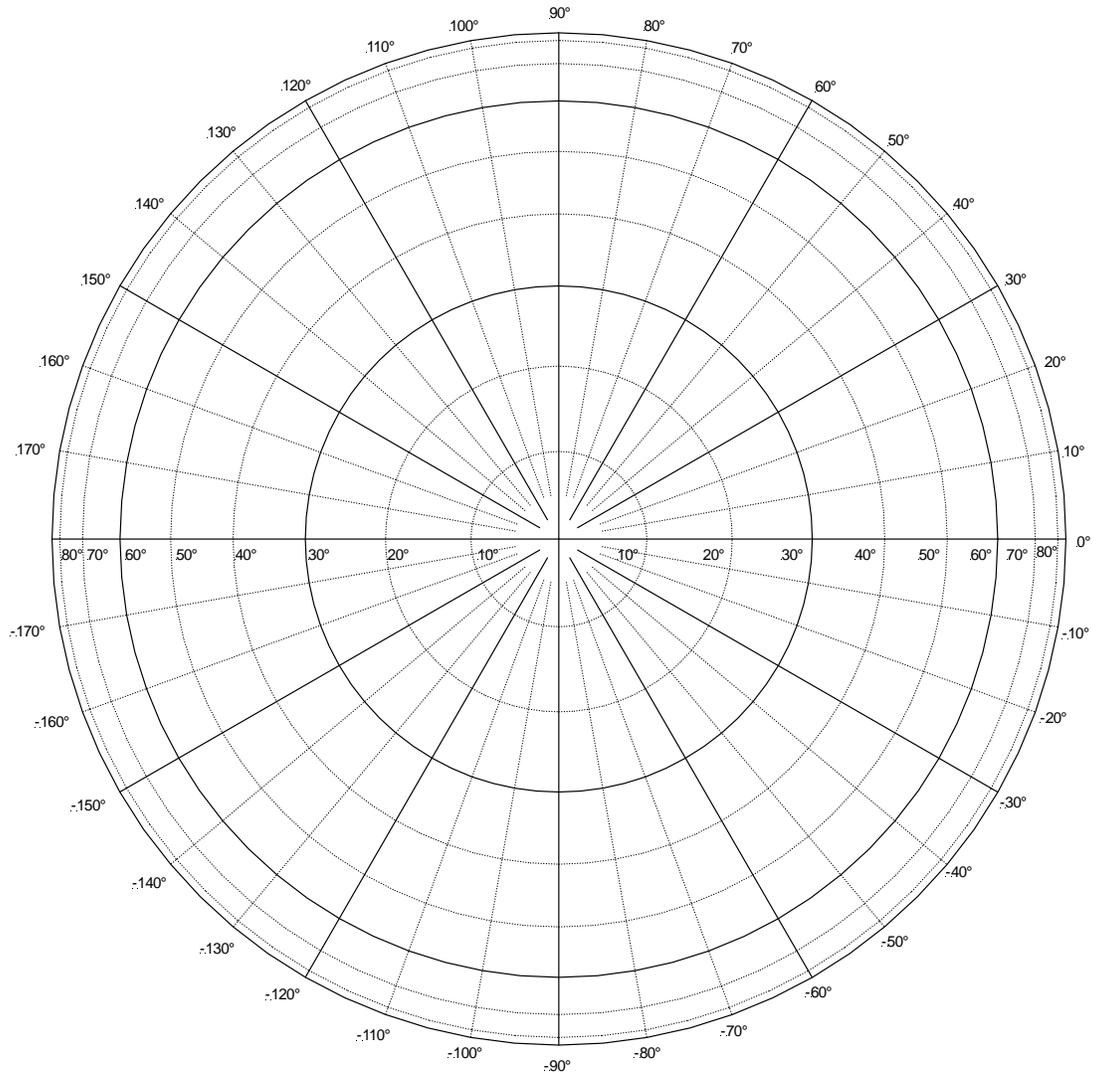


FIGURE 3 The reflectance hemisphere.