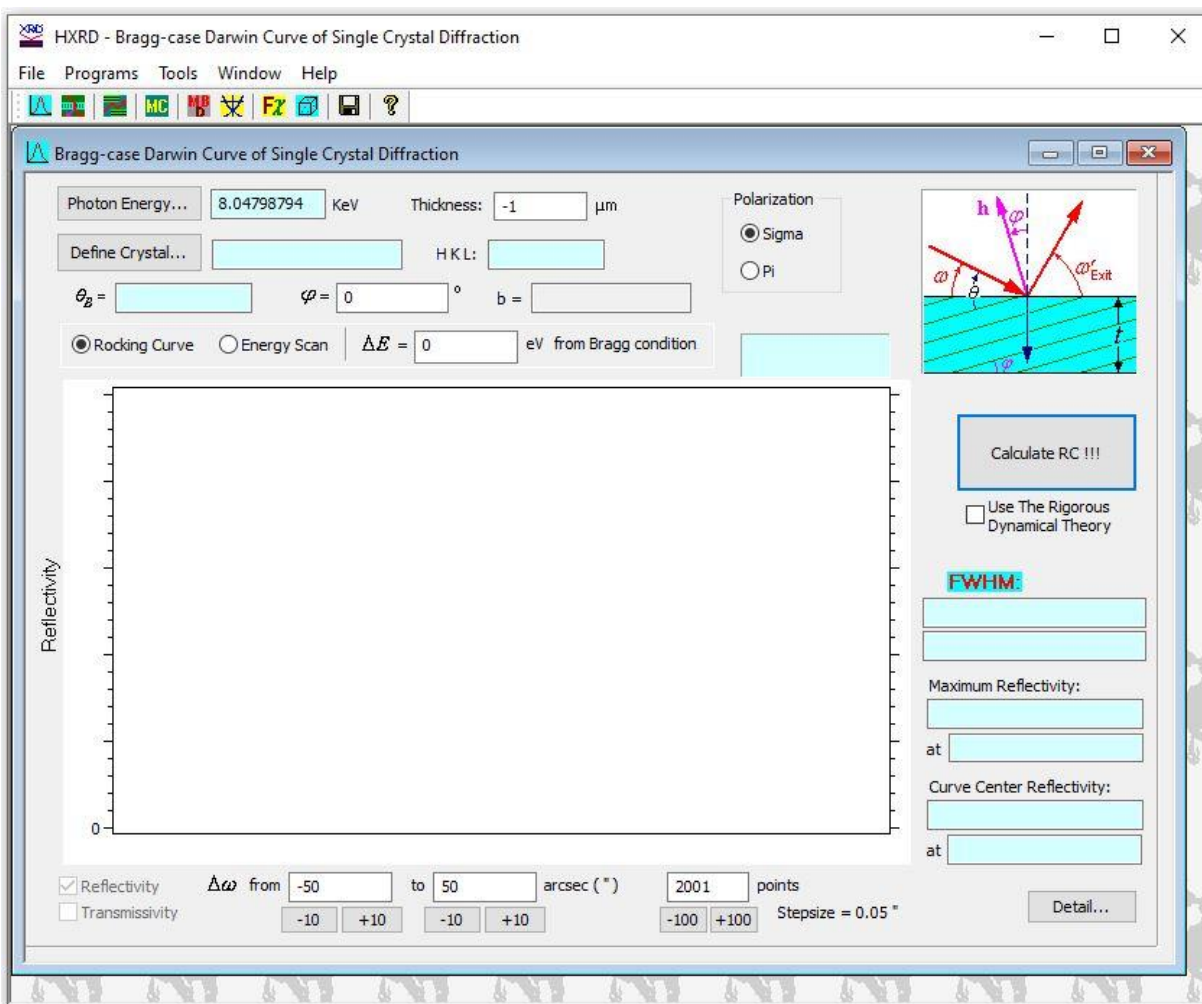# DXRD Help

The **DXRD** program suite is for accurately computing **X-ray diffraction from perfect single crystals** using the **X-ray dynamical theory**. It consists of the following programs.

1. Bragg-case Darwin Curve of Single Crystal Diffraction (for plane wave)

    This program allows you to calculate the **Darwin Curve** of **Bragg-case X-ray diffraction** from a semi-infinite-thickness (-1) crystal or a thin crystal plate. The Curve can be a function of either the *Incidence Angle* (**Rocking Curve**) or the *Photon Energy* (**Energy Scan**, showing the **Bandpass/Bandwidth** of a monochromator).

    Click the "**Photon Energy**" button, and you can set the photon energy (must be < 100 keV) by selecting from a list of characteristic X-ray energies, or by directly typing any energy value you want. The "**Define Crystal**" button allows you to import a **Crystal Structure** and select the **Reflection Indices** *HKL*.

    The program then calculates the **Structure Factors** and the corresponding **Chi (χ) Factors** involved. By default, **DXRD** uses tabulated coefficients to calculate structure factors for photon energies < 100 keV, which is similar to the XOP package (https://www.aps.anl.gov/Science/Scientific-Software/XOP, https://www.esrf.fr/Instrumentation/software/data-analysis/xop2.4). DXRD also provides another program to "**Calculate Structure Factors of Crystals Using Brennan's Method**" [S. Brennan and P. L. Cowan, *Rev. Sci. Instrum.* **63**, 850 (1992), https://doi.org/10.1063/1.1142625]. This method may give slightly different structure factors for **Sigma (σ) and Pi (π) polarization** states. Therefore, the "**Define or Modify**

Crystal and its Parameters" dialog has additional **π-polarization χ factors**. The tabulated-coefficient method gives the same χ factors for both σ- and π-polarization. You can also **manually set your own χ factors** from other sources in the **"Define or Modify Crystal and its Parameters"** dialog.

When you calculate the rocking curve, the energy is set to the Photon Energy (**Bragg energy**) you have set in the above. However, the ΔE parameter allows you to slightly deviate the energy from the Bragg energy, so that you can see how the rocking curve shifts with energy. The **horizontal axis $\Delta\omega$** is always relative to the **Bragg Angle θ_B** calculated with the **Photon Energy** without ΔE. For **Energy Scan**, the **Incidence Angle** is fixed at θ_B by default, but you can slightly deviate it from θ_B by setting the $\Delta\omega$ edit box. The horizontal axis for Energy Scan is ΔE relative to the **Photon Energy**.

The **Asymmetric Angle φ** is **positive** along the direction in the diagram, and negative along the other direction. For nearly backward diffraction, determining the sign of φ may be difficult, but just make sure that the incidence angle is $\omega_B = \theta_B - \varphi$ and the exit angle is $\omega_B' = \theta_B + \varphi$. The **Asymmetric Factor** is defined here as $b = -\sin\omega_B'/\sin\omega_B$. Note that in some papers or books, the asymmetric factor may be defined as b^{-1}. So we list both values in the "**b =**" **edit box**.

When you change any of the parameters, you need to click on the "**Calculate RC !!!**" button to update the results. Afterwards, you may click on any point on the Curve, and there is a box at the top-right of the curve showing the coordinates of the clicked point.

If the crystal has a **finite thickness** ($t > 0$), you can also plot the **Transmissivity Curve** by checking the "**Tranmissitivity**" checkbox at the bottom-left corner.

For grazing-incidence/exit geometry where the Incidence or Exit angle is very small, close to the critical angle of X-ray specular reflection, the conventional X-ray dynamical theory could fail. So, the program provides a check box "**Use The Rigorous Dynamical Theory**" under the "**Calculate RC !!!**" button to calculate the Curve using the so-called "**Extended Dynamical Theory**". For non-grazing geometry, this method gives the same result (checking/unchecking the checkbox does not matter), but for grazing geometry, the results may be noticeably different.

The box below the sign "**FWHM**" shows the FWHM width of the calculated Curve. Note that for **Asymmetric Reflection Geometry** ($b \neq -1$), the incidence and exit angle have different divergence. So, the box first shows the FWHM of the rocking curve in terms of the incidence angle, followed by the FWHM in terms of the exit angle (indicated by "**Exit**") in the parentheses. The unit here is **arcsec**. For Energy Scan, the FWHM is the bandwidth, but the value in the parentheses is still the angular FWHM in terms of the exit angle. The reason is that, for a fixed incidence angle, the exit angle still varies with the photon energy for asymmetric reflection --- **dispersion**! (No dispersion for symmetric Bragg reflection geometry.) The next edit box shows the same results but in the unit of **µrad**.

A complete Curve has the **Maximum Reflectivity peak**, besides which there are two **Half-Maximum** points. The midpoint of these two points is defined as the **Curve Center** and its reflectivity is the **Curve Center Reflectivity**.

You can use Menu "**File → Export RC Data**" to save the Curve data to a file. If the crystal has a **finite thickness** ($t > 0$), you can also export the **Tranmissitivity**. If you have checked "**Use the Rigorous Dynamical Theory**", you can also export the **Specular Reflectivity** (usually very small except for grazing geometry).

Clicking the "**Detail…**" button gives you more information about the Curve, though most of the time you may not be interested in those data.

2. Laue-case Single Crystal Diffraction (for Plane Wave)

This program is similar to the above Bragg-case program. The major difference is that the "**Incident Angle ω**" and the "**Exit angle ω'**" are defined differently with respect to the Crystal Surface, see the diagram. Also see the definition of the **Asymmetric Angle φ**. The crystal thickness for the Laue case must always be finite (> 0, NOT -1). The Reflectivity (R) Curve for the Laue cases show oscillation fringes in most cases. In particular, thick crystals have rapid reflectivity oscillation.

For a constant incidence angle, the reflectivity also changes periodically with crystal thickness, which is called the "**Pendellösung**" phenomenon. The periodicity is called the "**Pendellösung distance**", denoted by $\tau(\Delta\omega)$. When the crystal thickness is $t = N\tau$, the reflectivity becomes 0 at $\Delta\omega$. The reflectivity is maximized when at $t = (N + \frac{1}{2})\tau$. Here $N = 0, 1, 2, ...$ is an integer. In the "**Detail…**" dialog, both the analytical "**Pendellösung distance**" and "**Half Pendellösung distance**" derived from analytical equations are provided at the Curve Center. The analytical values may be accurate for low-absorption cases. Numerical calculations of τ has not been implemented yet.

3. Convoluted Rocking Curve for Divergent & Polychromatic Incident Beam

The above two programs are for the **plane-wave incident beam**. In practical experiments, the incident beam always has **divergence** and energy spread (**spectral bandwidth**), which can make the measured rocking curve MUCH WIDER than the intrinsic Darwin curve in most cases. This program is for calculating the crystal rocking curve based on an X-ray beam with finite divergence and energy spread.

The default set-up of this program is that the divergent and polychromatic incident beam is first monochromatized by a fixed **double-crystal monochromator** (DCM), and then incident on a sample. The rocking curve is measured (computed) with the DCM fixed while you rock the Sample. This is the typical setup at synchrotron beamlines. The incident spectrum is assumed to be the Gaussian spectrum with a spectral bandwidth of the **FWHM** value that you can set. Usually, the X-ray beam upstream the DCM is a white beam, so you can give set a very large FWHM value. The bandpass of a DCM is usually 1 eV, so as long as the FWHM is large enough, its detailed values have little effect on the results. The **Spectrum Range** is the Energy Range you use for integration over the energy. You can choose a large Spectrum Range value with adequate points. The **divergence of the incident beam** may greatly affect the final rocking curve width. Therefore, you have to carefully set this value based on your beamline parameters (including the slits used).

Before a full computation, you must make sure that the parameters you set are adequately large enough to achieve convergence of the integration and meanwhile, the computing fast enough. To do so, you can keep increasing each parameter, and compare the results with the previous results. The program can plot both the current rocking curve and the previous curve by checking "**Show Previous RC**". When there is no noticeable difference between the current and previous curves, it is likely that you reach the convergence requirements [for the testing parameter(s)]. But in general, the **Beam Divergence** parameter is a real condition of the beam and you should not change it significantly, though you can freely change the **Points.**

For the **non-dispersive** configuration, when the **Monochromator** and the **Sample** are of the same kind of crystal and have the same Bragg reflection (or the two Bragg angles are very close to each other), the convoluted rocking curve width is nearly independent of the divergence and spectrum of the incident beam. This is usually called "**double-crystal rocking curve**". It is a very accurate and reliable method for measuring the rocking curve widths of crystals. This method is accurate even if the incident beam is a laboratory source with large divergence. The disadvantage of this method is that for different samples/reflections, you have to switch to different monochromators (if they are available), which is very inconvenient. For a Lab-source-based double-crystal diffractometer, the DCM may not be necessary, a single monochromator may be enough. In this case, you can **uncheck the "DCM"** choice. For Cu Kα1 source, we suggest the following typical parameters: **Random polarization** (half Sigma and half Pi), **spectral FWHM 2.6 eV**, the **Spectrum Range 15 eV**, and the **Beam Divergence** about ~ **1.5 mrad**.

As is well known and can be easily demonstrated by the above "**Bragg-case Darwin Curve of Single-Crystal Diffraction**" program, the diffraction peak is always **slightly shifted upward** (typically by a few arcsecs) from the geometrical Bragg angle θ_B due to the small X-ray **refraction** effect. Therefore, the **principal incident angle of the monochromator** is not exactly the Bragg angle. It should be corrected by the small Bragg peak shift, and the **Angular Center** parameter must be equal to this shift. You can use the "**Bragg-case Darwin Curve of Single-Crystal Diffraction**"

program to quickly find the Bragg peak shift (i.e. the **relative Curve Center position**) of the monochromator and fill the <mark>Angular Center</mark> with the shift value.

You can also choose the "**Dispersive Configuration**" if necessary. For a **DCM**, the **Non-dispersive** or **Dispersive Configuration** is based on the <mark>relationship between the second crystal of the DCM and the Sample</mark>.

You can check the "**Channel Cut**" checkbox below the "**Define Sample…**" button if the sample crystal is a channel-cut crystal (which is not common though).

4. Multiple-Crystal Monochromator

The goal of this program is to calculate the **bandwidth** and **angular acceptance** of **arbitrary multiple-crystal monochromators**, but the development is still in the early stage.

First, if you check the "**Only 1st**" checkbox, you can compute the rocking curve or bandwidth of the **1st crystal** just like the "**Bragg-case Darwin Curve of Single Crystal Diffraction**" program does. But here you can also check the "**Channel-cut**" checkbox of the **first crystal** to compute the rocking curve of a channel-cut crystal.

If you uncheck "**Only 1st**", you can bring in the **2nd crystal**, which again can be either a single crystal or a channel-cut. You can set the second crystal in the "**Non-dispersive**" or "**Dispersive**" setup. Although the schematic diagram is similar to that of the above "Double-Crystal Diffraction" setup, there is a major difference here. That is, here the relative orientations between the two crystals are fixed, and the incident beam is a plane wave. You can only scan the **Incidence Angle** or Incident **Photon Energy**, similar to the program "**Bragg-case Darwin Curve of Single Crystal Diffraction**". By comparison, in the "**Double-Crystal Diffraction**" setup, the incident beam is not a plane wave. It is a divergent beam with a finite spectral bandwidth. Meanwhile, the 1st crystal is fixed and you can only rotate the 2nd crystal.

As mentioned before, the diffraction peak of a Bragg-case reflection **shifts slightly toward the high-angle direction** from the **geometrical Bragg angle** due to the slight X-ray refraction effect. To compute multiple-crystal diffraction, you must "align" each of the crystal to the peak position by taking into account these slight peak shifts. The <mark>Φ = angle</mark> is the relative orientation between the two crystals calculated without taking into account the slight peak shift; it is only based on the two geometrical Bragg angles and the asymmetric cut angles. The <mark>$\Delta\Phi$ = angle</mark> is the overall corrections calculated from the slight peak shifts of the two crystals. You can click the "**Auto Set…**" button to let the program calculate the angles. Then you may manually **tweak** it to optimize the overall reflectivity or bandwidth. Or you can input the values yourself (from single-crystal Darwin curve calculations). <mark>Note that if you do not set the two angles correctly, the reflectivity (efficiency) of the monochromator may be very low!</mark>

After all the parameters of the crystals and their relative orientations are set, you can perform the **Angular Scan** or **Energy scan** of the **entire monochromator**, similar to the "**Bragg-case Darwin Curve of Single Crystal Diffraction**" program. For Energy Scan, the "**$\Delta\omega$ =**" editbox allows you to slightly deviate the incidence angle (of the first crystal) from the Bragg angle, mainly for compensating the slight diffraction peak shift. **Setting it to 0** usually does not affect the Curve shape and width, but may induces a slight shift of the entire Curve.

A typical application of this program is that you set both crystals as channel cuts and place them in the **dispersive** configuration. Then it becomes a **Bartels Monochromator**, and you can calculate its **bandwidth** and **angular acceptance**. Especially you can vary the **asymmetric angles** (of both crystals) to tune the bandwidth and angular acceptance --- Don't forget to set and tweak the <mark>$\Delta\Phi$ =</mark> angle correctly, otherwise the efficiency would be very low.

5. Dynamical-Theory Computation of Multiple-Beam Diffraction

6. Multiple-Beam Diffraction Lines (Monochromator Glitches) in Azimuth-Energy MapMultiple-Beam Diffraction

The **Help File** of these two programs is "**MBD-Help.pdf**". You can open it directly in the main folder of DXRD, or you can open the "**Dynamical-Theory Computation of Multiple-Beam Diffraction**" program and click the "**Help**" button.