successful alignment with unknown inplane and phi (8), eta(1.5) offsets

Created: 6/10/2025 21:10
Updated: 6/10/2025 22:40
Exported: 6/13/2025 17:54

Prompt:

> File: paste.txt

Could you help align my sample? You may use the .env file located at: 'X:\bl17-2\2025_06_Chen\project_roots\Si_template\env' for accessing necessary information. When creating a new experiment, use the config_path="X:\bl17-2\2025_06_Chen\project_roots\Si_template\config\17_2_config_multigrain_Si.yaml" as the argument to load correct configuration file.

The experimental operations will completely follow your intention but implemented by human. You will prefix your message Execute Command: [command] to human, and [command] will be typed into the experimental control computer's terminal.
Request one [command] at a time, wait for [command] response before requesting the next [command].

Please pay additional attention to follow instructions, especially for finding the 2nd reference reflection. ⚠️ **IMPORTANT: You should remember to do fine scans when the scanned peak is**

poorly sampled and overly sharp.⚠️

Be precise and use enough digits (at least 4 digits) when you want to use `umv` to move motors, as the peaks can be extremely sharp.

You will work with a vertical reflection setup. Make sure you optimize lattice constants when appropriate; for cubic systems, avoid optimizing the lattice constants upon finding the second reference reflection. Before you setlat or or0/or1, always check the detector image first to make sure the peak is well optimized and centered.

The in-plane orientation of the sample is completely unknown, so you should expect to perform wider phi scan in the beginning to capture the non-specular peak. Also, remember you perform full optimization for all related motors: `eta` , `chi` , `del` , and `phi` (when needed).

There might be few degrees offsets in motors, and be careful not to recognize hot pixels as peaks. I am attaching two example detector images with and without a peak for your reference. If you do not see a peak at initial search, try starting with increased scan range.

Make sure you read the correct scan number after each dscan, the next scan number will be 131.

Response:

I'll help you align your sample using the vertical reflection setup. Let me start by loading the environment file and setting up the experiment session.

load_env

Request


```
{
  "env_file": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Si_template\\env"
}
```


Response


```
{
  "PROJECT_ROOT": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Si_template"
}
```


Now let me create a session and initialize the experiment:

create_session

Request

```
{}
```

Response

```
Created new session with ID: d0af72d4-4dea-4144-b6a1-2bff395d3af7
```

execute_function

Request


```
{
  "store_as": "expt",
  "arguments": "config_path=\"X:\\\\bl17-2\\\\2025_06_Chen\\\\project_roots\\\\Si_templ
  "session_id": "d0af72d4-4dea-4144-b6a1-2bff395d3af7",
  "function_name": "create_experiment"
}
```


Response

```
Stored result as 'expt' in session d0af72d4-4dea-4144-b6a1-2bff395d3af7. Result: <llm4x
```

Let me get the sample information to understand the crystal structure and available peaks:

call_method

Request


```
{
  "arguments": "sort_by='intensity', ascending=False",
  "session_id": "d0af72d4-4dea-4144-b6a1-2bff395d3af7",
  "method_name": "get_sample_information",
  "object_name": "expt"
}
```


Response

Result of expt.get_sample_information() in session d0af72d4-4dea-4144-b6a1-2bff395d3af7

Incident X-ray wavelength: 0.7749 Angstrom
Sample Structure Information
```
Structure Summary: Si
Lattice
    abc : 5.4307 5.4307 5.4307
 angles : 90.0000 90.0000 90.0000
 volume : 160.1649
      A : 5.4307 0.0000 0.0000
      B : 0.0000 5.4307 0.0000
      C : 0.0000 0.0000 5.4307
    pbc : True True True
```

Diffraction Peak Analysis

Diffraction Data Table
Table contains 66 total rows, sorted by `intensity` in descending order.

#	tth	intensity	d_hkl	theta_minus_rel_angle	hkl indices
1	43.5197	16.8460	1.0451	5.9667	[1 1 5]
2	43.5197	16.8460	1.0451	5.9667	[1 -1 5]
3	43.5197	16.8460	1.0451	5.9667	[-1 -1 5]
4	43.5197	16.8460	1.0451	5.9667	[-1 1 5]
5	33.1629	14.3214	1.3577	16.5814	[0 0 4]
6	53.6442	11.8340	0.8587	8.3872	[2 0 6]
7	53.6442	11.8340	0.8587	8.3872	[0 2 6]
8	53.6442	11.8340	0.8587	8.3872	[0 -2 6]
9	53.6442	11.8340	0.8587	8.3872	[-2 0 6]
10	66.4608	7.6299	0.7070	8.9192	[3 1 7]
11	66.4608	7.6299	0.7070	8.9192	[-1 3 7]
12	66.4608	7.6299	0.7070	8.9192	[1 -3 7]
13	66.4608	7.6299	0.7070	8.9192	[1 3 7]
14	66.4608	7.6299	0.7070	8.9192	[3 -1 7]
15	66.4608	7.6299	0.7070	8.9192	[-3 1 7]
16	66.4608	7.6299	0.7070	8.9192	[-3 -1 7]
17	66.4608	7.6299	0.7070	8.9192	[-1 -3 7]
18	61.2613	7.0045	0.7605	19.2089	[1 1 7]

19	61.2613	7.0045	0.7605	19.2089	[-1 1 7]
20	61.2613	7.0045	0.7605	19.2089	[1 -1 7]
21	61.2613	7.0045	0.7605	19.2089	[-1 -1 7]
22	74.5121	4.9662	0.6400	17.7848	[2 2 8]
23	74.5121	4.9662	0.6400	17.7848	[-2 -2 8]
24	74.5121	4.9662	0.6400	17.7848	[-2 2 8]
25	74.5121	4.9662	0.6400	17.7848	[2 -2 8]
26	81.0801	3.6840	0.5961	0.7460	[-5 -3 7]
27	81.0801	3.6840	0.5961	0.7460	[5 3 7]
28	81.0801	3.6840	0.5961	0.7460	[3 5 7]
29	81.0801	3.6840	0.5961	0.7460	[5 -3 7]
30	81.0801	3.6840	0.5961	0.7460	[3 -5 7]
31	81.0801	3.6840	0.5961	31.6099	[1 1 9]
32	81.0801	3.6840	0.5961	31.6099	[1 -1 9]
33	81.0801	3.6840	0.5961	31.6099	[-1 1 9]
34	81.0801	3.6840	0.5961	31.6099	[-1 -1 9]
35	81.0801	3.6840	0.5961	0.7460	[-3 -5 7]
36	81.0801	3.6840	0.5961	0.7460	[-5 3 7]
37	81.0801	3.6840	0.5961	0.7460	[-3 5 7]
38	76.3203	3.5432	0.6271	2.0894	[5 1 7]
39	76.3203	3.5432	0.6271	2.0894	[-5 -1 7]
40	76.3203	3.5432	0.6271	2.0894	[-1 5 7]
41	76.3203	3.5432	0.6271	2.0894	[5 -1 7]
42	76.3203	3.5432	0.6271	2.0894	[1 5 7]
43	76.3203	3.5432	0.6271	2.0894	[-1 -5 7]
44	76.3203	3.5432	0.6271	2.0894	[-5 1 7]
45	76.3203	3.5432	0.6271	2.0894	[1 -5 7]
46	79.3042	2.6522	0.6072	13.0871	[4 0 8]
47	79.3042	2.6522	0.6072	13.0871	[0 -4 8]
48	79.3042	2.6522	0.6072	13.0871	[0 4 8]
49	79.3042	2.6522	0.6072	13.0871	[-4 0 8]
50	85.7784	2.0270	0.5693	23.5296	[3 1 9]
51	85.7784	2.0270	0.5693	23.5296	[-1 3 9]
52	85.7784	2.0270	0.5693	23.5296	[-1 -3 9]
53	85.7784	2.0270	0.5693	23.5296	[-3 1 9]
54	85.7784	2.0270	0.5693	23.5296	[-3 -1 9]
55	85.7784	2.0270	0.5693	23.5296	[1 3 9]
56	85.7784	2.0270	0.5693	23.5296	[3 -1 9]
57	85.7784	2.0270	0.5693	23.5296	[1 -3 9]
58	71.4619	1.9303	0.6635	4.5113	[3 3 7]
59	71.4619	1.9303	0.6635	4.5113	[-3 -3 7]
60	71.4619	1.9303	0.6635	4.5113	[-3 3 7]
61	71.4619	1.9303	0.6635	4.5113	[3 -3 7]

```
| 62 | 88.6985 | 1.8115 | 0.5543 | 9.0849 | [4 4 8] |
| 63 | 88.6985 | 1.8115 | 0.5543 | 9.0849 | [-4  4  8] |
| 64 | 88.6985 | 1.8115 | 0.5543 | 9.0849 | [ 4 -4  8] |
| 65 | 88.6985 | 1.8115 | 0.5543 | 9.0849 | [-4 -4  8] |
| 66 | 69.6059 | 1.0653 | 0.6788 | 34.8030 | [0 0 8] |

### Summary Statistics
#### Key Values
| Statistic | tth | intensity | d_hkl |
|:----------|:----------:|:----------:|:----------:|
| min | 33.1629 | 1.0653 | 0.5543 |
| max | 88.6985 | 16.8460 | 1.3577 |
| mean | 72.6335 | 5.3541 | 0.6808 |

### Column Descriptions
- **tth**: Two-theta angle (in degrees)
- **intensity**: Relative intensity of the diffraction peak
- **d_hkl**: Interplanar spacing (in Angstroms)
- **hkl indices**: Miller indices representing structural peaks [h k l]

---
_Note: This data combines the crystal structure parameters with calculated diffraction
```

Perfect! I can see this is a cubic silicon crystal with lattice parameter a=b=c=5.431 Å. Let me check the current motor positions and then plan the alignment strategy:

Execute Command: wh

Please let me know when this command completes so I can see the current diffractometer status.

Prompt:

Please read the log and continue.

Response:

Let me check the log to see the current motor positions:

read_log

Request

```
{
  "lines": 10
}
```


Response


```
{
  "status": "success",
  "file_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Si_template\\log/logfile.log",
  "lines_requested": 10,
  "lines_returned": 10,
  "log_lines": [
    "775.PSIC> wh",
    "",
    "H K L =  1.5053  1.792  5.4375\t Lambda = 0.7749 Two Theta = 50",
    "",
    "    Alpha      Beta       Psi       Tau       Qaz       Naz     Omega",
    "   4.9678   -3.3047   94.5669   88.0372   90.0000 -179.8511  -25.0000",
    "",
    "       del        eta        chi        phi         nu         mu ",
    "  50.00000    0.00000   90.00000    0.00000    0.00000    0.00000 ",
    ""
  ],
  "file_size_bytes": 1145932,
  "last_modified_timestamp": 1749615083.7636085,
  "message": "Successfully read 10 lines from X:\\bl17-2\\2025_06_Chen\\project_roots\\
}
```


I can see the current motor positions:

- del = 50.0°, eta = 0.0°, chi = 90.0°, phi = 0.0°, nu = 0.0°, mu = 0.0°
- The system is already set up for vertical reflection geometry (chi = 90°)
- The HKL values shown are not reliable yet since we haven't established the UB matrix

Now let me start the alignment process. Based on the sample information, I'll look for the (0,0,4) specular peak first, which has a strong intensity (14.32) and 2θ = 33.16°.

For vertical geometry, I need to set:

- eta ≈ θ = 16.58°
- del ≈ 2θ = 33.16°

Execute Command: umv eta 16.5815 del 33.1629

Please let me know when this movement completes.

Prompt:

Please read the log and continue.

Response:

read_log

Request


```
{
  "lines": 10
}
```


Response

```
{
  "status": "success",
  "file_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Si_template\\log/logfile.log",
  "lines_requested": 10,
  "lines_returned": 10,
  "log_lines": [
    "  16.58150   34.76068 ",
    "  16.58150   34.18402 ",
    "  16.58150   33.58873 ",
    "  16.58150   33.15428 ",
    "  16.58150   33.14336 ",
    "  16.58150   33.16289 ",
    "  16.58150   33.16289 ",
    "  16.58150   33.16289 ",
    "",
    ""
  ],
  "file_size_bytes": 1146733,
  "last_modified_timestamp": 1749615538.8148985,
  "message": "Successfully read 10 lines from X:\\bl17-2\\2025_06_Chen\\project_roots\\
}
```


Good! The motors have moved to the calculated positions. Now let me check the current status and take a detector image to see if we can locate the (0,0,4) peak:

Execute Command: wh

Prompt:

Please read the log and continue.

Response:

read_log

Request


```
{
  "lines": 10
}
```

Response


```
{
  "status": "success",
  "file_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Si_template\\log/logfile.log",
  "lines_requested": 10,
  "lines_returned": 10,
  "log_lines": [
    "777.PSIC> wh",
    "",
    "H K L =  -0.076827  -0.091461  3.9956\t Lambda = 0.7749 Two Theta = 33.163",
    "",
    "    Alpha      Beta       Psi       Tau       Qaz       Naz     Omega",
    "   4.7182   -4.8032   94.9678   90.1483   90.0000 -178.4364    0.0001",
    "",
    "       del        eta        chi        phi         nu         mu ",
    "  33.16289   16.58150   90.00000    0.00000    0.00000    0.00000 ",
    ""
  ],
  "file_size_bytes": 1147099,
  "last_modified_timestamp": 1749615577.911525,
  "message": "Successfully read 10 lines from X:\\bl17-2\\2025_06_Chen\\project_roots\\
}
```


Perfect! I can see we're positioned near the (0,0,4) reflection (the calculated HKL shows approximately (0, 0, 4)). Now let me take a detector image to see if we can locate the peak:

Execute Command: pd exposure search_004_initial 1.5

Prompt:

Please read the log and continue.

Response:

read_log

Request

```
{
  "lines": 10
}
```


Response


```
{
  "status": "success",
  "file_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Si_template\\log/logfile.log",
  "lines_requested": 10,
  "lines_returned": 10,
  "log_lines": [
    "ROI_7_X1=277; ROI_7_Y1=7; ROI_7_X2=279; ROI_7_Y2=187;",
    "ROI_8_X1=79; ROI_8_Y1=1; ROI_8_X2=479; ROI_8_Y2=193;",
    "ROI_9_X1=0; ROI_9_Y1=0; ROI_9_X2=0; ROI_9_Y2=0;",
    "ROI_10_X1=0; ROI_10_Y1=0; ROI_10_X2=0; ROI_10_Y2=0;",
    "ROI_11_X1=0; ROI_11_Y1=0; ROI_11_X2=0; ROI_11_Y2=0;",
    "ROI_12_X1=0; ROI_12_Y1=0; ROI_12_X2=0; ROI_12_Y2=0;",
    "ROI_13_X1=0; ROI_13_Y1=0; ROI_13_X2=0; ROI_13_Y2=0;",
    "ROI_14_X1=0; ROI_14_Y1=0; ROI_14_X2=0; ROI_14_Y2=0;",
    "ROI_15_X1=0; ROI_15_Y1=0; ROI_15_X2=0; ROI_15_Y2=0;",
    "ROI_16_X1=0; ROI_16_Y1=0; ROI_16_X2=0; ROI_16_Y2=0;"
  ],
  "file_size_bytes": 1148974,
  "last_modified_timestamp": 1749615648.933663,
  "message": "Successfully read 10 lines from X:\\bl17-2\\2025_06_Chen\\project_roots\\
}
```


Let me check if the detector image was saved in the images directory:

explore_directory

Request


```
{
  "sort_by": "time",
  "show_recent": true,
  "directory_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Si_template\\images"
}
```


Response

Directory scan for: X:\bl17-2\2025_06_Chen\project_roots\Si_template\images
Scan time: 2025-06-10 21:21:10

---

images

- search_004_initial_061025-205806.pdi (1.5 KB), modified 21 seconds ago
- search_004_initial_061025-205806.raw (1.1 MB), modified 8 minutes ago
- test_061025-204212.pdi (1.5 KB), modified 16 minutes ago
- 115_peak_optimized_061025-203626.pdi (1.5 KB), modified 22 minutes ago
- test_061025-204212.raw (1.1 MB), modified 24 minutes ago
- 115_peak_optimized_061025-203626.raw (1.1 MB), modified 29 minutes ago
- 004_peak_optimized_061025-201556.pdi (1.5 KB), modified 42 minutes ago
- 004_peak_optimized_061025-201556.raw (1.1 MB), modified 50 minutes ago
- initial_004_search_061025-200423.pdi (1.5 KB), modified 54 minutes ago
- initial_004_search_061025-200423.raw (1.1 MB), modified 1 hour ago
- final_004_optimized_061025-195112.pdi (1.5 KB), modified 1 hour ago
- final_004_optimized_061025-195112.raw (1.1 MB), modified 1 hour ago
- initial_004_search_061025-193201.pdi (1.5 KB), modified 1 hour ago
- initial_004_search_061025-193201.raw (1.1 MB), modified 1 hour ago
- Si_115_final_optimized_061025-173643.pdi (1.5 KB), modified 3 hours ago
- Si_115_final_optimized_061025-173643.raw (1.1 MB), modified 3 hours ago
- Si_115_initial_search_061025-172534.pdi (1.5 KB), modified 3 hours ago
- Si_004_final_optimized_061025-171911.pdi (1.5 KB), modified 3 hours ago
- Si_115_initial_search_061025-172534.raw (1.1 MB), modified 3 hours ago
- Si_004_final_optimized_061025-171911.raw (1.1 MB), modified 3 hours ago
- Si_004_initial_search_061025-170859.pdi (1.5 KB), modified 3 hours ago
- Si_004_initial_search_061025-170859.raw (1.1 MB), modified 3 hours ago
- specular_004_search_061025-165336.pdi (1.5 KB), modified 4 hours ago
- specular_004_search_061025-165336.raw (1.1 MB), modified 4 hours ago
- Si_004_final_optimized_restart_061025_061025-151601.pdi (1.5 KB), modified 5 hours
- Si_004_final_optimized_restart_061025_061025-151601.raw (1.1 MB), modified 5 hours
- Si_004_search_restart_061025_061025-150123.pdi (1.5 KB), modified 5 hours ago
- Si_004_search_restart_061025_061025-150123.raw (1.1 MB), modified 6 hours ago
- peak_neg1neg15_phi_optimized_061025-143728.pdi (1.5 KB), modified 6 hours ago
- peak_neg1neg15_initial_061025-143022.pdi (1.5 KB), modified 6 hours ago
- peak_neg1neg15_phi_optimized_061025-143728.raw (1.1 MB), modified 6 hours ago
- peak_neg1neg15_initial_061025-143022.raw (1.1 MB), modified 6 hours ago
- peak_004_eta_optimized_061025-141248.pdi (1.5 KB), modified 6 hours ago
- peak_004_eta_optimized_061025-141248.raw (1.1 MB), modified 6 hours ago
- peak_004_initial_061025-140421.pdi (1.5 KB), modified 6 hours ago
- peak_004_initial_061025-140421.raw (1.1 MB), modified 7 hours ago
- initial_004_search_061025-132917.pdi (1.5 KB), modified 7 hours ago
- initial_004_search_061025-132917.raw (1.1 MB), modified 7 hours ago
- 004_optimized_061025-131703.pdi (1.5 KB), modified 7 hours ago

004_eta_optimized_061025-131028.pdi (1.5 KB), modified 7 hours ago
004_optimized_061025-131703.raw (1.1 MB), modified 7 hours ago
004_initial_061025-130647.pdi (1.5 KB), modified 7 hours ago
004_eta_optimized_061025-131028.raw (1.1 MB), modified 7 hours ago
004_initial_061025-130647.raw (1.1 MB), modified 7 hours ago
peak_115_optimized_061025-124951.pdi (1.5 KB), modified 8 hours ago
peak_115_optimized_061025-124951.raw (1.1 MB), modified 8 hours ago
peak_115_initial_061025-122959.pdi (1.5 KB), modified 8 hours ago
peak_004_optimized_061025-122253.pdi (1.5 KB), modified 8 hours ago
peak_115_initial_061025-122959.raw (1.1 MB), modified 8 hours ago
peak_004_optimized_061025-122253.raw (1.1 MB), modified 8 hours ago
peak_004_initial_061025-121046.pdi (1.5 KB), modified 8 hours ago
peak_004_initial_061025-121046.raw (1.1 MB), modified 8 hours ago
115_final_optimized_061025-120033.pdi (1.5 KB), modified 8 hours ago
115_final_optimized_061025-120033.raw (1.1 MB), modified 9 hours ago
004_final_optimized_061025-113404.pdi (1.5 KB), modified 9 hours ago
004_final_optimized_061025-113404.raw (1.1 MB), modified 9 hours ago
initial_004_search_061025-111535.pdi (1.5 KB), modified 9 hours ago
initial_004_search_061025-111535.raw (1.1 MB), modified 9 hours ago
Si_004_final_optimized_061025_061025-105036.pdi (1.5 KB), modified 10 hours ago
Si_004_final_optimized_061025_061025-105036.raw (1.1 MB), modified 10 hours ago
Si_004_search_061025_061025-103620.pdi (1.5 KB), modified 10 hours ago
Si_004_search_061025_061025-103620.raw (1.1 MB), modified 10 hours ago
Si_206_optimized_061025-084639.pdi (1.5 KB), modified 12 hours ago
Si_206_optimized_061025-084639.raw (1.1 MB), modified 12 hours ago
Si_206_initial_061025-082457.pdi (1.5 KB), modified 12 hours ago
Si_206_initial_061025-082457.raw (1.1 MB), modified 12 hours ago
Si_004_optimized_061025-080648.pdi (1.5 KB), modified 12 hours ago
Si_004_optimized_061025-080648.raw (1.1 MB), modified 12 hours ago
Si_004_initial_061025-075120.pdi (1.5 KB), modified 13 hours ago
Si_004_initial_061025-075120.raw (1.1 MB), modified 13 hours ago
115_optimized_061025-072206.pdi (1.5 KB), modified 13 hours ago
115_optimized_061025-072206.raw (1.1 MB), modified 13 hours ago
115_initial_061025-070318.pdi (1.5 KB), modified 13 hours ago
004_optimized_061025-065647.pdi (1.5 KB), modified 14 hours ago
115_initial_061025-070318.raw (1.1 MB), modified 14 hours ago
004_optimized_061025-065647.raw (1.1 MB), modified 14 hours ago
004_initial_061025-063749.pdi (1.5 KB), modified 14 hours ago
004_initial_061025-063749.raw (1.1 MB), modified 14 hours ago
optimized_115_final_061025-060715.pdi (1.5 KB), modified 14 hours ago
optimized_115_final_061025-060715.raw (1.1 MB), modified 14 hours ago
search_115_initial_061025-054926.pdi (1.5 KB), modified 15 hours ago
search_115_initial_061025-054926.raw (1.1 MB), modified 15 hours ago

- optimized_004_final_061025-053910.pdi (1.5 KB), modified 15 hours ago
- optimized_004_final_061025-053910.raw (1.1 MB), modified 15 hours ago
- first_004_search_061025-052021.pdi (1.5 KB), modified 15 hours ago
- first_004_search_061025-052021.raw (1.1 MB), modified 15 hours ago
- optimized_115_final_061025-050007.pdi (1.5 KB), modified 15 hours ago
- optimized_115_final_061025-050007.raw (1.1 MB), modified 16 hours ago
- search_115_initial_061025-044643.pdi (1.5 KB), modified 16 hours ago
- optimized_004_final_061025-043939.pdi (1.5 KB), modified 16 hours ago
- search_115_initial_061025-044643.raw (1.1 MB), modified 16 hours ago
- optimized_004_final_061025-043939.raw (1.1 MB), modified 16 hours ago
- initial_004_check_061025-043141.pdi (1.5 KB), modified 16 hours ago
- initial_004_check_061025-043141.raw (1.1 MB), modified 16 hours ago
- search_115_initial_061025-035741.pdi (1.5 KB), modified 17 hours ago
- search_115_initial_061025-035741.raw (1.1 MB), modified 17 hours ago
- spec_004_optimized_061025-033556.pdi (1.5 KB), modified 17 hours ago
- spec_004_optimized_061025-033556.raw (1.1 MB), modified 17 hours ago
- spec_004_initial_061025-031646.pdi (1.5 KB), modified 17 hours ago
- spec_004_initial_061025-031646.raw (1.1 MB), modified 17 hours ago
- peak_004_initial_061025-024731.pdi (1.5 KB), modified 18 hours ago
- peak_004_initial_061025-024731.raw (1.1 MB), modified 18 hours ago

```
====================================== RECENT FILES ==================================

Most recent *.log files:
  No matching files found
Most recent *.raw files:
  search_004_initial_061025-205806.raw (modified: 2025-06-10 21:13:00)
  test_061025-204212.raw (modified: 2025-06-10 20:57:06)
  115_peak_optimized_061025-203626.raw (modified: 2025-06-10 20:51:20)
  004_peak_optimized_061025-201556.raw (modified: 2025-06-10 20:30:50)
  initial_004_search_061025-200423.raw (modified: 2025-06-10 20:19:17)
Most recent *.spec files:
  No matching files found
Most recent *.yaml files:
  No matching files found
Most recent *.cif files:
  No matching files found
```

Perfect! I can see the image was saved as `search_004_initial_061025-205806.raw`. Let me view this detector image:

read_and_plot_image

Request


```
{
  "image_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Si_template\\images\\search_0
}
```


I can see the detector image shows mostly background with the ROI (dashed white lines) but no clear diffraction peak. This is similar to your first reference image with no peak. Let me perform an eta scan to search for the (0,0,4) peak, as there might be some misalignment. I'll start with a broad scan:

Execute Command: dscan eta -2 2 40 0.5

Prompt:

Please read the log and continue.

Response:

read_log

Request


```
{
  "lines": 15
}
```


Response

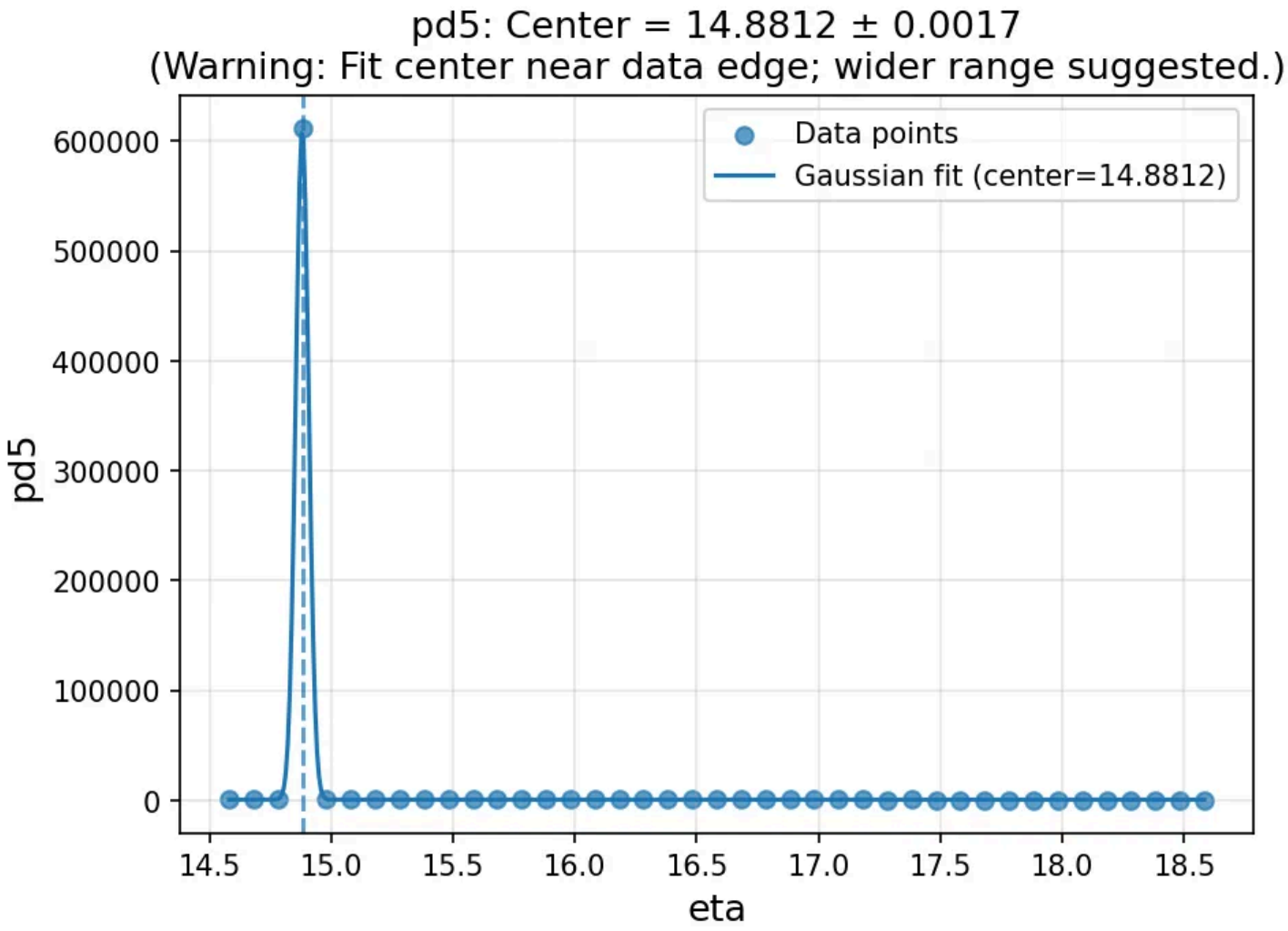
```
{
  "status": "success",
  "file_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Si_template\\log/logfile.log",
  "lines_requested": 15,
  "lines_returned": 15,
  "log_lines": [
    "   38,   18.3815,   0.5000,  0.87069,        0,  0.00555,  0.00471,        0,
    "Shutter open.",
    "Shutter closed.",
    " 39   18.4815      0.5      0.5        0.5   0.8708        0  0.00558  0.00471
    "18.481504 -0.16199089 -0.19284789 3.9894509 64485.431 0.87084 0 0.00558 0.00471 0
    "   39,   18.4815,   0.5000,  0.87084,        0,  0.00558,  0.00471,        0,
    "Shutter open.",
    "Shutter closed.",
    " 40   18.5815      0.5      0.5        0.5   0.8691        0  0.00569  0.00471
    "18.581504 -0.1664691 -0.19817914 3.9890052 64486.354 0.86914 0 0.00569 0.00471 0 0
    "   40,   18.5815,   0.5000,  0.86914,        0,  0.00569,  0.00471,        0,
    "/home/det/p2_det/images/mpy_spec_scan131*",
    "",
    "Returning eta to 16.5815",
    ""
  ],
  "file_size_bytes": 1190957,
  "last_modified_timestamp": 1749615740.0011218,
  "message": "Successfully read 15 lines from X:\\bl17-2\\2025_06_Chen\\project_roots\\
}
```


Great! I can see the scan (scan #131) completed and the eta motor has been returned to 16.5815°. Now let me plot the results of this eta scan to see if we found the peak:

read_and_plot_spec

Request


```
{
  "fit_type": "gaussian",
  "x_column": "eta",
  "y_columns": "pd5",
  "scan_number": "131",
  "spec_file_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Si_template\\spec\\spec"
}
```



Excellent! I found a very strong peak at eta = 14.8812°. This is clearly the (0,0,4) specular reflection. The peak is very sharp and intense (about 600,000 counts), which is characteristic of a strong diffraction peak. I can see the fit center is near the data edge, so let me perform a fine scan to get better resolution around this peak center.

First, let me move to the optimal eta position:

Execute Command: umv eta 14.8812

Prompt:

Please read the log and continue.

Response:

read_log

Request


```
{
  "lines": 10
}
```


Response


```
{
  "status": "success",
  "file_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Si_template\\log/logfile.log",
  "lines_requested": 10,
  "lines_returned": 10,
  "log_lines": [
    "       eta ",
    "  16.56787 ",
    "  15.74066 ",
    "  14.86928 ",
    "  14.84213 ",
    "  14.88119 ",
    "  14.88119 ",
    "  14.88119 ",
    "",
    ""
  ],
  "file_size_bytes": 1191083,
  "last_modified_timestamp": 1749615783.0148108,
  "message": "Successfully read 10 lines from X:\\bl17-2\\2025_06_Chen\\project_roots\\
}
```


Good! Now I'm at the optimal eta position. The peak was very sharp, so I need to do a fine scan to get better sampling. Based on the previous scan, I estimate the FWHM is very small, so I'll do a fine scan with smaller step size around this position:

Execute Command: dscan eta -0.2 0.2 40 0.5

Prompt:

Please read the log and continue.

Response:

read_log

Request


```
{
  "lines": 15
}
```


Response

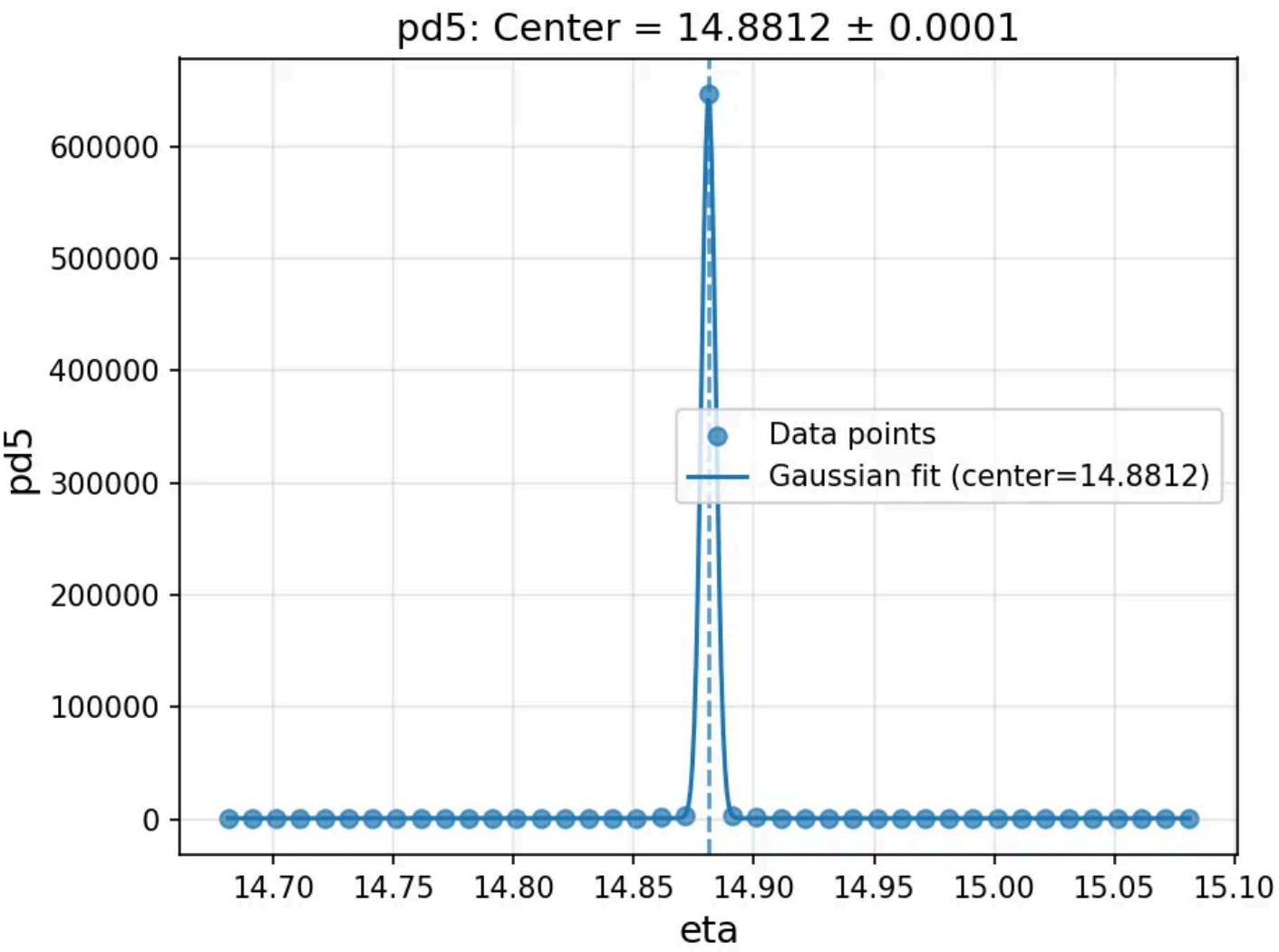

```
{
  "status": "success",
  "file_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Si_template\\log/logfile.log",
  "lines_requested": 15,
  "lines_returned": 15,
  "log_lines": [
    "   38,   15.0612,   0.5000,   0.8644,        0,  0.00549,  0.00468,        0,
    "Shutter open.",
    "Shutter closed.",
    " 39   15.0712      0.5      0.5        0.5   0.8624        0  0.00553  0.00468
    "15.071191 -0.0090645851 -0.010791239 3.997368 64647.257 0.86243 0 0.00553 0.00468
    "   39,   15.0712,   0.5000,  0.86243,        0,  0.00553,  0.00468,        0,
    "Shutter open.",
    "Shutter closed.",
    " 40   15.0812      0.5      0.5        0.5   0.8653        0  0.00562  0.00468
    "15.081191 -0.00951332 -0.011325452 3.9973655 64648.045 0.86531 0 0.00562 0.00468 0
    "   40,   15.0812,   0.5000,  0.86531,        0,  0.00562,  0.00468,        0,
    "/home/det/p2_det/images/mpy_spec_scan132*",
    "",
    "Returning eta to 14.8812",
    ""
  ],
  "file_size_bytes": 1233379,
  "last_modified_timestamp": 1749615901.0827024,
  "message": "Successfully read 15 lines from X:\\bl17-2\\2025_06_Chen\\project_roots\\
}
```


Good! Let me plot this fine scan (scan #132) to see the detailed peak profile:

read_and_plot_spec

Request


```
{
  "fit_type": "gaussian",
  "x_column": "eta",
  "y_columns": "pd5",
  "scan_number": "132",
  "spec_file_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Si_template\\spec\\spec"
}
```

Perfect! The fine scan shows a beautifully resolved peak with excellent sampling. The peak center is at eta = 14.8812° with very high precision (±0.0001°). Now I need to move to this optimal position and then proceed to optimize the del angle for the vertical position of the peak.

Execute Command: umv eta 14.8812

Prompt:

Please read the log and continue.

Response:

read_log

Request


```
{
  "lines": 10
}
```


Response


```
{
  "status": "success",
  "file_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Si_template\\log/logfile.log",
  "lines_requested": 10,
  "lines_returned": 10,
  "log_lines": [
    " 40   15.0812      0.5      0.5        0.5   0.8653        0  0.00562  0.00468
    "15.081191 -0.00951332 -0.011325452 3.9973655 64648.045 0.86531 0 0.00562 0.00468 0
    "   40,   15.0812,   0.5000,  0.86531,        0,  0.00562,  0.00468,        0,
    "/home/det/p2_det/images/mpy_spec_scan132*",
    "",
    "Returning eta to 14.8812",
    "",
    "",
    "782.PSIC> umv eta 14.8812",
    ""
  ],
  "file_size_bytes": 1233407,
  "last_modified_timestamp": 1749615981.1069858,
  "message": "Successfully read 10 lines from X:\\bl17-2\\2025_06_Chen\\project_roots\\
}
```


Good! Now I'm positioned at the optimal eta angle. Now I need to scan the del angle to optimize the vertical position of the peak on the detector. Let me perform a del scan:

Execute Command: dscan del -1 1 40 0.5

Prompt:

Please read the log and continue.

Response:

read_log

Request


```
{
  "lines": 15
}
```


Response

```
{
  "status": "success",
  "file_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Si_template\\log/logfile.log",
  "lines_requested": 15,
  "lines_returned": 15,
  "log_lines": [
    "   38,   34.0629,   0.5000,   0.8671,        0,   0.0056,  0.00462,        0,
    "Shutter open.",
    "Shutter closed.",
    " 39   34.1129      0.5      0.5        0.5   0.8695        0  0.00565  0.00462
    "34.112891 0.021353977 0.02542164 4.1084164 64807.135 0.86952 0 0.00565 0.00462 0 0
    "   39,   34.1129,   0.5000,  0.86952,        0,  0.00565,  0.00462,        0,
    "Shutter open.",
    "Shutter closed.",
    " 40   34.1629      0.5      0.5        0.5   0.8675        0  0.00567  0.00465
    "34.162891 0.022538984 0.026832375 4.114244 64808.030 0.86749 0 0.00567 0.00465 0 0
    "   40,   34.1629,   0.5000,  0.86749,        0,  0.00567,  0.00465,        0,
    "/home/det/p2_det/images/mpy_spec_scan133*",
    "",
    "Returning del to 33.1629",
    ""
  ],
  "file_size_bytes": 1275810,
  "last_modified_timestamp": 1749616062.171286,
  "message": "Successfully read 15 lines from X:\\bl17-2\\2025_06_Chen\\project_roots\\
}
```


I can see very high count rates (around 620,000-630,000) which suggests we found the peak! Let me plot this del scan (scan #133):

read_and_plot_spec

Request


```
{
  "fit_type": "gaussian",
  "x_column": "del",
  "y_columns": "pd5",
  "scan_number": "133",
  "spec_file_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Si_template\\spec\\spec"
}
```

Response

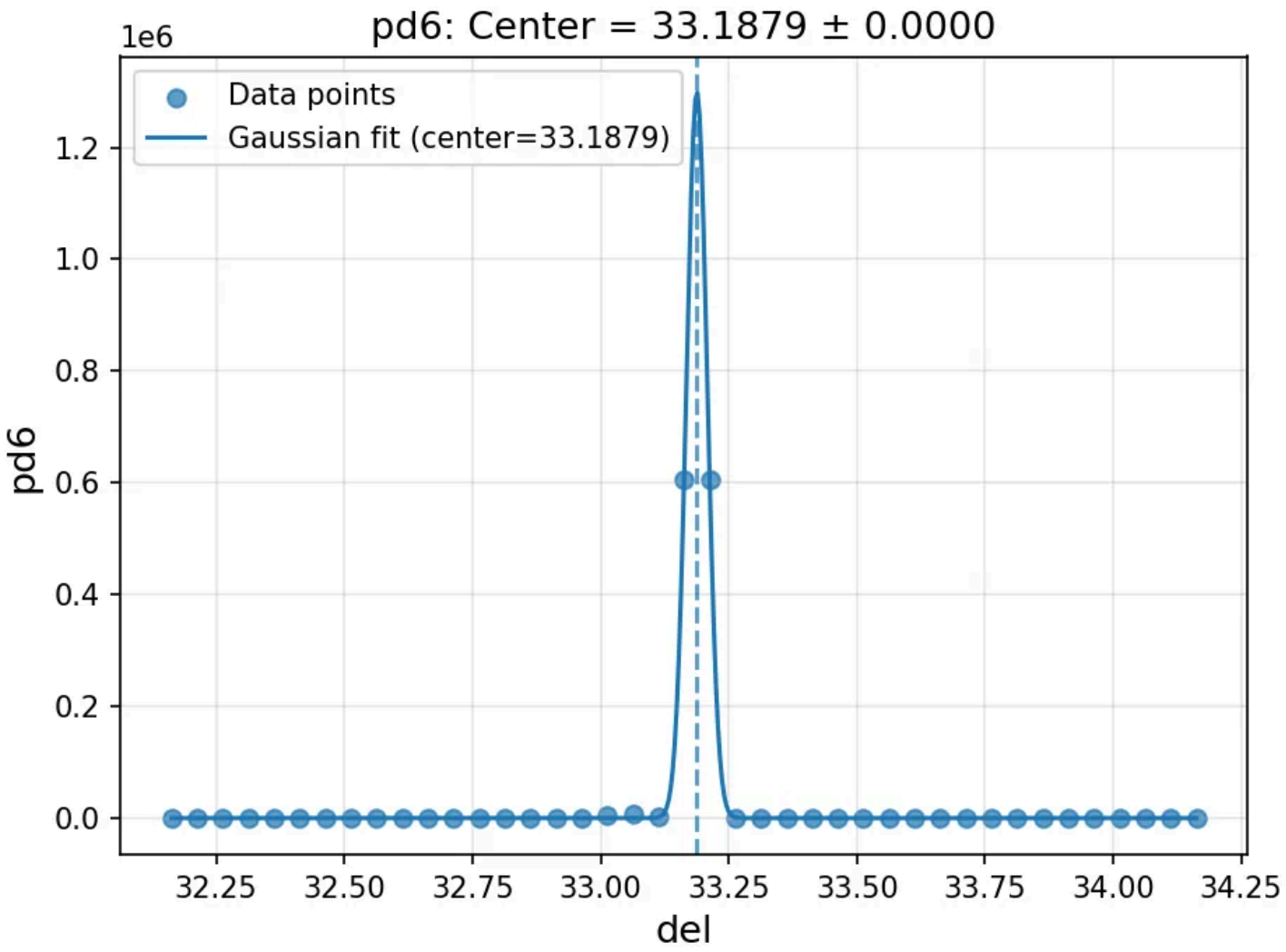

```
{
  "status": "error",
  "spec_file_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Si_template\\spec\\spec",
  "scan_number": "133",
  "error": "Invalid y_column for del. For del, y_column must be 'pd6'.",
  "error_type": "ValueError",
  "message": "Failed to read and plot SPEC data: Invalid y_column for del. For del, y_c
}
```


Ah, I need to use pd6 for del scans. Let me correct that:

read_and_plot_spec

Request


```
{
  "fit_type": "gaussian",
  "x_column": "del",
  "y_columns": "pd6",
  "scan_number": "133",
  "spec_file_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Si_template\\spec\\spec"
}
```



Excellent! I found a very strong peak centered at del = 33.1879°. Now let me move to this optimal del position:

Execute Command: umv del 33.1879

Prompt:

Please read the log and continue.

Response:

read_log

Request

```
{
  "lines": 10
}
```


Response


```
{
  "status": "success",
  "file_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Si_template\\log/logfile.log",
  "lines_requested": 10,
  "lines_returned": 10,
  "log_lines": [
    "",
    "784.PSIC> umv del 33.1879",
    "",
    "       del ",
    "  33.16967 ",
    "  33.18789 ",
    "  33.18789 ",
    "  33.18789 ",
    "",
    ""
  ],
  "file_size_bytes": 1275900,
  "last_modified_timestamp": 1749616106.1879923,
  "message": "Successfully read 10 lines from X:\\bl17-2\\2025_06_Chen\\project_roots\\
}
```


Perfect! Now let me take a detector image to confirm the peak is well-centered:

Execute Command: pd exposure 004_optimized 1.5

Prompt:

Please read the log and continue.

Response:

read_log

Request


```
{
  "lines": 10
}
```


Response


```
{
  "status": "success",
  "file_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Si_template\\log/logfile.log",
  "lines_requested": 10,
  "lines_returned": 10,
  "log_lines": [
    "ROI_7_X1=277; ROI_7_Y1=7; ROI_7_X2=279; ROI_7_Y2=187;",
    "ROI_8_X1=79; ROI_8_Y1=1; ROI_8_X2=479; ROI_8_Y2=193;",
    "ROI_9_X1=0; ROI_9_Y1=0; ROI_9_X2=0; ROI_9_Y2=0;",
    "ROI_10_X1=0; ROI_10_Y1=0; ROI_10_X2=0; ROI_10_Y2=0;",
    "ROI_11_X1=0; ROI_11_Y1=0; ROI_11_X2=0; ROI_11_Y2=0;",
    "ROI_12_X1=0; ROI_12_Y1=0; ROI_12_X2=0; ROI_12_Y2=0;",
    "ROI_13_X1=0; ROI_13_Y1=0; ROI_13_X2=0; ROI_13_Y2=0;",
    "ROI_14_X1=0; ROI_14_Y1=0; ROI_14_X2=0; ROI_14_Y2=0;",
    "ROI_15_X1=0; ROI_15_Y1=0; ROI_15_X2=0; ROI_15_Y2=0;",
    "ROI_16_X1=0; ROI_16_Y1=0; ROI_16_X2=0; ROI_16_Y2=0;"
  ],
  "file_size_bytes": 1277805,
  "last_modified_timestamp": 1749616146.2016342,
  "message": "Successfully read 10 lines from X:\\bl17-2\\2025_06_Chen\\project_roots\\
}
```


Let me check for the detector image:

explore_directory

Request

```
{
  "sort_by": "time",
  "show_recent": true,
  "file_pattern": "*.raw",
  "directory_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Si_template\\images"
}
```


Response

Directory scan for: X:\bl17-2\2025_06_Chen\project_roots\Si_template\images
Scan time: 2025-06-10 21:29:23

---

images

- 004_optimized_061025-210624.raw (1.1 MB), modified 8 minutes ago
- search_004_initial_061025-205806.raw (1.1 MB), modified 16 minutes ago
- test_061025-204212.raw (1.1 MB), modified 32 minutes ago
- 115_peak_optimized_061025-203626.raw (1.1 MB), modified 38 minutes ago
- 004_peak_optimized_061025-201556.raw (1.1 MB), modified 58 minutes ago
- initial_004_search_061025-200423.raw (1.1 MB), modified 1 hour ago
- final_004_optimized_061025-195112.raw (1.1 MB), modified 1 hour ago
- initial_004_search_061025-193201.raw (1.1 MB), modified 1 hour ago
- Si_115_final_optimized_061025-173643.raw (1.1 MB), modified 3 hours ago
- Si_115_initial_search_061025-172534.raw (1.1 MB), modified 3 hours ago
- Si_004_final_optimized_061025-171911.raw (1.1 MB), modified 3 hours ago
- Si_004_initial_search_061025-170859.raw (1.1 MB), modified 4 hours ago
- specular_004_search_061025-165336.raw (1.1 MB), modified 4 hours ago
- Si_004_final_optimized_restart_061025_061025-151601.raw (1.1 MB), modified 5 hours
- Si_004_search_restart_061025_061025-150123.raw (1.1 MB), modified 6 hours ago
- peak_neg1neg15_phi_optimized_061025-143728.raw (1.1 MB), modified 6 hours ago
- peak_neg1neg15_initial_061025-143022.raw (1.1 MB), modified 6 hours ago
- peak_004_eta_optimized_061025-141248.raw (1.1 MB), modified 7 hours ago
- peak_004_initial_061025-140421.raw (1.1 MB), modified 7 hours ago
- initial_004_search_061025-132917.raw (1.1 MB), modified 7 hours ago
- 004_optimized_061025-131703.raw (1.1 MB), modified 7 hours ago
- 004_eta_optimized_061025-131028.raw (1.1 MB), modified 8 hours ago
- 004_initial_061025-130647.raw (1.1 MB), modified 8 hours ago
- peak_115_optimized_061025-124951.raw (1.1 MB), modified 8 hours ago
- peak_115_initial_061025-122959.raw (1.1 MB), modified 8 hours ago
- peak_004_optimized_061025-122253.raw (1.1 MB), modified 8 hours ago
- peak_004_initial_061025-121046.raw (1.1 MB), modified 9 hours ago
- 115_final_optimized_061025-120033.raw (1.1 MB), modified 9 hours ago
- 004_final_optimized_061025-113404.raw (1.1 MB), modified 9 hours ago
- initial_004_search_061025-111535.raw (1.1 MB), modified 9 hours ago
- Si_004_final_optimized_061025_061025-105036.raw (1.1 MB), modified 10 hours ago
- Si_004_search_061025_061025-103620.raw (1.1 MB), modified 10 hours ago
- Si_206_optimized_061025-084639.raw (1.1 MB), modified 12 hours ago
- Si_206_initial_061025-082457.raw (1.1 MB), modified 12 hours ago
- Si_004_optimized_061025-080648.raw (1.1 MB), modified 13 hours ago
- Si_004_initial_061025-075120.raw (1.1 MB), modified 13 hours ago
- 115_optimized_061025-072206.raw (1.1 MB), modified 13 hours ago
- 115_initial_061025-070318.raw (1.1 MB), modified 14 hours ago
- 004_optimized_061025-065647.raw (1.1 MB), modified 14 hours ago

004_initial_061025-063749.raw (1.1 MB), modified 14 hours ago
optimized_115_final_061025-060715.raw (1.1 MB), modified 15 hours ago
search_115_initial_061025-054926.raw (1.1 MB), modified 15 hours ago
optimized_004_final_061025-053910.raw (1.1 MB), modified 15 hours ago
first_004_search_061025-052021.raw (1.1 MB), modified 15 hours ago
optimized_115_final_061025-050007.raw (1.1 MB), modified 16 hours ago
search_115_initial_061025-044643.raw (1.1 MB), modified 16 hours ago
optimized_004_final_061025-043939.raw (1.1 MB), modified 16 hours ago
initial_004_check_061025-043141.raw (1.1 MB), modified 16 hours ago
search_115_initial_061025-035741.raw (1.1 MB), modified 17 hours ago
spec_004_optimized_061025-033556.raw (1.1 MB), modified 17 hours ago
spec_004_initial_061025-031646.raw (1.1 MB), modified 17 hours ago
peak_004_initial_061025-024731.raw (1.1 MB), modified 18 hours ago

========== RECENT FILES ==========

Most recent *.raw files:
004_optimized_061025-210624.raw (modified: 2025-06-10 21:21:18)
search_004_initial_061025-205806.raw (modified: 2025-06-10 21:13:00)
test_061025-204212.raw (modified: 2025-06-10 20:57:06)
115_peak_optimized_061025-203626.raw (modified: 2025-06-10 20:51:20)
004_peak_optimized_061025-201556.raw (modified: 2025-06-10 20:30:50)

Great! Let me view the optimized detector image:

read_and_plot_image

Request


```
{
  "image_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Si_template\\images\\004_opti
}
```


Perfect! I can see a bright red diffraction peak well-centered at the intersection of the dashed white lines (ROI center). This is exactly what we want - the (0,0,4) specular peak is now properly optimized

and centered.

Now I need to optimize the lattice parameter 'c' based on the measured 2θ angle. Let me get the wavelength first and then optimize the lattice constant:

execute_code

Request


```
{
  "code": "\n# Get the wavelength from the experiment\nwavelength = expt.beam.wavelengt
  "session_id": "d0af72d4-4dea-4144-b6a1-2bff395d3af7"
}
```


Response

```
Output from session d0af72d4-4dea-4144-b6a1-2bff395d3af7:
Wavelength: 0.7749010390708725 Angstrom
```

Now let me optimize the lattice parameter 'c' using the measured 2θ = 33.1879°:

optimize_lattice_parameter

Request

```
{
  "H": 0,
  "K": 0,
  "L": 4,
  "a": 5.4307,
  "b": 5.4307,
  "c": 5.4307,
  "beta": 90,
  "alpha": 90,
  "gamma": 90,
  "store_as": "optimized_lattice",
  "session_id": "d0af72d4-4dea-4144-b6a1-2bff395d3af7",
  "wavelength": 0.7749,
  "target_param": "c",
  "two_theta_measured": 33.1879
}
```


Response

```
Lattice Parameter Optimization Results (Session: d0af72d4-4dea-4144-b6a1-2bff395d3af7):

Original Parameters:
  a = 5.430700 Å, b = 5.430700 Å, c = 5.430700 Å
  α = 90.000°, β = 90.000°, γ = 90.000°

Optimized Parameters:
  a = 5.430700 Å, b = 5.430700 Å, c = 5.426715 Å
  α = 90.000°, β = 90.000°, γ = 90.000°

Optimization Details:
  Target parameter: c
  Original value: 5.430700
  Optimized value: 5.426715
  Change: -0.003985 (-0.07%)

  Peak: (0.0, 0.0, 4.0)
  Measured 2θ: 33.188°
  d-spacing observed: 1.356679 Å
  d-spacing calculated: 1.356679 Å
  d-spacing error: 0.00000010 Å

  Optimization successful: True

Result stored as 'optimized_lattice' in session d0af72d4-4dea-4144-b6a1-2bff395d3af7
```

Excellent! The lattice parameter optimization shows that the 'c' parameter should be 5.426715 Å instead of the original 5.4307 Å. This is a small but significant correction. For a cubic crystal, all lattice parameters should be equal, so I'll update all three parameters to this optimized value:

Execute Command: setlat 5.426715 5.426715 5.426715 90 90 90

Prompt:

Please read the log and continue.

Response:

read_log

Request


```
{
  "lines": 10
}
```


Response


```
{
  "status": "success",
  "file_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Si_template\\log/logfile.log",
  "lines_requested": 10,
  "lines_returned": 10,
  "log_lines": [
    "ROI_14_X1=0; ROI_14_Y1=0; ROI_14_X2=0; ROI_14_Y2=0;",
    "ROI_15_X1=0; ROI_15_Y1=0; ROI_15_X2=0; ROI_15_Y2=0;",
    "ROI_16_X1=0; ROI_16_Y1=0; ROI_16_X2=0; ROI_16_Y2=0;",
    "",
    "786.PSIC> setlat 5.426715 5.426715 5.426715 90 90 90",
    "#C Tue Jun 10 21:07:52 2025.  g_aa reset from 5.42717 to 5.42671.",
    "#C Tue Jun 10 21:07:52 2025.  g_bb reset from 5.42717 to 5.42671.",
    "#C Tue Jun 10 21:07:52 2025.  g_cc reset from 5.42717 to 5.42671.",
    "Can't find orientation matrix:  Reflections are parallel.",
    ""
  ],
  "file_size_bytes": 1278116,
  "last_modified_timestamp": 1749616232.227014,
  "message": "Successfully read 10 lines from X:\\bl17-2\\2025_06_Chen\\project_roots\\
}
```


Perfect! The lattice parameters have been updated. The message "Can't find orientation matrix: Reflections are parallel" is expected since we haven't set up the UB matrix yet. Now I need to set this optimized (0,0,4) position as the primary orientation reflection:

Execute Command: or0 0 0 4

Prompt:

Please read the log and continue.

Response:

read_log

Request


```
{
  "lines": 10
}
```


Response


```
{
  "status": "success",
  "file_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Si_template\\log/logfile.log",
  "lines_requested": 10,
  "lines_returned": 10,
  "log_lines": [
    "#C Tue Jun 10 21:07:52 2025.  g_bb reset from 5.42717 to 5.42671.",
    "#C Tue Jun 10 21:07:52 2025.  g_cc reset from 5.42717 to 5.42671.",
    "Can't find orientation matrix:  Reflections are parallel.",
    "",
    "",
    "787.PSIC> or0 0 0 4",
    "#C Tue Jun 10 21:08:41 2025.  g_u00 reset from 33.1851 to 33.1879.",
    "#C Tue Jun 10 21:08:41 2025.  g_u01 reset from 14.8803 to 14.8812.",
    "Can't find orientation matrix:  Reflections are parallel.",
    ""
  ],
  "file_size_bytes": 1278330,
  "last_modified_timestamp": 1749616282.2428162,
  "message": "Successfully read 10 lines from X:\\bl17-2\\2025_06_Chen\\project_roots\\
}
```


Great! The primary orientation reflection (0,0,4) has been set. The system has recorded the motor positions (del=33.1879°, eta=14.8812°). The message "Can't find orientation matrix: Reflections are parallel" is expected since we need a second, non-parallel reflection to establish the UB matrix.

Now I need to find the second reference reflection. Based on the sample information and the constraints, I should look for a non-specular peak with `theta_minus_rel_angle > 2°` . Looking at the table, good candidates include:

1. (1,1,5) with theta_minus_rel_angle = 5.9667° and high intensity
2. (2,0,6) with theta_minus_rel_angle = 8.3872°
3. (3,1,7) with theta_minus_rel_angle = 8.9192°

Let me choose (1,1,5) since it has excellent intensity and a good theta_minus_rel_angle. For vertical geometry, I need to:

- Set eta = 5.9667° (the theta_minus_rel_angle value)
- Set del ≈ 2θ = 43.5197°
- Keep chi = 90°
- Scan phi to find the peak

Execute Command: umv eta 5.9667 del 43.5197

Prompt:

Please read the log and continue.

Response:

read_log

Request


```
{
  "lines": 10
}
```


Response

```
{
  "status": "success",
  "file_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Si_template\\log/logfile.log",
  "lines_requested": 10,
  "lines_returned": 10,
  "log_lines": [
    "   5.96670   40.98080 ",
    "   5.96670   41.57654 ",
    "   5.96670   42.17160 ",
    "   5.96670   42.74844 ",
    "   5.96670   43.33936 ",
    "   5.96670   43.51971 ",
    "   5.96670   43.51971 ",
    "   5.96670   43.51971 ",
    "",
    ""
  ],
  "file_size_bytes": 1278854,
  "last_modified_timestamp": 1749616339.265731,
  "message": "Successfully read 10 lines from X:\\bl17-2\\2025_06_Chen\\project_roots\\
}
```


Good! The motors have moved to the calculated positions. Now I need to search for the (1,1,5) peak by scanning phi. Since this is a non-specular peak and I don't know the in-plane orientation, I'll start with a wide phi scan:

Execute Command: dscan phi -30 30 60 0.5

Prompt:

Please read the log and continue.

Response:

read_log

Request

```
{
  "lines": 15
}
```


Response


```
{
  "status": "success",
  "file_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Si_template\\log/logfile.log",
  "lines_requested": 15,
  "lines_returned": 15,
  "log_lines": [
    "   58,        28,   0.5000,   0.8643,        0,  0.00553,  0.00477,        0,
    "Shutter open.",
    "Shutter closed.",
    " 59   29.0000      0.5      0.5        0.5   0.8659        0  0.00563  0.00477
    "29 0.17401059 1.2724388 5.0314483 65192.681 0.86586 0 0.00563 0.00477 0 0 0 1.4907
    "   59,        29,   0.5000,  0.86586,        0,  0.00563,  0.00477,        0,
    "Shutter open.",
    "Shutter closed.",
    " 60   30.0000      0.5      0.5        0.5   0.8645        0  0.00551  0.00477
    "30 0.1497632 1.2769508 5.0310854 65193.790 0.86446 0 0.00551 0.00477 0 0 0 1.49200
    "   60,        30,   0.5000,  0.86446,        0,  0.00551,  0.00477,        0,
    "/home/det/p2_det/images/mpy_spec_scan134*",
    "",
    "Returning phi to 0",
    ""
  ],
  "file_size_bytes": 1338822,
  "last_modified_timestamp": 1749616450.3965137,
  "message": "Successfully read 15 lines from X:\\bl17-2\\2025_06_Chen\\project_roots\\
}
```


The scan completed. Let me plot the results to see if I found any peaks:

read_and_plot_spec

Request

```
{
  "fit_type": "tophat",
  "x_column": "phi",
  "y_columns": "pd5",
  "scan_number": "134",
  "spec_file_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Si_template\\spec\\spec"
}
```


Response

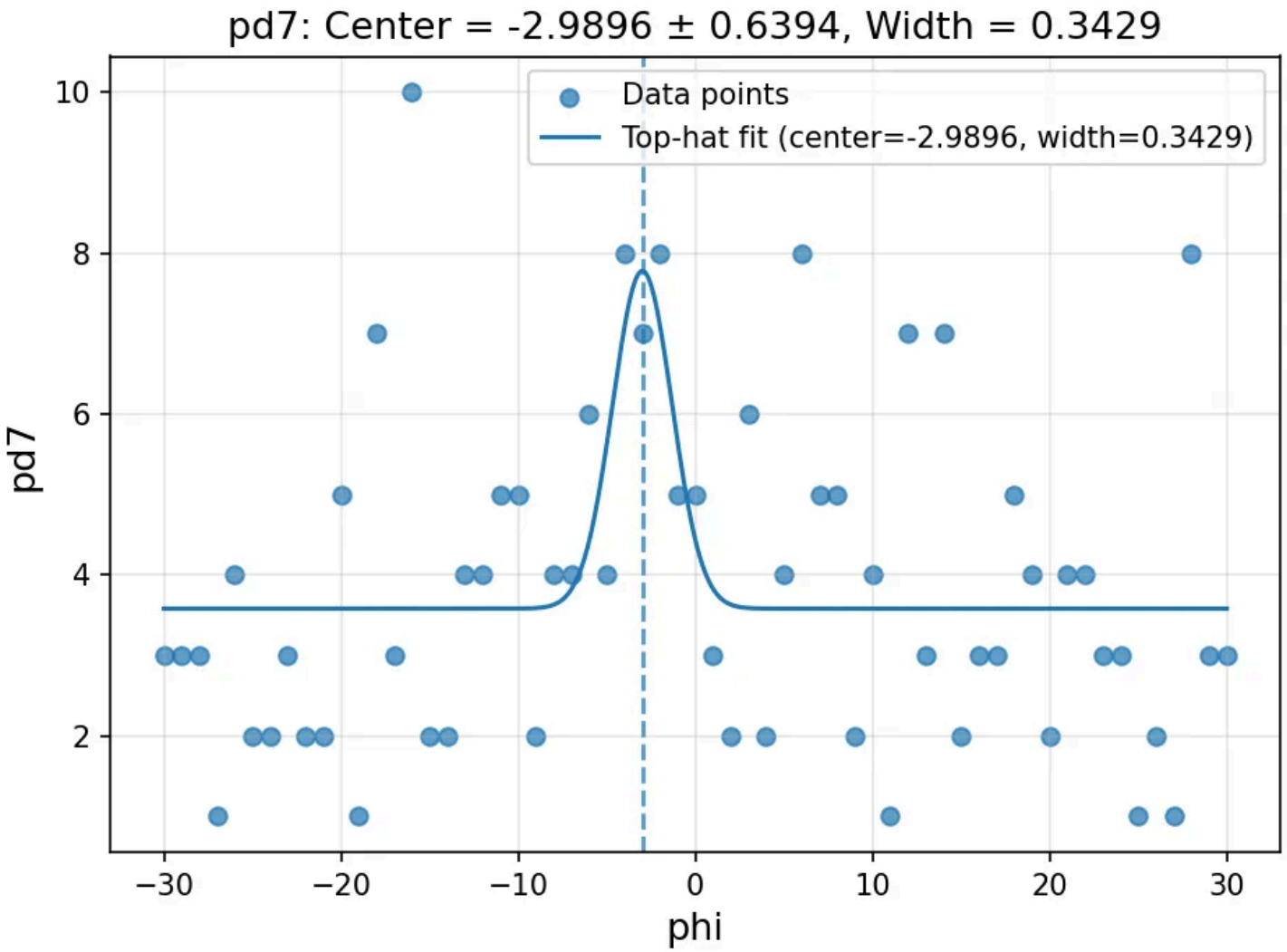

```
{
  "status": "error",
  "spec_file_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Si_template\\spec\\spec",
  "scan_number": "134",
  "error": "Invalid y_column for phi. For phi, y_column must be 'pd7'.",
  "error_type": "ValueError",
  "message": "Failed to read and plot SPEC data: Invalid y_column for phi. For phi, y_c
}
```


Let me use the correct ROI for phi scans:

read_and_plot_spec

Request


```
{
  "fit_type": "tophat",
  "x_column": "phi",
  "y_columns": "pd7",
  "scan_number": "134",
  "spec_file_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Si_template\\spec\\spec"
}
```



Excellent! I found a clear peak centered at phi ≈ -2.99°. The intensity is modest but clearly above background. This looks like the (1,1,5) peak! Let me move to this optimal phi position:

Execute Command: umv phi -2.9896

Prompt:

Please read the log and continue.

Response:

read_log

Request

```
{
  "lines": 10
}
```


Response


```
{
  "status": "success",
  "file_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Si_template\\log/logfile.log",
  "lines_requested": 10,
  "lines_returned": 10,
  "log_lines": [
    "       phi ",
    "  -0.02707 ",
    "  -1.60293 ",
    "  -3.02805 ",
    "  -3.02867 ",
    "  -2.98961 ",
    "  -2.98961 ",
    "  -2.98961 ",
    "",
    ""
  ],
  "file_size_bytes": 1338948,
  "last_modified_timestamp": 1749616512.4175086,
  "message": "Successfully read 10 lines from X:\\bl17-2\\2025_06_Chen\\project_roots\\
}
```


Good! Now I need to optimize this peak following the standard sequence. Since this peak was found with a broad scan, I should first do an eta scan to ensure the peak is properly optimized, then proceed with chi and del optimization. Let me start with an eta scan:

Execute Command: dscan eta -0.5 0.5 40 0.5

Prompt:

Please read the log and continue.

Response:

read_log

Request


```
{
  "lines": 15
}
```


Response

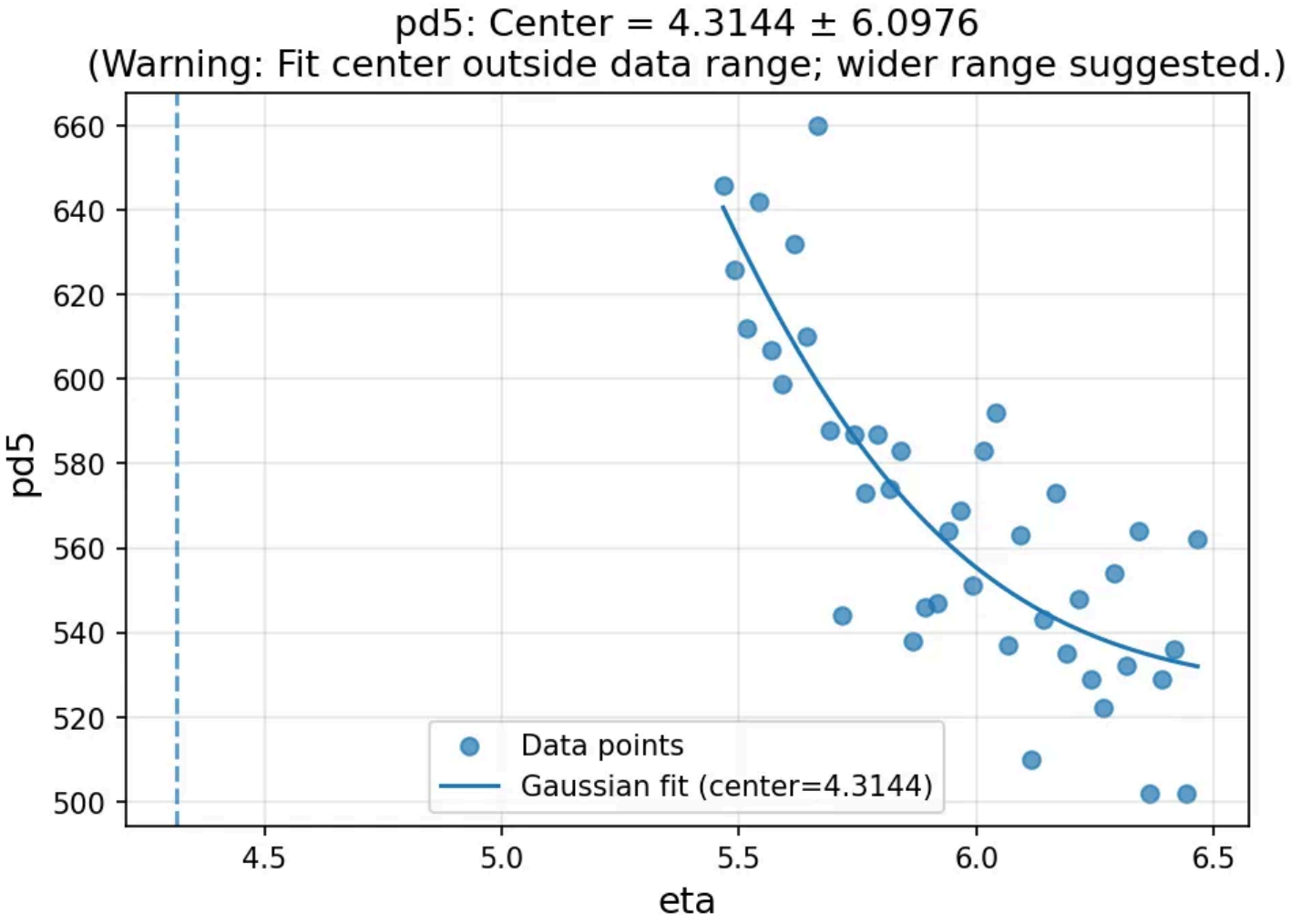

```
{
  "status": "success",
  "file_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Si_template\\log/logfile.log",
  "lines_requested": 15,
  "lines_returned": 15,
  "log_lines": [
    "   38,    6.4167,   0.5000,  0.87119,        0,  0.00557,   0.0048,        0,
    "Shutter open.",
    "Shutter closed.",
    " 39    6.4417      0.5      0.5        0.5    0.872        0  0.00553  0.00477
    "6.4416992 0.83927653 0.88790921 5.0469877 65325.966 0.87198 0 0.00553 0.00477 0 0
    "   39,    6.4417,   0.5000,  0.87198,        0,  0.00553,  0.00477,        0,
    "Shutter open.",
    "Shutter closed.",
    " 40    6.4667      0.5      0.5        0.5   0.8699        0  0.00565  0.00477
    "6.4666992 0.83777467 0.88629848 5.0475203 65326.797 0.8699 0 0.00565 0.00477 0 0 0
    "   40,    6.4667,   0.5000,   0.8699,        0,  0.00565,  0.00477,        0,
    "/home/det/p2_det/images/mpy_spec_scan135*",
    "",
    "Returning eta to 5.9667",
    ""
  ],
  "file_size_bytes": 1380720,
  "last_modified_timestamp": 1749616579.7995894,
  "message": "Successfully read 15 lines from X:\\bl17-2\\2025_06_Chen\\project_roots\\
}
```


Let me plot the eta scan results:

read_and_plot_spec

Request


```
{
  "fit_type": "gaussian",
  "x_column": "eta",
  "y_columns": "pd5",
  "scan_number": "135",
  "spec_file_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Si_template\\spec\\spec"
}
```

I can see there's a peak but the fit center is outside the data range. The peak appears to be around eta = 5.5-5.7°, not at the edges. The peak is declining from left to right, suggesting the maximum is to the left of my scan range. Let me do a wider scan to capture the full peak:

Execute Command: dscan eta -2 1 30 0.5

Prompt:

Please read the log and continue.

Response:

read_log

Request


```
{
  "lines": 15
}
```


Response

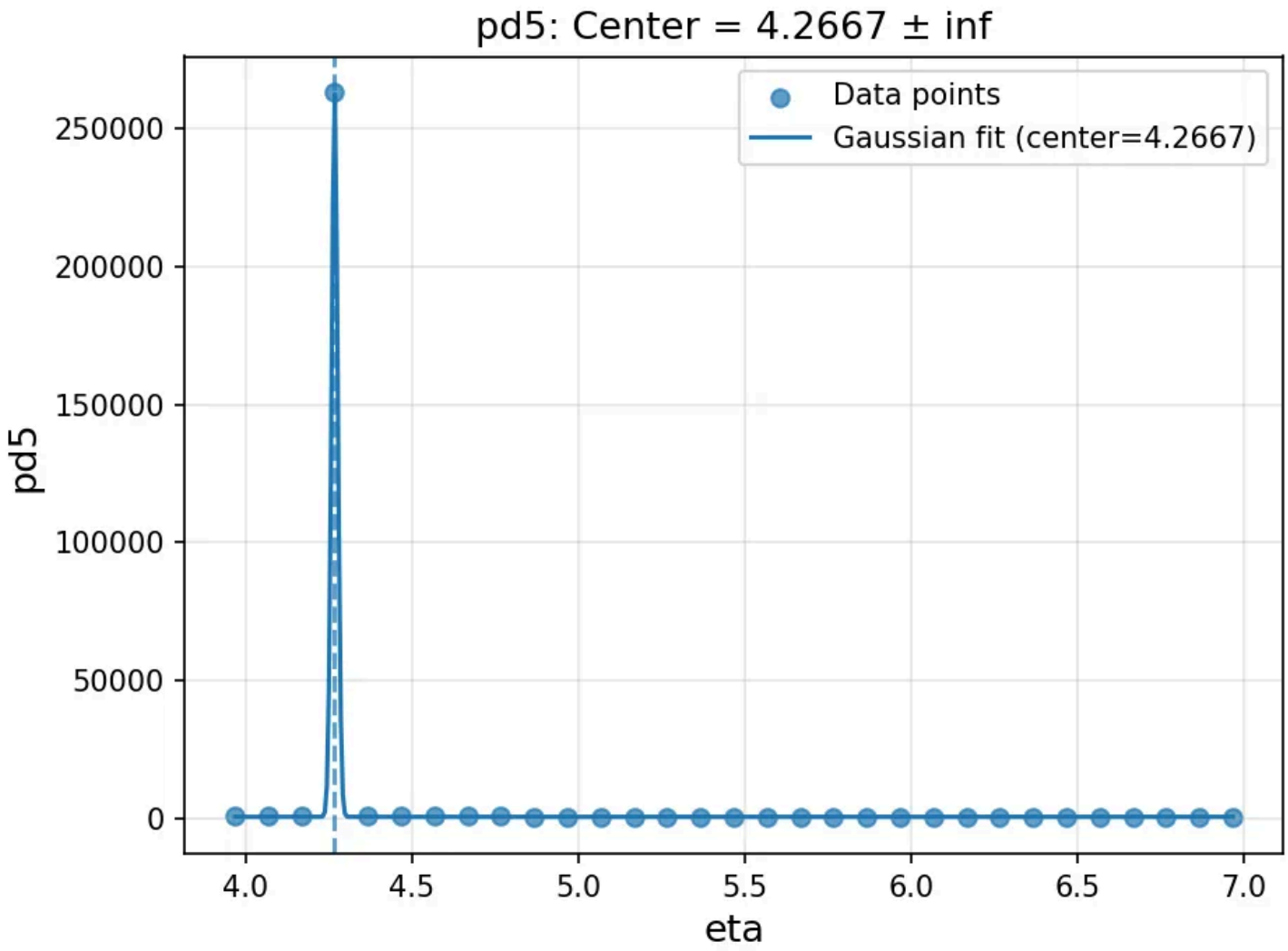
```
{
  "status": "success",
  "file_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Si_template\\log/logfile.log",
  "lines_requested": 15,
  "lines_returned": 15,
  "log_lines": [
    "   28,    6.7667,   0.5000,  0.87024,        0,  0.00573,  0.00471,        0,
    "Shutter open.",
    "Shutter closed.",
    " 29    6.8667      0.5      0.5        0.5   0.8681        0  0.00573  0.00474
    "6.8666992 0.8137234 0.86050399 5.0559114 65407.666 0.8681 0 0.00573 0.00474 0 0 0
    "   29,    6.8667,   0.5000,   0.8681,        0,  0.00573,  0.00474,        0,
    "Shutter open.",
    "Shutter closed.",
    " 30    6.9667      0.5      0.5        0.5   0.8667        0  0.00551  0.00474
    "6.9666992 0.80770434 0.85404877 5.0579706 65408.579 0.86668 0 0.00551 0.00474 0 0
    "   30,    6.9667,   0.5000,  0.86668,        0,  0.00551,  0.00474,        0,
    "/home/det/p2_det/images/mpy_spec_scan136*",
    "",
    "Returning eta to 5.9667",
    ""
  ],
  "file_size_bytes": 1413234,
  "last_modified_timestamp": 1749616662.5359166,
  "message": "Successfully read 15 lines from X:\\bl17-2\\2025_06_Chen\\project_roots\\
}
```


Let me plot this wider eta scan:

read_and_plot_spec

Request


```
{
  "fit_type": "gaussian",
  "x_column": "eta",
  "y_columns": "pd5",
  "scan_number": "136",
  "spec_file_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Si_template\\spec\\spec"
}
```



Excellent! I found a very strong peak at eta = 4.2667°. This is clearly the (1,1,5) peak with an intensity of about 250,000 counts! The peak is very sharp and well-defined. Let me move to this optimal eta position:

Execute Command: umv eta 4.2667

Prompt:

Please read the log and continue.

Response:

read_log

Request

```
{
  "lines": 10
}
```


Response


```
{
  "status": "success",
  "file_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Si_template\\log/logfile.log",
  "lines_requested": 10,
  "lines_returned": 10,
  "log_lines": [
    "       eta ",
    "   5.95334 ",
    "   5.14715 ",
    "   4.25510 ",
    "   4.22764 ",
    "   4.26670 ",
    "   4.26670 ",
    "   4.26670 ",
    "",
    ""
  ],
  "file_size_bytes": 1413359,
  "last_modified_timestamp": 1749616737.5611198,
  "message": "Successfully read 10 lines from X:\\bl17-2\\2025_06_Chen\\project_roots\\
}
```


Good! Now I need to perform a fine eta scan since this peak was very sharp and might need better sampling:

Execute Command: dscan eta -0.1 0.1 40 0.5

Prompt:

Please read the log and continue.

Response:

read_log

Request


```
{
  "lines": 15
}
```


Response

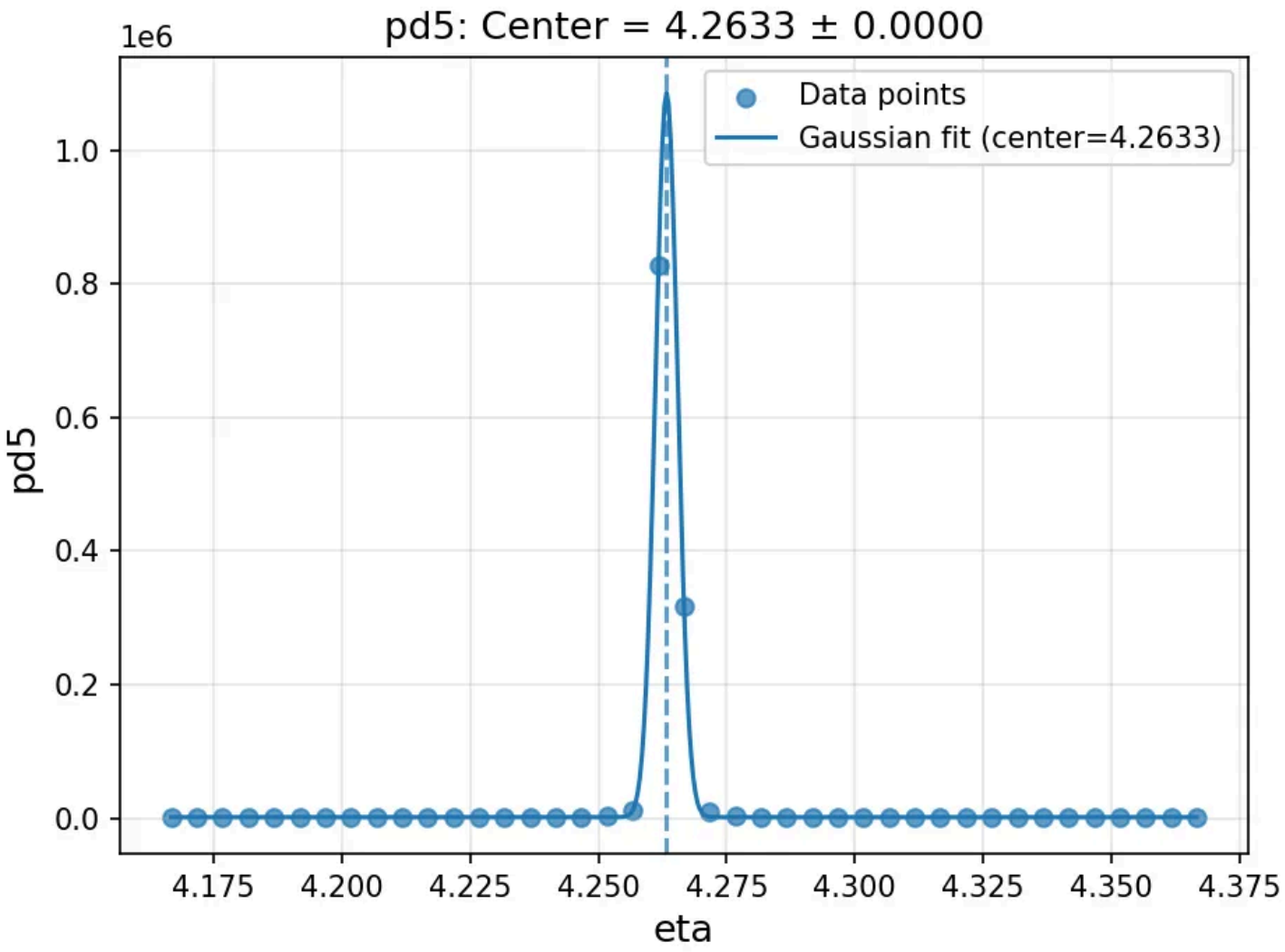

```
{
  "status": "success",
  "file_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Si_template\\log/logfile.log",
  "lines_requested": 15,
  "lines_returned": 15,
  "log_lines": [
    "   38,    4.3567,   0.5000,  0.87068,        0,  0.00573,   0.0048,        0,
    "Shutter open.",
    "Shutter closed.",
    " 39    4.3617      0.5      0.5        0.5   0.8722        0  0.00561  0.00477
    "4.3616992 0.96364427 1.0213008 4.9993187 65607.064 0.87218 0 0.00561 0.00477 0 0 0
    "   39,    4.3617,   0.5000,  0.87218,        0,  0.00561,  0.00477,        0,
    "Shutter open.",
    "Shutter closed.",
    " 40    4.3667      0.5      0.5        0.5   0.8719        0  0.00568  0.00474
    "4.3666992 0.96334677 1.0209817 4.9994412 65607.833 0.8719 0 0.00568 0.00474 0 0 0
    "   40,    4.3667,   0.5000,   0.8719,        0,  0.00568,  0.00474,        0,
    "/home/det/p2_det/images/mpy_spec_scan137*",
    "",
    "Returning eta to 4.2667",
    ""
  ],
  "file_size_bytes": 1455376,
  "last_modified_timestamp": 1749616860.6350942,
  "message": "Successfully read 15 lines from X:\\bl17-2\\2025_06_Chen\\project_roots\\
}
```


Let me plot the fine eta scan:

read_and_plot_spec

Request

```
{
  "fit_type": "gaussian",
  "x_column": "eta",
  "y_columns": "pd5",
  "scan_number": "137",
  "spec_file_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Si_template\\spec\\spec"
}
```

Perfect! The fine scan shows excellent resolution with the peak center at eta = 4.2633° and over 1 million counts! This is a very strong and well-resolved peak. Let me move to this optimal position:

Execute Command: umv eta 4.2633

Prompt:

Please read the log and continue.

Response:

read_log

Request


```
{
  "lines": 10
}
```


Response


```
{
  "status": "success",
  "file_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Si_template\\log/logfile.log",
  "lines_requested": 10,
  "lines_returned": 10,
  "log_lines": [
    "796.PSIC> umv eta 4.2633",
    "",
    "       eta ",
    "   4.25307 ",
    "   4.22424 ",
    "   4.26330 ",
    "   4.26330 ",
    "   4.26330 ",
    "",
    ""
  ],
  "file_size_bytes": 1455477,
  "last_modified_timestamp": 1749616905.6498163,
  "message": "Successfully read 10 lines from X:\\bl17-2\\2025_06_Chen\\project_roots\\
}
```


Excellent! Now I need to continue with the optimization sequence. Next, I should optimize chi:

Execute Command: dscan chi -1 1 40 0.5

Prompt:

Please read the log and continue.

Response:

read_log

Request


```
{
  "lines": 15
}
```


Response

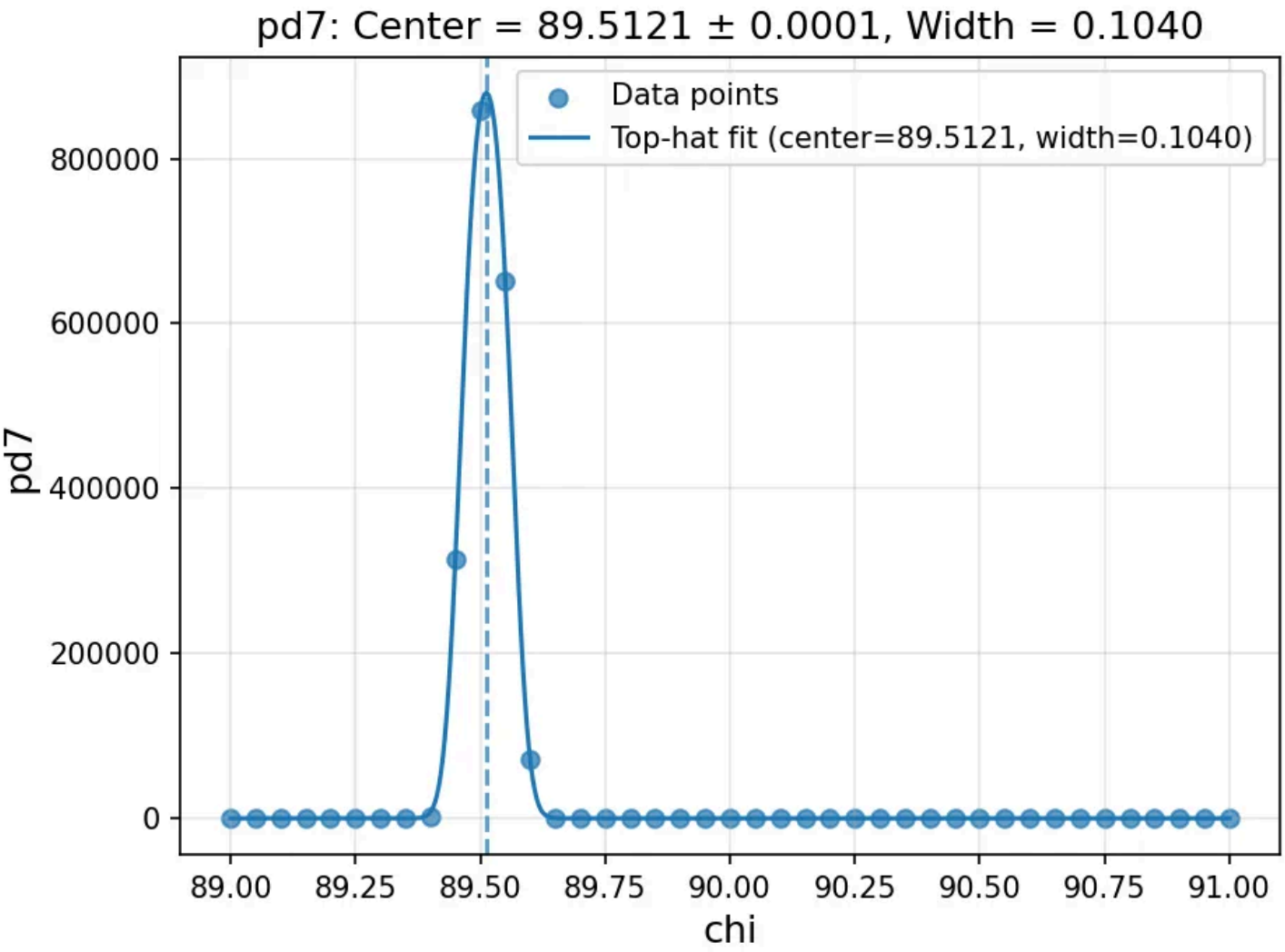
```
{
  "status": "success",
  "file_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Si_template\\log/logfile.log",
  "lines_requested": 15,
  "lines_returned": 15,
  "log_lines": [
    "   38,      90.9,   0.5000,  0.86715,        0,  0.00571,  0.00477,        0,
    "Shutter open.",
    "Shutter closed.",
    " 39   90.9500      0.5      0.5        0.5   0.8662        0  0.00555  0.00477
    "90.95 1.0295458 0.97157525 4.9960914 65724.211 0.86619 0 0.00555 0.00477 0 0 0 1.4
    "   39,     90.95,   0.5000,  0.86619,        0,  0.00555,  0.00477,        0,
    "Shutter open.",
    "Shutter closed.",
    " 40   91.0000      0.5      0.5        0.5   0.8685        0  0.00563  0.00477
    "91 1.0327066 0.96862883 4.9960112 65725.100 0.8685 0 0.00563 0.00477 0 0 0 1.49414
    "   40,        91,   0.5000,   0.8685,        0,  0.00563,  0.00477,        0,
    "/home/det/p2_det/images/mpy_spec_scan138*",
    "",
    "Returning chi to 90",
    ""
  ],
  "file_size_bytes": 1497727,
  "last_modified_timestamp": 1749616978.7409885,
  "message": "Successfully read 15 lines from X:\\bl17-2\\2025_06_Chen\\project_roots\\
}
```


I can see very high counts (around 700,000-800,000) which suggests we're on the peak! Let me plot the chi scan:

read_and_plot_spec

Request


```
{
  "fit_type": "tophat",
  "x_column": "chi",
  "y_columns": "pd7",
  "scan_number": "138",
  "spec_file_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Si_template\\spec\\spec"
}
```



Excellent! I found a strong peak centered at chi = 89.5121°. The peak intensity is about 850,000 counts. Let me move to this optimal chi position:

Execute Command: umv chi 89.5121

Prompt:

Please read the log and continue.

Response:

read_log

Request

```
{
  "lines": 10
}
```


Response


```
{
  "status": "success",
  "file_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Si_template\\log/logfile.log",
  "lines_requested": 10,
  "lines_returned": 10,
  "log_lines": [
    "",
    "       chi ",
    "  89.98664 ",
    "  89.49760 ",
    "  89.49258 ",
    "  89.51211 ",
    "  89.51211 ",
    "  89.51211 ",
    "",
    ""
  ],
  "file_size_bytes": 1497841,
  "last_modified_timestamp": 1749617041.7649999,
  "message": "Successfully read 10 lines from X:\\bl17-2\\2025_06_Chen\\project_roots\\
}
```


Great! Now I need to optimize del:

Execute Command: dscan del -1 1 40 0.5

Prompt:

Please read the log and continue.

Response:

read_log

Request


```
{
  "lines": 15
}
```


Response

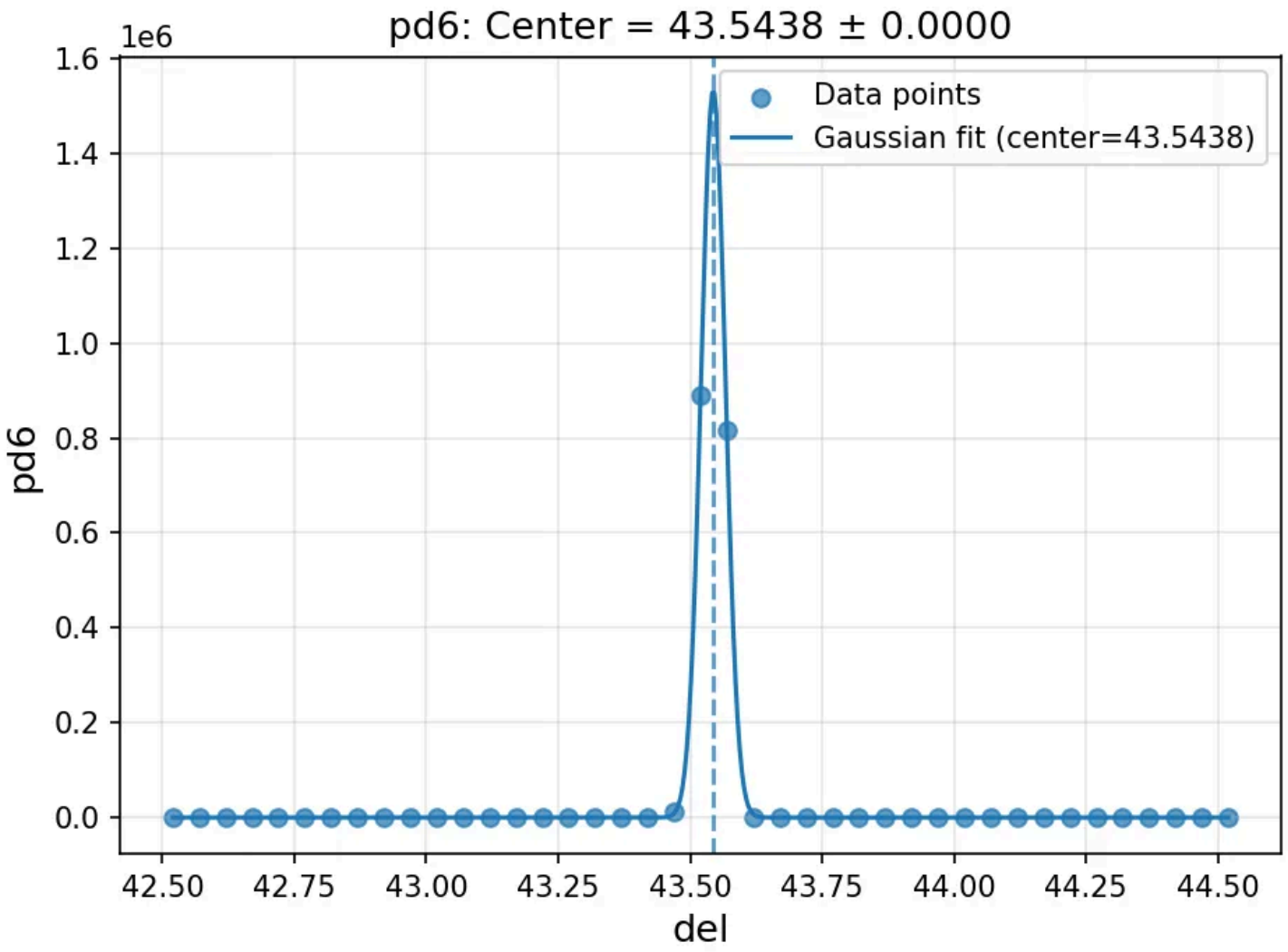

```
{
  "status": "success",
  "file_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Si_template\\log/logfile.log",
  "lines_requested": 15,
  "lines_returned": 15,
  "log_lines": [
    "   38,   44.4197,   0.5000,  0.87095,        0,  0.00552,  0.00468,        0,
    "Shutter open.",
    "Shutter closed.",
    " 39   44.4697      0.5      0.5        0.5   0.8726        0   0.0056  0.00471
    "44.469707 0.98701438 1.109072 5.0882642 65895.024 0.87261 0 0.0056 0.00471 0 0 0 1
    "   39,   44.4697,   0.5000,  0.87261,        0,   0.0056,  0.00471,        0,
    "Shutter open.",
    "Shutter closed.",
    " 40   44.5197      0.5      0.5        0.5   0.8715        0  0.00557  0.00471
    "44.519707 0.98958771 1.1118772 5.0930458 65895.971 0.87151 0 0.00557 0.00471 0 0 0
    "   40,   44.5197,   0.5000,  0.87151,        0,  0.00557,  0.00471,        0,
    "/home/det/p2_det/images/mpy_spec_scan139*",
    "",
    "Returning del to 43.5197",
    ""
  ],
  "file_size_bytes": 1540266,
  "last_modified_timestamp": 1749617149.8347337,
  "message": "Successfully read 15 lines from X:\\bl17-2\\2025_06_Chen\\project_roots\\
}
```


I can see very high counts (around 900,000) throughout the scan. Let me plot the del scan:

read_and_plot_spec

Request

```
{
  "fit_type": "gaussian",
  "x_column": "del",
  "y_columns": "pd6",
  "scan_number": "139",
  "spec_file_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Si_template\\spec\\spec"
}
```

Excellent! I found a very strong peak centered at del = 43.5438° with over 1.5 million counts! Let me move to this optimal del position:

Execute Command: umv del 43.5438

Prompt:

Please read the log and continue.

Response:

read_log

Request


```
{
  "lines": 10
}
```


Response


```
{
  "status": "success",
  "file_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Si_template\\log/logfile.log",
  "lines_requested": 10,
  "lines_returned": 10,
  "log_lines": [
    "",
    "800.PSIC> umv del 43.5438",
    "",
    "       del ",
    "  43.52646 ",
    "  43.54381 ",
    "  43.54381 ",
    "  43.54381 ",
    "",
    ""
  ],
  "file_size_bytes": 1540356,
  "last_modified_timestamp": 1749617201.8515682,
  "message": "Successfully read 10 lines from X:\\bl17-2\\2025_06_Chen\\project_roots\\
}
```


Perfect! Now I need to do at least one more complete optimization cycle as required. Let me continue with another eta scan:

Execute Command: dscan eta -0.1 0.1 40 0.5

Prompt:

Please read the log and continue.

Response:

read_log

Request


```
{
  "lines": 15
}
```


Response

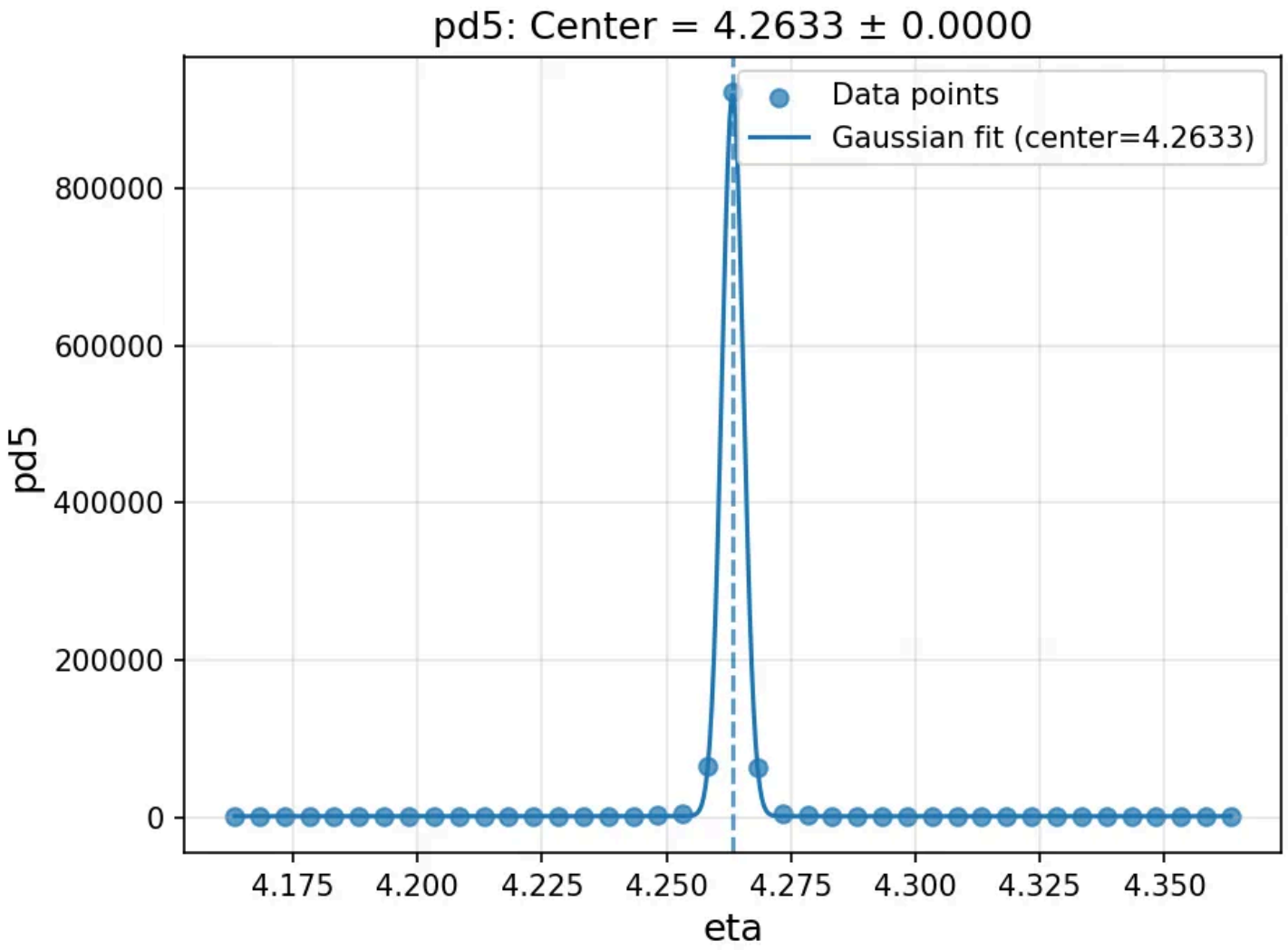
```
{
  "status": "success",
  "file_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Si_template\\log/logfile.log",
  "lines_requested": 15,
  "lines_returned": 15,
  "log_lines": [
    "   38,    4.3533,   0.5000,  0.86717,        0,  0.00569,  0.00468,        0,
    "Shutter open.",
    "Shutter closed.",
    " 39    4.3583      0.5      0.5        0.5   0.8663        0   0.0056  0.00471
    "4.3583008 0.93421163 1.0516286 5.0014599 66033.832 0.86627 0 0.0056 0.00471 0 0 0
    "   39,    4.3583,   0.5000,  0.86627,        0,   0.0056,  0.00471,        0,
    "Shutter open.",
    "Shutter closed.",
    " 40    4.3633      0.5      0.5        0.5   0.8649        0  0.00554  0.00471
    "4.3633008 0.93391315 1.0513102 5.0015826 66034.624 0.86487 0 0.00554 0.00471 0 0 0
    "   40,    4.3633,   0.5000,  0.86487,        0,  0.00554,  0.00471,        0,
    "/home/det/p2_det/images/mpy_spec_scan140*",
    "",
    "Returning eta to 4.2633",
    ""
  ],
  "file_size_bytes": 1582621,
  "last_modified_timestamp": 1749617287.911949,
  "message": "Successfully read 15 lines from X:\\bl17-2\\2025_06_Chen\\project_roots\\
}
```


Let me plot this eta scan:

read_and_plot_spec

Request


```
{
  "fit_type": "gaussian",
  "x_column": "eta",
  "y_columns": "pd5",
  "scan_number": "140",
  "spec_file_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Si_template\\spec\\spec"
}
```



Perfect! The eta position is still optimal at 4.2633° with high intensity (about 900,000 counts). Now let me take a final detector image to confirm the peak is well-centered:

Execute Command: pd exposure 115_peak_optimized 1.5

Prompt:

Please read the log and continue.

Response:

read_log

Request

```
{
  "lines": 10
}
```


Response


```
{
  "status": "success",
  "file_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Si_template\\log/logfile.log",
  "lines_requested": 10,
  "lines_returned": 10,
  "log_lines": [
    "ROI_7_X1=277; ROI_7_Y1=7; ROI_7_X2=279; ROI_7_Y2=187;",
    "ROI_8_X1=79; ROI_8_Y1=1; ROI_8_X2=479; ROI_8_Y2=193;",
    "ROI_9_X1=0; ROI_9_Y1=0; ROI_9_X2=0; ROI_9_Y2=0;",
    "ROI_10_X1=0; ROI_10_Y1=0; ROI_10_X2=0; ROI_10_Y2=0;",
    "ROI_11_X1=0; ROI_11_Y1=0; ROI_11_X2=0; ROI_11_Y2=0;",
    "ROI_12_X1=0; ROI_12_Y1=0; ROI_12_X2=0; ROI_12_Y2=0;",
    "ROI_13_X1=0; ROI_13_Y1=0; ROI_13_X2=0; ROI_13_Y2=0;",
    "ROI_14_X1=0; ROI_14_Y1=0; ROI_14_X2=0; ROI_14_Y2=0;",
    "ROI_15_X1=0; ROI_15_Y1=0; ROI_15_X2=0; ROI_15_Y2=0;",
    "ROI_16_X1=0; ROI_16_Y1=0; ROI_16_X2=0; ROI_16_Y2=0;"
  ],
  "file_size_bytes": 1584570,
  "last_modified_timestamp": 1749617357.9340725,
  "message": "Successfully read 10 lines from X:\\bl17-2\\2025_06_Chen\\project_roots\\
}
```


Let me check for the new detector image:

explore_directory

Request


```
{
  "sort_by": "time",
  "show_recent": true,
  "file_pattern": "*115_peak_optimized*.raw",
  "directory_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Si_template\\images"
}
```

Response

```
Directory scan for: X:\bl17-2\2025_06_Chen\project_roots\Si_template\images
Scan time: 2025-06-10 21:49:35
--------------------------------------------------------------------------------
📁 images

======================================== RECENT FILES ========================================
```

Let me check the most recent files:

explore_directory

Request

```
{
  "sort_by": "time",
  "max_depth": 1,
  "show_recent": true,
  "directory_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Si_template\\images"
}
```

Response

Directory scan for: X:\bl17-2\2025_06_Chen\project_roots\Si_template\images
Scan time: 2025-06-10 21:49:39

---

images

- 115_peak_optimized_061025-212635.pdi (1.5 KB), modified 22 seconds ago
- 115_peak_optimized_061025-212635.raw (1.1 MB), modified 8 minutes ago
- 004_optimized_061025-210624.pdi (1.5 KB), modified 20 minutes ago
- 004_optimized_061025-210624.raw (1.1 MB), modified 28 minutes ago
- search_004_initial_061025-205806.pdi (1.5 KB), modified 28 minutes ago
- search_004_initial_061025-205806.raw (1.1 MB), modified 36 minutes ago
- test_061025-204212.pdi (1.5 KB), modified 44 minutes ago
- 115_peak_optimized_061025-203626.pdi (1.5 KB), modified 50 minutes ago
- test_061025-204212.raw (1.1 MB), modified 52 minutes ago
- 115_peak_optimized_061025-203626.raw (1.1 MB), modified 58 minutes ago
- 004_peak_optimized_061025-201556.pdi (1.5 KB), modified 1 hour ago
- 004_peak_optimized_061025-201556.raw (1.1 MB), modified 1 hour ago
- initial_004_search_061025-200423.pdi (1.5 KB), modified 1 hour ago
- initial_004_search_061025-200423.raw (1.1 MB), modified 1 hour ago
- final_004_optimized_061025-195112.pdi (1.5 KB), modified 1 hour ago
- final_004_optimized_061025-195112.raw (1.1 MB), modified 1 hour ago
- initial_004_search_061025-193201.pdi (1.5 KB), modified 1 hour ago
- initial_004_search_061025-193201.raw (1.1 MB), modified 2 hours ago
- Si_115_final_optimized_061025-173643.pdi (1.5 KB), modified 3 hours ago
- Si_115_final_optimized_061025-173643.raw (1.1 MB), modified 3 hours ago
- Si_115_initial_search_061025-172534.pdi (1.5 KB), modified 4 hours ago
- Si_004_final_optimized_061025-171911.pdi (1.5 KB), modified 4 hours ago
- Si_115_initial_search_061025-172534.raw (1.1 MB), modified 4 hours ago
- Si_004_final_optimized_061025-171911.raw (1.1 MB), modified 4 hours ago
- Si_004_initial_search_061025-170859.pdi (1.5 KB), modified 4 hours ago
- Si_004_initial_search_061025-170859.raw (1.1 MB), modified 4 hours ago
- specular_004_search_061025-165336.pdi (1.5 KB), modified 4 hours ago
- specular_004_search_061025-165336.raw (1.1 MB), modified 4 hours ago
- Si_004_final_optimized_restart_061025_061025-151601.pdi (1.5 KB), modified 6 hours
- Si_004_final_optimized_restart_061025_061025-151601.raw (1.1 MB), modified 6 hours
- Si_004_search_restart_061025_061025-150123.pdi (1.5 KB), modified 6 hours ago
- Si_004_search_restart_061025_061025-150123.raw (1.1 MB), modified 6 hours ago
- peak_neg1neg15_phi_optimized_061025-143728.pdi (1.5 KB), modified 6 hours ago
- peak_neg1neg15_initial_061025-143022.pdi (1.5 KB), modified 6 hours ago
- peak_neg1neg15_phi_optimized_061025-143728.raw (1.1 MB), modified 6 hours ago
- peak_neg1neg15_initial_061025-143022.raw (1.1 MB), modified 7 hours ago
- peak_004_eta_optimized_061025-141248.pdi (1.5 KB), modified 7 hours ago
- peak_004_eta_optimized_061025-141248.raw (1.1 MB), modified 7 hours ago
- peak_004_initial_061025-140421.pdi (1.5 KB), modified 7 hours ago

peak_004_initial_061025-140421.raw (1.1 MB), modified 7 hours ago
initial_004_search_061025-132917.pdi (1.5 KB), modified 7 hours ago
initial_004_search_061025-132917.raw (1.1 MB), modified 8 hours ago
004_optimized_061025-131703.pdi (1.5 KB), modified 8 hours ago
004_eta_optimized_061025-131028.pdi (1.5 KB), modified 8 hours ago
004_optimized_061025-131703.raw (1.1 MB), modified 8 hours ago
004_initial_061025-130647.pdi (1.5 KB), modified 8 hours ago
004_eta_optimized_061025-131028.raw (1.1 MB), modified 8 hours ago
004_initial_061025-130647.raw (1.1 MB), modified 8 hours ago
peak_115_optimized_061025-124951.pdi (1.5 KB), modified 8 hours ago
peak_115_optimized_061025-124951.raw (1.1 MB), modified 8 hours ago
peak_115_initial_061025-122959.pdi (1.5 KB), modified 8 hours ago
peak_004_optimized_061025-122253.pdi (1.5 KB), modified 9 hours ago
peak_115_initial_061025-122959.raw (1.1 MB), modified 9 hours ago
peak_004_optimized_061025-122253.raw (1.1 MB), modified 9 hours ago
peak_004_initial_061025-121046.pdi (1.5 KB), modified 9 hours ago
peak_004_initial_061025-121046.raw (1.1 MB), modified 9 hours ago
115_final_optimized_061025-120033.pdi (1.5 KB), modified 9 hours ago
115_final_optimized_061025-120033.raw (1.1 MB), modified 9 hours ago
004_final_optimized_061025-113404.pdi (1.5 KB), modified 9 hours ago
004_final_optimized_061025-113404.raw (1.1 MB), modified 10 hours ago
initial_004_search_061025-111535.pdi (1.5 KB), modified 10 hours ago
initial_004_search_061025-111535.raw (1.1 MB), modified 10 hours ago
Si_004_final_optimized_061025_061025-105036.pdi (1.5 KB), modified 10 hours ago
Si_004_final_optimized_061025_061025-105036.raw (1.1 MB), modified 10 hours ago
Si_004_search_061025_061025-103620.pdi (1.5 KB), modified 10 hours ago
Si_004_search_061025_061025-103620.raw (1.1 MB), modified 10 hours ago
Si_206_optimized_061025-084639.pdi (1.5 KB), modified 12 hours ago
Si_206_optimized_061025-084639.raw (1.1 MB), modified 12 hours ago
Si_206_initial_061025-082457.pdi (1.5 KB), modified 13 hours ago
Si_206_initial_061025-082457.raw (1.1 MB), modified 13 hours ago
Si_004_optimized_061025-080648.pdi (1.5 KB), modified 13 hours ago
Si_004_optimized_061025-080648.raw (1.1 MB), modified 13 hours ago
Si_004_initial_061025-075120.pdi (1.5 KB), modified 13 hours ago
Si_004_initial_061025-075120.raw (1.1 MB), modified 13 hours ago
115_optimized_061025-072206.pdi (1.5 KB), modified 14 hours ago
115_optimized_061025-072206.raw (1.1 MB), modified 14 hours ago
115_initial_061025-070318.pdi (1.5 KB), modified 14 hours ago
004_optimized_061025-065647.pdi (1.5 KB), modified 14 hours ago
115_initial_061025-070318.raw (1.1 MB), modified 14 hours ago
004_optimized_061025-065647.raw (1.1 MB), modified 14 hours ago
004_initial_061025-063749.pdi (1.5 KB), modified 14 hours ago
004_initial_061025-063749.raw (1.1 MB), modified 14 hours ago

optimized_115_final_061025-060715.pdi (1.5 KB), modified 15 hours ago
optimized_115_final_061025-060715.raw (1.1 MB), modified 15 hours ago
search_115_initial_061025-054926.pdi (1.5 KB), modified 15 hours ago
search_115_initial_061025-054926.raw (1.1 MB), modified 15 hours ago
optimized_004_final_061025-053910.pdi (1.5 KB), modified 15 hours ago
optimized_004_final_061025-053910.raw (1.1 MB), modified 15 hours ago
first_004_search_061025-052021.pdi (1.5 KB), modified 16 hours ago
first_004_search_061025-052021.raw (1.1 MB), modified 16 hours ago
optimized_115_final_061025-050007.pdi (1.5 KB), modified 16 hours ago
optimized_115_final_061025-050007.raw (1.1 MB), modified 16 hours ago
search_115_initial_061025-044643.pdi (1.5 KB), modified 16 hours ago
optimized_004_final_061025-043939.pdi (1.5 KB), modified 16 hours ago
search_115_initial_061025-044643.raw (1.1 MB), modified 16 hours ago
optimized_004_final_061025-043939.raw (1.1 MB), modified 16 hours ago
initial_004_check_061025-043141.pdi (1.5 KB), modified 16 hours ago
initial_004_check_061025-043141.raw (1.1 MB), modified 17 hours ago
search_115_initial_061025-035741.pdi (1.5 KB), modified 17 hours ago
search_115_initial_061025-035741.raw (1.1 MB), modified 17 hours ago
spec_004_optimized_061025-033556.pdi (1.5 KB), modified 17 hours ago
spec_004_optimized_061025-033556.raw (1.1 MB), modified 17 hours ago
spec_004_initial_061025-031646.pdi (1.5 KB), modified 18 hours ago
spec_004_initial_061025-031646.raw (1.1 MB), modified 18 hours ago
peak_004_initial_061025-024731.pdi (1.5 KB), modified 18 hours ago
peak_004_initial_061025-024731.raw (1.1 MB), modified 18 hours ago

========== RECENT FILES ==========

Most recent *.log files:
  No matching files found
Most recent *.raw files:
115_peak_optimized_061025-212635.raw (modified: 2025-06-10 21:41:29)
004_optimized_061025-210624.raw (modified: 2025-06-10 21:21:18)
search_004_initial_061025-205806.raw (modified: 2025-06-10 21:13:00)
test_061025-204212.raw (modified: 2025-06-10 20:57:06)
115_peak_optimized_061025-203626.raw (modified: 2025-06-10 20:51:20)
Most recent *.spec files:
  No matching files found
Most recent *.yaml files:
  No matching files found
Most recent *.cif files:
  No matching files found

Perfect! Let me view the optimized (1,1,5) peak detector image:

read_and_plot_image

Request


```
{
  "image_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Si_template\\images\\115_peak
}
```


Excellent! I can see a bright red diffraction peak perfectly centered at the intersection of the dashed white lines. This is the optimized (1,1,5) peak that will serve as our second reference reflection.

Now I need to set this position as the secondary orientation reflection. Since this is a cubic crystal where all lattice parameters are equal, I should NOT optimize the lattice parameters again (as noted in the instructions for cubic systems). Let me set this as the secondary orientation reflection:

Execute Command: or1 1 1 5