转靶微焦斑单晶衍射仪简易操作规程

一、 设备状态检查确认 ：靶电压电流、温度状态等
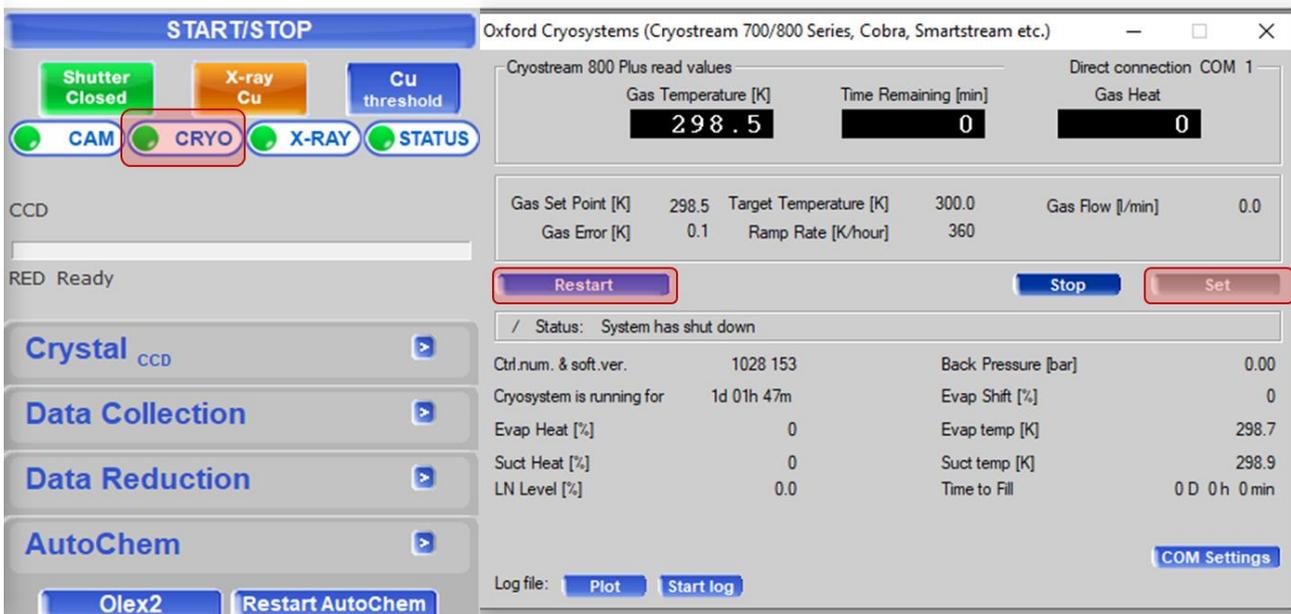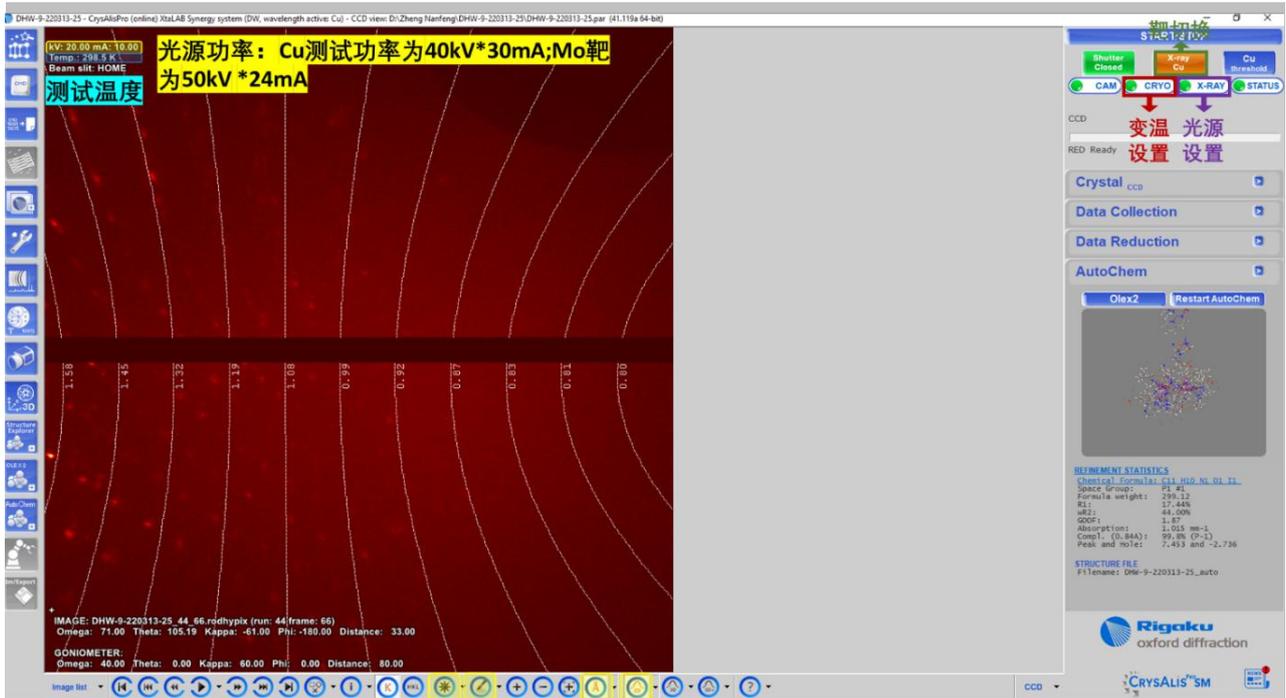
二、测试设置

1. 开始新实验：
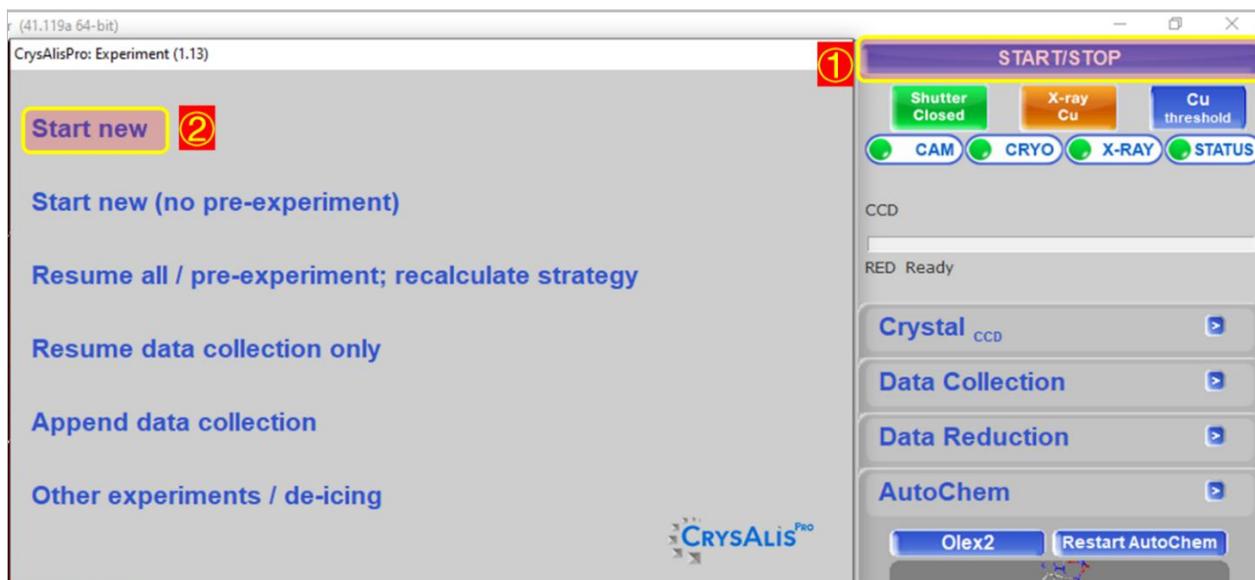
2. 挑选高质量晶体，对心；
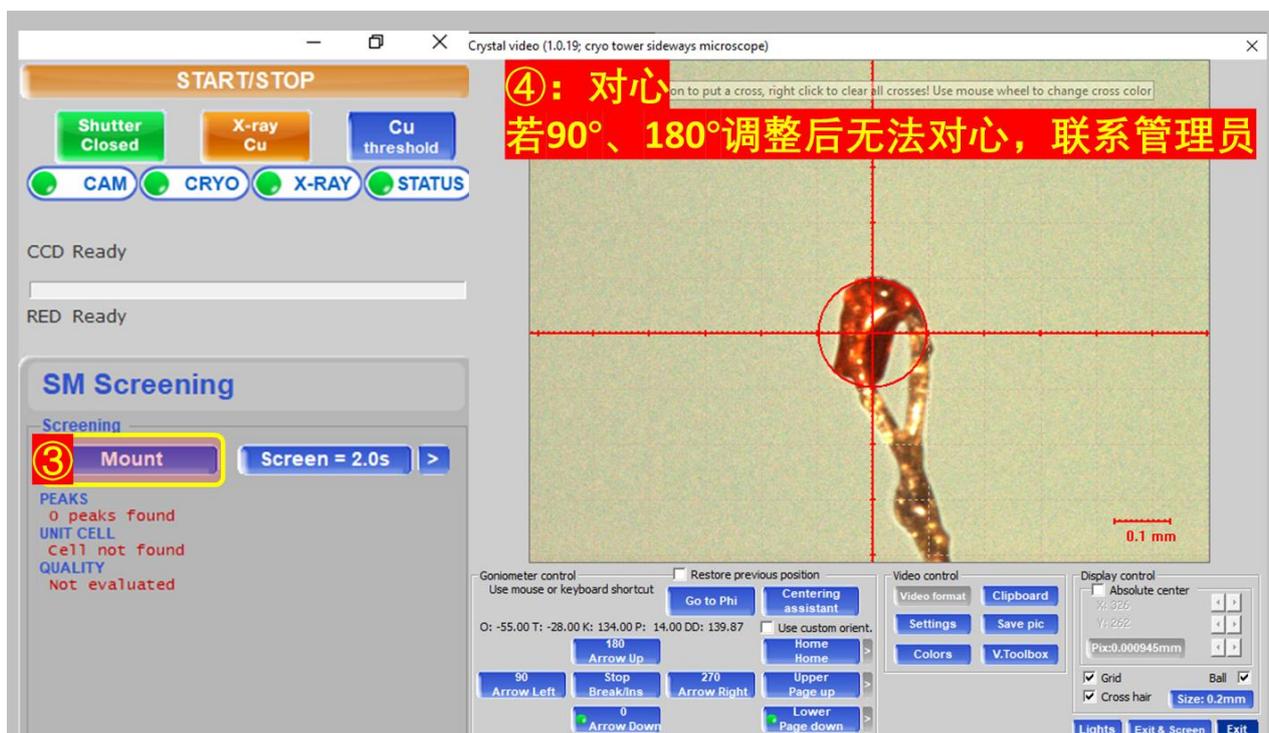
3. 快扫（也可以拍单张照片）：获取预实验拟采用参数；
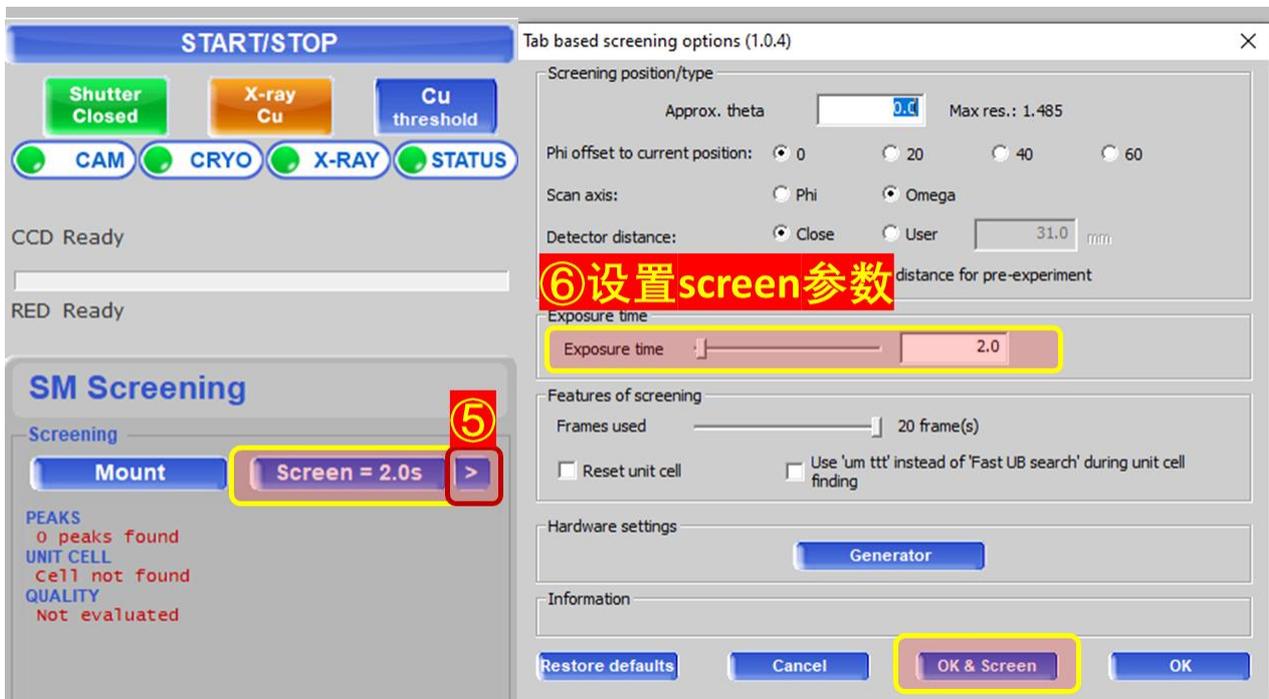
4、预实验：为采集完整晶体数据获取策略条件

5、数据收集：根据预实验设置数据收集策略条件

Experiment S ⑧根据预实验情况设置空间群和曝光时间等参数 CRYSALIS^Pro

Unit cell for Strategy Calculation [CSD:
Cell: 12.0221(14) 16.6089(18)

P-lattice 6.04% (800 of 833 reflections) **Lattice Wizard**

Strategy parameters

○ Resolution ○ Theta ○ 2Theta 0.837

○ Laue group ○ Point group ○ Other mmm

☑ Friedel mates are equivalent (uncheck for high quality absolute configuration data)

Detector Distance 30.80 **Advanced**

Strategy mode ☑ Use run list sorting with scan inversion

Complete data (default mode)

limit 100.0 **IUCr limit** Max 100.0 %

Generates runs that reach
completeness limit

Time prediction based on data to 0.837 Ang

○ Fill time
○ Fill I/sigma
○ The same time for all theta positions
● Different time for each theta positions

Predicted resolution beyond 0.84
Scan width: 0.50

	exp time	individual I/sigma	merged I/sigma
	0.05	15.13	30.46
[-49.78; 49.78]	0.05	23.98	36.58
[-99.00; 10-53]	0.08	14.80	26.79
Total I/sigma:		17.49	35.21

Automatic experiment settings

Mode: 16bit no dead-time **Frequency: 100.0Hz**

Options (CNOS)

Autochem/Movie/Cryo/Red

Current Strategy

No. runs/frames: 16/1124
Total experiment time: 0h 04m
Expected experiment finish time: Mon Aug 12 14:47:09 2024

Calculate New Strategy **Manually Edit Run List** **Update Completeness**

● Completeness/Coverage curves ○ Completeness/Coverage tables ☐ Completeness/Predicted resolution

Completeness in mmm

Full sphere (P1)
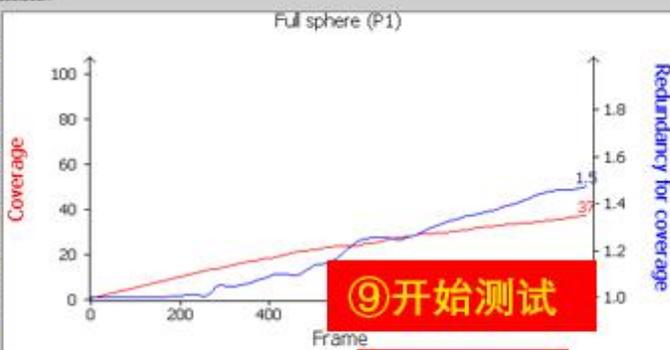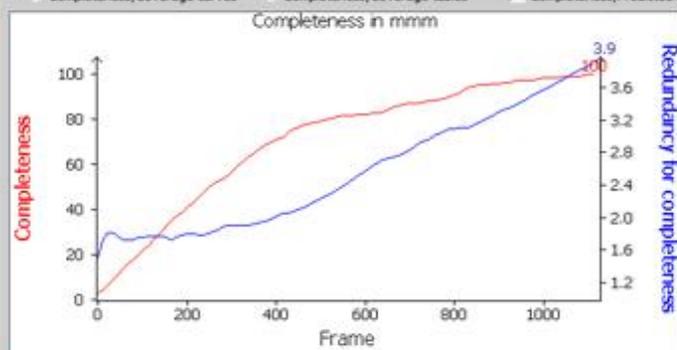
⑨开始测试

Help **Start named experiment** **Start experiment** **Cancel**