## CONTENTS

1 **Introduction** 3  
  1.1 Mouse Interaction in Image Views and Spectrum Views 3  
  1.2 Image Color Scale and Contrast 3  

2 **Calibration Procedure** 5  
  2.1 Preparation 5  
  2.2 Peak Picking 5  
  2.3 The Calibration and Refinement Process 7  

3 **Mask Creation** 9  
  3.1 Selection Tools 9  
  3.2 Threshold Masking and Cosmic Removal 10  
  3.3 Control Buttons 10  
  3.4 File Handling 10  

4 **Integration Module** 11  
  4.1 File Handling 12  
  4.2 Overlays 12  
  4.3 Phases 13  
  4.4 Background subtraction 14  
  4.5 Special (X-Tab) 16
Contents:
Dioptas is a GUI program for fast analysis of powder X-ray diffraction images. It provides the capability of calibrating, integrating, creating masks, showing multiple spectrum overlays and display phases line positions. The basis of the integration and calibration algorithm is the pyFAI library pyFAI. The usage of pyFAI allows integration times on the order of 20 milliseconds and calibration of every possible detector geometry.

Dioptas has three different modules which can all be accessed by the tab indicators on the left side of the user interface: Calibration, Mask, Integration.

The Calibration module enables you to calibrate the detector geometry. Within the mask module you can select regions you want to exclude from the image integration and the Integration module is the heart for data exploration. It shows both, the image and integrated spectra. One can overlay different spectra and show line position of phases.

1.1 Mouse Interaction in Image Views and Spectrum Views

*Left Click:* Action depends on the module you are in. In the calibration view it will search for peaks. In the Mask view it is the primary tool for creating the geometric objects used to build up the mask and in the integration view it draws a line at the current two theta value.

*Left Drag:* Zooms into the selected area. It will try to scale images accordingly, but will not perfectly zoom in to the selected area, because pixels are kept as square objects on the screen.

*Right Click (Command+Right Click on Mac):* Zoom out.

*Right Double Click (Command + Right Double Click on Mac):* Completely zoom out.

*Mouse Wheel:* Zoom in and zoom out based on the current cursor position.

1.2 Image Color Scale and Contrast

Every image view has a color bar and a histogram either on the side of the image (Mask module and Calibration Module) or on the top (integration view). The colors of the color bars can be easily adjusted. You can switch to a completely different color-scale by right clicking the color bar. This creates a pop-up where one of the predefined color scales can be selected. The position of the individual colors can be adjusted by dragging the triangle of this color. Further the colors can be changed completely by double clicking (left) it, which will pop up a color chooser. It is in addition also possible to add a complete new color by double clicking (left) next to the color bar. The histogram next to the color bar shows the intensity distribution of the loaded image on a log scale. The sliders two lines define the scaling of the image in the image view. Please feel free to adjust their position by dragging them.
CHAPTER TWO

CALIBRATION PROCEDURE

Make sure you are in the calibration module, which should be selected on the left side of the window.

2.1 Preparation

Load the calibration image by clicking the “load image” button on the upper right side of the window. Now you can insert the starting values for the calibration in the menu on the right. The calibration procedure will define distance and center position of the x-ray. Therefore, wavelength and pixel width/height have to be defined based on the experimental setup and detector used. Please choose the correct calibrant from the Calibrant drop-down list. Additionally the image can be rotated, or flipped in order to accommodate for different detector orientations. These image transformations will be applied to all subsequent loaded images in the calibration module and in the integration module.

![Start values for calibration](image)

Figure 2.1: Start values for calibration

2.2 Peak Picking

The parameters for peak selection are given in the peak selection section on the right site of the calibration module, when “Calibration Parameters” is selected.

By default automatic peak search is selected, which tries to automatically find peaks on a clicked ring. To search on the first ring please click on it with the left mouse button. If the peak search was successful it should look like this:

If the automatic peak searching fails (if it does select other peaks in addition to the first diffraction ring) there are several options:
Figure 2.2: Peak Selection Options

Figure 2.3: LaB₆ 2D diffraction image with the first ring selected.
• perform the automatic peak search on a different ring.
  – change the current ring number
  – and select the a peak on this ring
• choose single peak search, which will search the highest intensity peak around the click position, whereby the size of the search area is defined by the search size
  – then search one peak for one diffraction ring (the current peak number will automatically increase)
  – or deselect the automatic increase checkbox and click several spots on the first ring, or any ring you like (with the corresponding peak number selected)

2.3 The Calibration and Refinement Process

After the peaks/ring(s) have been selected we can start the calibration procedure. This is done by clicking the “Calibrate” Button on the lower left of the interface. This will calculate the geometric parameters based on the current peak selection and then do automatically refine the calibration parameters.

After refinement Dioptas will automatically create a 360 degree cake image and an integrated spectrum. When the procedure is finished it will jump to the “Cake” tab (top tab-bar above the image) and show the cake image. In this image you can easily check if the calibration was successful (by checking if the cake lines are straight). Additionally, the spectrum is plotted with calculated calibrant positions in the “Spectrum” Tab. All peak maxima should coincide with phase line positions. The resulting calibration parameters are shown by clicking the pyFAI parameters or Fit2d Parameters tabs in the right control panel. The current calibration parameters can be saved by clicking the Save Calibration button on the lower right of the user interface. To fast reuse the current calibration later, the calibration can be reloaded by clicking Load Calibration.

If the calibration failed, either the start values are wrong, the initial peak selection was faulty or the refinement parameters need to be adjusted. For a new peak selection, just click “clear all peaks” and start the the peak selection again, make sure that current peak number belongs to the corresponding clicked ring. The meaning of each of the refinement options are explained in the next section.

2.3.1 Refinement Options

The refinement options are defined on the right control panel of the Calibration module, when “Calibration Parameters” is selected.

![Available options for calibration refinement](image)

Figure 2.4: Available options for calibration refinement

There are several options available:
**automatic refinement:** Defines if refinement is executed automatically after calibration.

**use mask/transparent:** The refinement can be constraint to a certain image area by using a mask previously defined in the mask module. The image of the mask can be made transparent to be able to “look behind”

**Peak search algorithm:** The algorithm used for searching peaks on the ring. The standard algorithm is “Massif” although “Blob” detection may give better results in some cases.

**Delta 2th:** This is the +- search range used for automatic peak search for each ring. The center value depends on the values, estimated by the calibration procedure, so ultimately by the initial choice of predefined peaks (Peak selection)

**Intensity Min factor:** This factor determines how many times the peak intensity has to be higher than the mean value of the search area (within the delta 2th value) for each individual ring. The lower this value is the more peaks will be selected, however, also the likelihood of selecting wrong background peaks increase.

**Intensity Max:** A threshold value which excludes all peaks above this value.

**Number of rings:** The number of rings on which peaks are searched.

If the calibration/refinement fails you can in principle play with all parameters. However, the most common adjustments are the number of rings and the **Intensity Min factor.**
CHAPTER THREE

MASK CREATION

In the mask module areas can be defined which will be excluded from integration or calibration. There are several geometries available to select different kind of areas. Additionally it is possible to mask based on threshold values and perform automatic cosmic removal. All tools are available on the right control panel in the Mask view. It can be either chosen to mask a certain region or unmask it (select either on the top of the control panel).

![Figure 3.1: The Mask module of Dioptas.](image)

3.1 Selection Tools

To select a specific geometry just click on it and an orange border will show which one is active right now. All geometric shapes are created by using left clicks:

- **Circle**: The first click defines the center of the circle and the second the radius of the circle.
**Rectangle:** The first click defines one corner and the second the corner on the opposite side.

**Point:** A click will mask an area as large as the circle floating around the mouse pointer. The size of the circle can be changed by changing the value next the the **Point** button or using just pressing the q and w keys.

**Polygon:** Subsequent clicks will define edges of the polygon. A double click will close the polygon (and add the position of the double click as last point to the polygon)

### 3.2 Threshold Masking and Cosmic Removal

In order to do threshold masking, please insert the wanted number next to the desired Thresh button and click the button.

Cosmic removal is an automatic optimization procedure trying to mask cosmic rays from the image. This procedure can take considerable amount of time, please be patient.

### 3.3 Control Buttons

**Grow:** Grows the current mask by one pixel in all directions.

**Shrink:** Shrinks the current mask by one pixel in all directions.

**Invert:** This will invert the mask so that unmasked areas become masked and vice versa.

**Clear:** This will remove the complete mask.

**Undo/Redo:** Enabling to undo the last action or redo them. You can undo up to 50 actions.

### 3.4 File Handling

**Save Mask:** Saves the current mask as a tiff file with intensities being 1 for masked areas and 0 for unmasked areas.

**Load Mask:** Loads a previously saved mask. Clears the current mask before.

**Add Mask:** Loads a previously saved mask and adds it to the current mask.
CHAPTER FOUR

INTEGRATION MODULE

The integration module is the heart of Dioptas. Here you can automatically integrate multiple of spectra, browse between images and integrated spectra, compare multiple spectra to each other, perform background subtraction and compare spectrum peak positions to the ones of known phases.

Figure 4.1: The integration module of Dioptas.

In the integration module the current image is displayed on the left side with the integrated spectrum shown on the lower right. The control panel has several tabs for different functions.

The “Img” and “Spec” tabs are primarily for loading and browsing images and spectra, respectively. In the “Overlay” tab integrated spectra can be loaded for comparing them to the currently loaded shown active spectrum. The “Phase” tab enables opening/editing jcpds files and changing the equation of state parameters of the loaded phases. The controls in the “Bkg” tab can be used to define an image as background prior to integration and the “X” (special) tab contains several additional optional features like cBN absorption correction, manual selection of the number of integrating bins.
4.1 File Handling

Images and spectra can be loaded by clicking the **Load** button in the respective modules. Images can be in different file formats: .img, .sfrm, .dm3, .edf, .xml, .cbf, .kccd, .msk, .spr, .tif, .mccd, .mar3450, .pnm, or any other common image formats. Spectrum files should be 2 column files. If there is a header present it should be commented by ‘#’ signs.

Images loaded will be automatically integrated if a calibration is available (either by performing it in the calibration window or by loading a previously saved calibration file (*.poni) file). There are too modes for file browsing (clicking the “<” and “>” buttons):

**By Name**: the next and previous filenames will be searched based on the last digits in the filename. For example the next file from *test_002.tif* will be *test_003.tif* and the previous will be *test_001.tif*

**By Time**: The next and previous files loaded will be search based on creation time of the files. This filemode does not need any numbers in the filenames it will just sort the files based on creation time and go forward and backwards in this list.

Any newly added file to the current img working directory can be opened by checking the **autoprocess** checkbox in the Image module.

By default the integrated spectra are not saved. If you want the spectra to be saved please choose an output folder in the Spec tab by clicking the “...” button and then check the **autoprocess** checkbox. All new integrated spectra will then be automatically saved in this folder with name being the same as the image but different file extension. The integrated spectra can be automatically saved in 3 different formats by checking their respective boxes in the lower right of the **Spec** tab:

- **.xy**: (Selected by default) A two column format with a header which contains the calibration parameters, polarization correction and integration unit (2th, Q or d)
- **.chi**: A two column format with a 5 line header containing the filename, integration unit and number of points. Based on Fit2d output format.
- **.dat**: A two column format without any header. It saved just the plain data.

In addition to file browsing and the “load” button, files can also be loaded by inserting their name folder in the respective text fields. The upper one is the filename and the lower one is the containing folder. If the file does not exist it the text field will revert to its previous state.

4.1.1 Quick Actions

The “**Img**” and the “**Spec**” tab exhibit several quick actions, which are basically shortcuts to some functions:

**Save Image**: Saves the currently shown image as either a *.png file for presentation or *.tiff file as data.

**Save Spectrum**: Saves the current spectrum either in a two-column format (*.xy) or the complete spectrum content in a *.png or vectorized *.svg format.

**As Overlay**: Adds the currently active spectrum (white) to overlays.

**As Bkg**: Adds the currently active spectrum (white) to overlays and sets it as background.

**Load Calibration**: Opens a dialog to open a *.poni calibration file and sets this as the new calibration parameters.

4.2 Overlays

In the overlay control panel you can add, delete or clear overlays and adjust their scaling and offset.
Add: Loads a spectrum file (2-column file) as overlay. It is possible to select multiple spectra and load them all at once.

Delete: Deletes the currently selected overlay in the overlay list.

Clear: Deletes all currently loaded overlays.

The list of overlays shows several widgets representing the state of each individual overlay. The first checkbox controls if the overlay is visible in the graph. The colored button shows the overlay color. Clicking on it will pop-up a color-chooser dialog where the color for this overlay can be changed. The name of an overlay is by default its filename, but it can be modified by double-clicking the name in the overlay list.

On the right side you can adjust the scale and offset of the overlays by either entering a specific number or using the spin-box controls. The step text fields control the steps of the spin-box.

An overlay can be used as a background for the spectrum. In order to do so, you have to activate the “Set as Background” button. This button sets the currently selected overlay as background for the spectrum file. It can be seen that an overlay is set as background by the Set as Background button being activated for a specific overlay and by the background overlay name being shown in the lower right of the graphical user interface (right below the graph). The scaling and offset of the overlay/background can still be adjusted by using the respective spin boxes. The background overlay remains active until it is deactivated, therefore the background will be automatically subtracted from each newly integrated image or newly loaded spectrum. If autosave for spectra is set, Dioptas will create a bkg_subtracted folder in the autosave folder and automatically save all subtracted spectra.

4.3 Phases

The basic controls for phases are similar to the ones in overlay:

Add: Loads a *.jcpds file, calculates the line positions in the range of the current spectrum and shows the phase lines in the graph. You can select multiple spectra in the phase dialog.

Edit: Opens a dialog where the jcpds file can be edited. For further details see the JCPDS editor section

Delete: Deletes the currently selected phase in the phase list.

Clear: Deletes all phases.

The list of phases shows several widgets representing the state of each individual phase overlay. The first checkbox controls if the phase lines are visible in the graph. The colored button shows the color of the phase lines. Clicking on it will pop-up a color-chooser dialog where the color for this phase can be changed. The name of an phase is by
default its filename, but can be changed by double-clicking the name in the phase list. Additionally the pressure and temperature for each phase is shown in the phase list. If for a particular phase thermal expansion is not in the jcpds file it will always display ‘- K’.

On the right side the pressure and temperatures of the loaded phases can be adjusted. If Apply to all phases is checked the pressure and temperature will be set for all loaded phases. By default the pressure and temperature values will be displayed in the phase legend in the spectrum if they differ from ambient conditions. For disabling this feature please uncheck the ‘Show in Spectrum’ checkbox.

4.3.1 JCPDS Editor

In the jcpds editor the content of the jcpds file can be modified. Every change will be immediately reflected in the position of the lines in the spectrum. You can edit the comment, the symmetry, lattice parameter and equation of state parameters. Reflections can be edited in the reflections table. h, k, l and intensities can be modified by double clicking in the table all other parameters are calculated correspondingly. A 0 after a parameters always means that this is the value at ambient condition and when there is no 0 the value corresponds to the current temperature and pressure conditions modified in the Phase tab. The changes can be saved as a new file by clicking the Save As button. If you want to revert all changes and reload the original files please press the Reload File button. If you like the changes you made you can close the JCPDS editor either by clicking the X button or the OK button on the lower right. The Cancel button will close the JCPDS editor and revert the changes made since the last opening of the JCPDS editor.

4.4 Background subtraction

In the Bkg tab an image can be loaded as background image. This image will be subtracted from the original image prior to the integration process. The intensity of the image can scaled or offset by using the corresponding spin boxes. The text fields next to the spinboxes define the individual steps for the spinbox. After each change, loading an image as background, removing it, or change the scale and offset of the background image, the image will be automatically reintegrated.

Load: Loads an image as background image.

Remove: Removes the currently loaded background image. The original image will then be integrated without any background subtraction.

Scale and Offset: The intensity of the background image is scaled by: scale x img_intensity + offset.
Figure 4.4: Graphical JCPDS editor
4.5 Special (X-Tab)

The currently available features:

**Mask - Transparent:** If a mask is used for integration it will be shown as transparent red over the image, compared to the usual solid red. This makes it possible to still be able to see what exactly is masked.

**Levels - Autoscale, Absolute, Percentage:** These 3 choices are different modes for intensity scaling when loading new files or browsing files. *Autoscale* will always perform autoscaling for each newly loaded image. When using *Absolute* the maximum and minimum levels remain the same and are independent of the img intensities and when using *Percentage* the levels are always scaled as percentage of the maximum intensity of the newly loaded image.

**cBN Seat Correction:** Enabling this option calculates the theoretical transmitted intensity through a diamond and cBN seat based on the parameters entered into the text boxes. Where:

- Diamond d is the diamond thickness in mm.
- Seat d is the seat thickness in mm
- Inner Seat r is the radius of the small opening of the cBN seat (close to the diamond) in mm
- Outer Seat r is the radius of the outer opening of the cBN seat in mm
- Cell Tilt is the tilting of the cell in respect to the primary beam in degrees.
- Tilt Rotation is the direction of the Cell tilt in degrees.

To see the calculated transmitted intensity distribution press the *Plot Cor* button. This will show the calculated absorption correction in the image view.

**Integration:** Here you can manually specify the number of integration bins and/or choose to supersample the image. Supersampling an image by a factor of n>1 results in of splitting of each pixel into n^2 pixels with equal distribution of intensities among the splitted pixels. For perfect powder samples this can result in smaller integrated peak widths and more points per peak if the physical pixel width is too high. However, it may result in unreasonable intensity distributions. Please use at your own risk.