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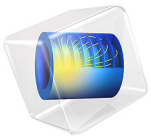

Rowland Circle Spectrometer

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Introduction

The Rowland circle is a circle of radius R that lies tangent to a concave curved diffraction grating of radius $2R$. The basic concept is illustrated in Figure 1; the Rowland circle itself and the concave grating are illustrated by the long and short solid black lines, respectively.

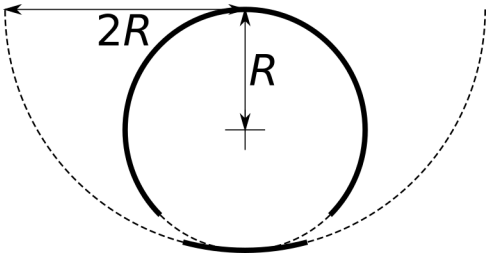

Figure 1: The Rowland circle.

If light enters through a narrow slit located anywhere along the Rowland circle and hits the diffraction grating, then the reflected light will be focused at some point along the same circle. If the incoming light is polychromatic, then the direction of the reflected light is a function of the wavelength and the diffraction order.

This tutorial model of a basic 2D Rowland circle spectrometer demonstrates how to define concave curved diffraction gratings using the **Grating** node, trace polychromatic light, specify which diffraction orders to release, and record the diffraction orders of released rays using an **Auxiliary Dependent Variable** node.

Model Definition

This tutorial model uses the Geometrical Optics interface to trace rays in a simple 2D geometry. The vacuum wavelength of the released light follows a uniform distribution between 400 nm and 700 nm. The built-in **Grating** boundary condition automatically detects which diffraction orders might be released, and a user-defined **Auxiliary Dependent Variable** is used to record which diffraction order each ray corresponds to.

RELEASE OF POLYCHROMATIC LIGHT

By default, the rays in a Geometrical Optics model are monochromatic. In this example, a distribution of wavelengths is released by selecting **Polychromatic, specify vacuum wavelength** from the **Wavelength distribution of released rays** list in the physics interface **Ray Release and Propagation** section. Then, in ray release features (such as **Release from Grid**), you can specify whether the released rays all have the same wavelength, a list of wavelength values, or values sampled from a normal, lognormal, or uniform distribution.

GRATING EQUATION

Some diffraction gratings can release both transmitted and reflected rays of various diffraction orders. This model concerns a purely reflective grating, so the transmitted orders are ignored.

The fundamental equation of rays reflected by a diffraction grating is

$$\frac{m\lambda}{d} = \sin\beta_m - \sin\alpha \tag{1}$$

where

- m (dimensionless integer) is the diffraction order,
- λ (SI unit: m) is the wavelength,
- d (SI unit: m) is the spacing between successive grooves or unit cells in the grating,
- α (SI unit: rad) is the angle of incidence, and
- β_m (SI unit: rad) is the angle of reflection of the mth diffraction order.

Here λ should not be confused with the vacuum wavelength λ_0; if the incident and reflected ray propagate through a medium with refractive index $n \neq 1$, then $\lambda = \lambda_0/n$.

In addition, different authors will use different sign conventions to designate positive or negative diffraction orders, or to indicate whether the angles of reflection should be positive or negative. The sign convention used here is such that the angle of incidence is positive, the angle or reflection for the 0th order (specular reflection) is positive ($\beta_0 = \alpha$), and higher positive diffraction orders bend farther away from the surface normal.

The **Grating constant** d that you specify in this model is actually somewhat smaller than the value of d used in Equation 1. For concave curved gratings, the classical interpretation of the grating constant is the projected distance between grooves in a tangent plane.

EXISTENCE OF DIFFRACTION ORDERS

A given diffraction order can exist if the value of m permits real values of α and β_m in Equation 1. If light can hit the grating from any direction, then this requirement can be expressed as

$$\left|\frac{m\lambda}{d}\right| < 2$$

If the angle of incidence α is known, then a stricter requirement can be applied,

$$\left|\frac{m\lambda}{d}\right| < 1 + |\sin\alpha| \tag{2}$$

The above formulas only indicate whether light of a certain diffraction order can be released at all. Even if a certain diffraction order can be released for some values of the angle of incidence, it might not be permitted for all values. In addition, these formulas alone cannot determine the relative intensity of rays of different diffraction orders, which would require a more in-depth understanding of the unit cell structure.

The Geometrical Optics interface is usable when the wavelength of radiation is much smaller than even the smallest geometric details in the model. Taking this requirement literally, it would seem impossible to use ray optics simulation to model diffraction gratings, which have details comparable to the wavelength. Instead of explicitly modeling the grating geometry on such a small scale, diffraction gratings are implemented using the **Grating** boundary condition, which takes a lumped approach by only tracing rays of each discrete diffraction order while not attempting to predict the pattern of evanescent waves in the near vicinity of the grating. When a ray hits the grating surface, then it is split into multiple reflected and/or transmitted rays depending on the number of **Diffraction Order** subnodes that have been added to the parent **Grating** node.

In the settings for the **Grating** node in the Geometrical Optics interface, a section called **Automatic Diffraction Order Calculation** is shown. You can click the **Add Diffraction Orders** button to automatically create a **Diffraction Order** subnode for every value of m that satisfies Equation 2.

ALLOCATION OF SECONDARY RAYS

If the **Grating** node has at least two **Diffraction Order** subnodes (or at least one **Diffraction Order** subnode with both reflected and transmitted diffraction orders released), then the degrees of freedom corresponding to the incident ray will be used to trace either the transmitted or reflected ray of the first **Diffraction Order** subnode to appear. All other orders must be traced using secondary rays.

In the Geometrical Optics interface, a secondary ray is a ray whose position and direction are not specified directly, but are instead triggered by the interaction of an existing ray with a boundary condition in the model. For example, during a deterministic ray split at a **Material Discontinuity** boundary, the refracted ray uses the incident ray's degrees of freedom, while the reflected ray is a secondary ray. Because a single ray can produce rays of many different diffraction order, the **Grating** boundary condition can potentially use up a large number of secondary rays.

You can specify the **Maximum number of secondary rays** in the physics interface **Ray Release and Propagation** section. If this number of secondary rays is reached, then the model will stop producing rays of higher diffraction orders, and a warning will be given when the study concludes.

RECORDING DIFFRACTION ORDERS

In this example an **Auxiliary Dependent Variable** node is used to store information about the diffraction order of each released ray. For every **Auxiliary Dependent Variable** node added to the model, the number of degrees of freedom solved for increases by 1 per ray. Optionally, you can enter a **Source**, i.e. a time derivative for these variables. In this example, the time derivative is zero so the auxiliary variable just stores information about which **Diffraction Order** subnode released each ray.

Results and Discussion

A Ray Trajectories plot is shown in Figure 2. The color expression on the rays indicates their diffraction order. The incident rays are the orange-colored rays entering from the top left and propagating towards the grating on the bottom; the orange-colored rays propagating towards the top right are the reflected rays of order 0.

A similar Ray Trajectories plot is shown in Figure 3, except that the color expression is now the wavelength of the rays. A plot **Filter** has been used to replace the incident rays and the reflected zero-order rays with thick black lines, since otherwise they could have any arbitrary color (since the $m = 0$ order does not separate rays by wavelength).

From both Figure 2 and Figure 3 it is evident that the rays of diffraction orders $m = -2$ and $m = -3$ overlap near the left side of the Rowland circle. Another way of visualizing this overlap is with a 2D **Histogram** plot, as shown in Figure 4. In this plot, the horizontal axis is the sector angle where the reflected rays hit the Rowland circle, while the vertical axis is their diffraction order. Columns with two or more nonzero entries carry some risk of overlapping diffraction orders. Comparison with the ray diagrams suggests that the overlap between the $m = -2$ and $m = -3$ orders is real, while the apparent overlap between the $m = 1$ and $m = 2$ orders may just be an artifact of the finite number of bins used in this histogram. Increasing the number of wavelengths in the model, and the number of bins in the x-direction, should assuage any concerns about overlap between these orders.

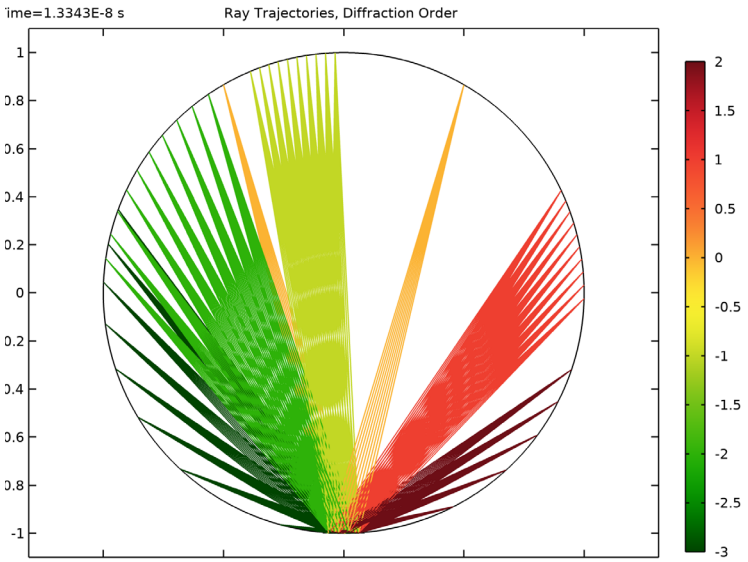

Figure 2: Ray diagram. The color expression represents diffraction order.

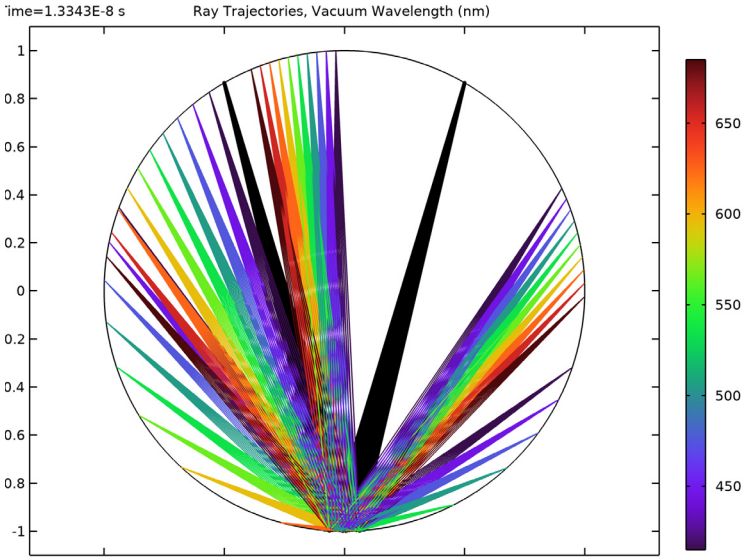

Figure 3: Ray diagram. The color represents the vacuum wavelength of each ray, except that incident rays and those of zero diffraction order are colored black.

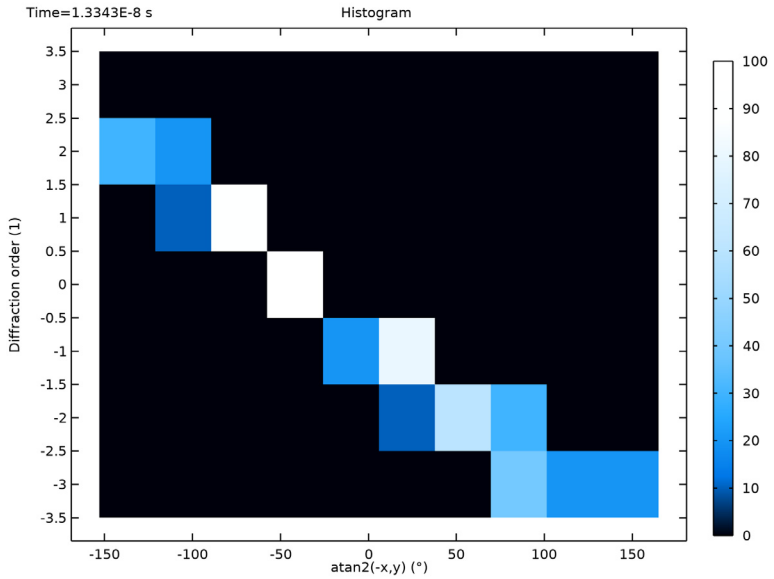

Figure 4: 2D Histogram plot comparing the sector angle of reflected rays, measured counterclockwise from the positive y-axis, to their diffraction order.

Application Library path: `Ray_Optics_Module/Tutorials/rowland_circle_spectrometer`

Modeling Instructions

From the **File** menu, choose **New**.

NEW

In the **New** window, click **Model Wizard**.

MODEL WIZARD

1 In the **Model Wizard** window, click **2D**.

2 In the **Select Physics** tree, select **Optics>Ray Optics>Geometrical Optics (gop)**.

3 Click **Add**.

4 Click **Study**.

5 In the **Select Study** tree, select **Preset Studies for Selected Physics Interfaces>Ray Tracing**.

6 Click **Done**.

GLOBAL DEFINITIONS

Parameters 1

1 In the **Model Builder** window, under **Global Definitions** click **Parameters 1**.

2 In the **Settings** window for **Parameters**, locate the **Parameters** section.

3 In the table, enter the following settings:

Name	Expression	Value	Description
R	1[m]	1 m	Rowland circle radius
alpha	5[deg]	0.087266 rad	Grating sector angle
phi0	30[deg]	0.5236 rad	Release angle (+CCW)

COMPONENT 1 (COMP1)

1 In the **Model Builder** window, click **Component 1 (comp1)**.

2 In the **Settings** window for **Component**, locate the **Curved Mesh Elements** section.

3 From the **Geometry shape function** list, choose **Cubic Lagrange**. The ray tracing algorithm used by the Geometrical Optics interface computes the refracted ray direction based on a discretized geometry via the underlying finite element mesh. A cubic geometry shape order usually introduces less discretization error compared to the default, which uses linear and quadratic polynomials.

GEOMETRY 1

Circle 1 (c1)

1 In the **Geometry** toolbar, click **Circle**.

2 In the **Settings** window for **Circle**, locate the **Object Type** section.

3 From the **Type** list, choose **Curve**.

4 Locate the **Size and Shape** section. In the **Radius** text field, type `R`.

5 In the **Sector angle** text field, type `360-2*alpha`.

6 Locate the **Rotation Angle** section. In the **Rotation** text field, type `-90+alpha`.

Circle 2 (c2)

1 In the **Geometry** toolbar, click **Circle**.

2 In the **Settings** window for **Circle**, locate the **Object Type** section.

3 From the **Type** list, choose **Curve**.

4 Locate the **Size and Shape** section. In the **Radius** text field, type `2*R`.

5 In the **Sector angle** text field, type `alpha`.

6 Locate the **Position** section. In the **y** text field, type `R`.

7 Locate the **Rotation Angle** section. In the **Rotation** text field, type `270-alpha/2`.

Delete Entities 1 (del1)

1 In the **Geometry** toolbar, click **Delete**.

2 In the **Settings** window for **Delete Entities**, locate the **Entities or Objects to Delete** section.

3 From the **Geometric entity level** list, choose **Boundary**.

4 On the object **c1**, select Boundaries 5 and 6 only.

5 On the object **c2**, select Boundaries 2 and 3 only.

These selected edges are the radii that bound each of the two circular arcs.

6 Click **Build All Objects**.

7 Click the **Zoom Extents** button in the **Graphics** toolbar.

GEOMETRICAL OPTICS (GOP)

By default monochromatic light will be traced. A quick adjustment to the physics interface settings will allow light to be released with a distribution of different wavelengths.

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Geometrical Optics (gop)**.

2 In the **Settings** window for **Geometrical Optics**, locate the **Ray Release and Propagation** section.

3 From the **Wavelength distribution of released rays** list, choose **Polychromatic, specify vacuum wavelength**.

4 Select the **Use geometry normals for ray-boundary interactions** check box.

Next add an **Auxiliary Dependent Variable**, an extra degree of freedom to track the diffraction order of each released secondary ray.

Auxiliary Dependent Variable 1

1 In the **Physics** toolbar, click **Global** and choose **Auxiliary Dependent Variable**.

2 In the **Settings** window for **Auxiliary Dependent Variable**, locate the **Auxiliary Dependent Variable** section.

3 In the **Field variable name** text field, type `m`.

Optionally a derivative with respect to time or optical path length can be specified in the **Source** field. In this example, the default of 0 will be used so that the variable does not change after the secondary rays are released.

Release from Grid 1

1 In the **Physics** toolbar, click **Global** and choose **Release from Grid**.

2 In the **Settings** window for **Release from Grid**, locate the **Initial Coordinates** section.

3 In the $q_{x,0}$ text field, type `-R*sin(phi0)`.

4 In the $q_{y,0}$ text field, type `R*cos(phi0)`.

5 Click **Preview Initial Coordinates** in the upper-right corner of the **Initial Coordinates** section. A red dot will be shown in the Graphics window, marking the location of the entrance pupil on the Rowland circle.

6 Locate the **Ray Direction Vector** section. From the **Ray direction vector** list, choose **Conical**.

7 In the N_w text field, type `10`.

8 Specify the **r** vector as

`-x`	`x`
`-(y+R)`	`y`

This expression for the cone axis will aim the incoming light at the center of the concave grating which will be located at the bottom of the Rowland circle.

9 In the α text field, type `2[deg]`.

10 Locate the **Vacuum Wavelength** section. From the **Distribution function** list, choose **Uniform**.

The default values of the minimum and maximum wavelength cover most of the visible part of the electromagnetic spectrum.

11 In the N text field, type `10`.

Grating 1

1 In the **Physics** toolbar, click **Boundaries** and choose **Grating**.

2 Select Boundary 3 only.

3 In the **Settings** window for **Grating**, locate the **Device Properties** section.

4 From the **Rays to release** list, choose **Reflected**.

5 In the d text field, type `1.5[um]`.

6 From the **Interpretation of grating constant** list, choose **Projected unit cell width**.

7 Locate the **Automatic Diffraction Order Calculation** section. Click **Add Diffraction Orders**.

Clicking the **Add Diffraction Orders** button will cause a set of **Diffraction Order** subnodes to be created.

INITIALIZING AUXILIARY VARIABLES FOR SECONDARY RAYS

For each of the **Diffraction Order** subnodes, repeat the following steps:

1 In the **Model Builder** window, click **Diffraction Order (m = -3)**.

2 Expand the **Auxiliary Dependent Variables, Reflected Ray** section.

3 Select the **Assign new value to auxiliary variable : m** check box.

4 In the text field, enter a numeric value corresponding to the diffraction order. For example, for the **Diffraction Order (m = -3)** node, type `-3`.

Wall 1

1 In the **Physics** toolbar, click **Boundaries** and choose **Wall**.

2 Select Boundaries 1, 2, 4, and 5 only.

3 Keep the default value from the **Wall condition** list, **Freeze**. Rays that hit the selected boundaries will stop propagating, but their final positions will still be available for postprocessing.

MESH 1

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Mesh 1**.

2 In the **Settings** window for **Mesh**, locate the **Physics-Controlled Mesh** section.

3 From the **Element size** list, choose **Extremely fine**.

4 Click **Build All**.

STUDY 1

Step 1: Ray Tracing

1 In the **Model Builder** window, under **Study 1** click **Step 1: Ray Tracing**.

2 In the **Settings** window for **Ray Tracing**, locate the **Study Settings** section.

3 From the **Time-step specification** list, choose **Specify maximum path length**.

4 In the **Lengths** text field, type `0 4*R`.

5 In the **Home** toolbar, click **Compute**.

RESULTS

Ray Trajectories, Diffraction Order

1 In the **Settings** window for **2D Plot Group**, type `Ray Trajectories, Diffraction Order` in the **Label** text field.

2 Click to expand the **Title** section. From the **Title type** list, choose **Label**.

3 In the **Model Builder** window, expand the **Ray Trajectories, Diffraction Order** node.

Color Expression 1

1 In the **Model Builder** window, expand the **Results>Ray Trajectories, Diffraction Order> Ray Trajectories 1** node, then click **Color Expression 1**.

2 In the **Settings** window for **Color Expression**, locate the **Expression** section.

3 In the **Expression** text field, type `m`.

4 Select the **Description** check box.

5 In the associated text field, type `Diffraction order number`.

6 Locate the **Coloring and Style** section. From the **Color table** list, choose **Traffic**.

7 In the **Ray Trajectories, Diffraction Order** toolbar, click **Plot**. Compare the resulting image to Figure 2.

Ray Trajectories, Vacuum Wavelength (nm)

1 In the **Model Builder** window, right-click **Ray Trajectories, Diffraction Order** and choose **Duplicate**.

2 In the **Settings** window for **2D Plot Group**, type `Ray Trajectories, Vacuum Wavelength (nm)` in the **Label** text field.

3 In the **Model Builder** window, expand the **Ray Trajectories, Vacuum Wavelength (nm)** node.

Color Expression 1

1 In the **Model Builder** window, expand the **Results>Ray Trajectories, Vacuum Wavelength (nm)>Ray Trajectories 1** node, then click **Color Expression 1**.

2 In the **Settings** window for **Color Expression**, click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Component 1 (comp1)> Geometrical Optics>Ray properties>gop.lambda0 - Vacuum wavelength - m**.

3 Locate the **Expression** section. From the **Unit** list, choose **nm**.

4 Locate the **Coloring and Style** section. From the **Color table** list, choose **Spectrum**.

Filter 1

1 In the **Model Builder** window, click **Filter 1**.

2 In the **Settings** window for **Filter**, locate the **Ray Selection** section.

3 From the **Rays to include** list, choose **Logical expression**.

4 In the **Logical expression for inclusion** text field, type `m!=0`.

Ray Trajectories, Vacuum Wavelength (nm)

In the **Model Builder** window, under **Results** click **Ray Trajectories, Vacuum Wavelength (nm)**.

Ray Trajectories 2

1 In the **Ray Trajectories, Vacuum Wavelength (nm)** toolbar, click **More Plots** and choose **Ray Trajectories**.

2 In the **Settings** window for **Ray Trajectories**, locate the **Coloring and Style** section.

3 Find the **Line style** subsection. From the **Type** list, choose **Tube**.

Filter 1

1 In the **Ray Trajectories, Vacuum Wavelength (nm)** toolbar, click **Filter**.

2 In the **Settings** window for **Filter**, locate the **Ray Selection** section.

3 From the **Rays to include** list, choose **Logical expression**.

4 In the **Logical expression for inclusion** text field, type `m==0`.

5 In the **Ray Trajectories, Vacuum Wavelength (nm)** toolbar, click **Plot**. Compare the resulting image to Figure 3.

2D Histogram

1 In the **Home** toolbar, click **Add Plot Group** and choose **2D Plot Group**.

2 In the **Settings** window for **2D Plot Group**, type `2D Histogram` in the **Label** text field.

3 Locate the **Data** section. From the **Dataset** list, choose **Ray 1**.

Histogram 1

1 In the **2D Histogram** toolbar, click **More Plots** and choose **Histogram**.

2 In the **Settings** window for **Histogram**, locate the **x-Expression** section.

3 In the **Expression** text field, type `atan2(-x,y)`.

4 From the **Unit** list, choose **°**.

5 Locate the **y-Expression** section. In the **Expression** text field, type `m`.

6 Select the **Description** check box.

7 In the associated text field, type `Diffraction order`.

8 Locate the **Bins** section. Find the **y bins** subsection. From the **Entry method** list, choose **Limits**.

9 Click  **Range**.

10 In the **Range** dialog box, type `-3.5` in the **Start** text field.

11 In the **Step** text field, type `1`.

12 In the **Stop** text field, type `3.5`.

13 Click **Replace**.

14 In the **Settings** window for **Histogram**, locate the **Output** section.

15 From the **Function** list, choose **Discrete**.

16 Locate the **Coloring and Style** section. From the **Color table** list, choose **JupiterAuroraBorealis**.

17 In the **2D Histogram** toolbar, click  **Plot**. Compare the resulting image to Figure 4.