

How to run Autograin on the NanoSIMS

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Pre-sputter

Take an Image

Define Particles

Measure each grain

Move Stage



Setup the following:

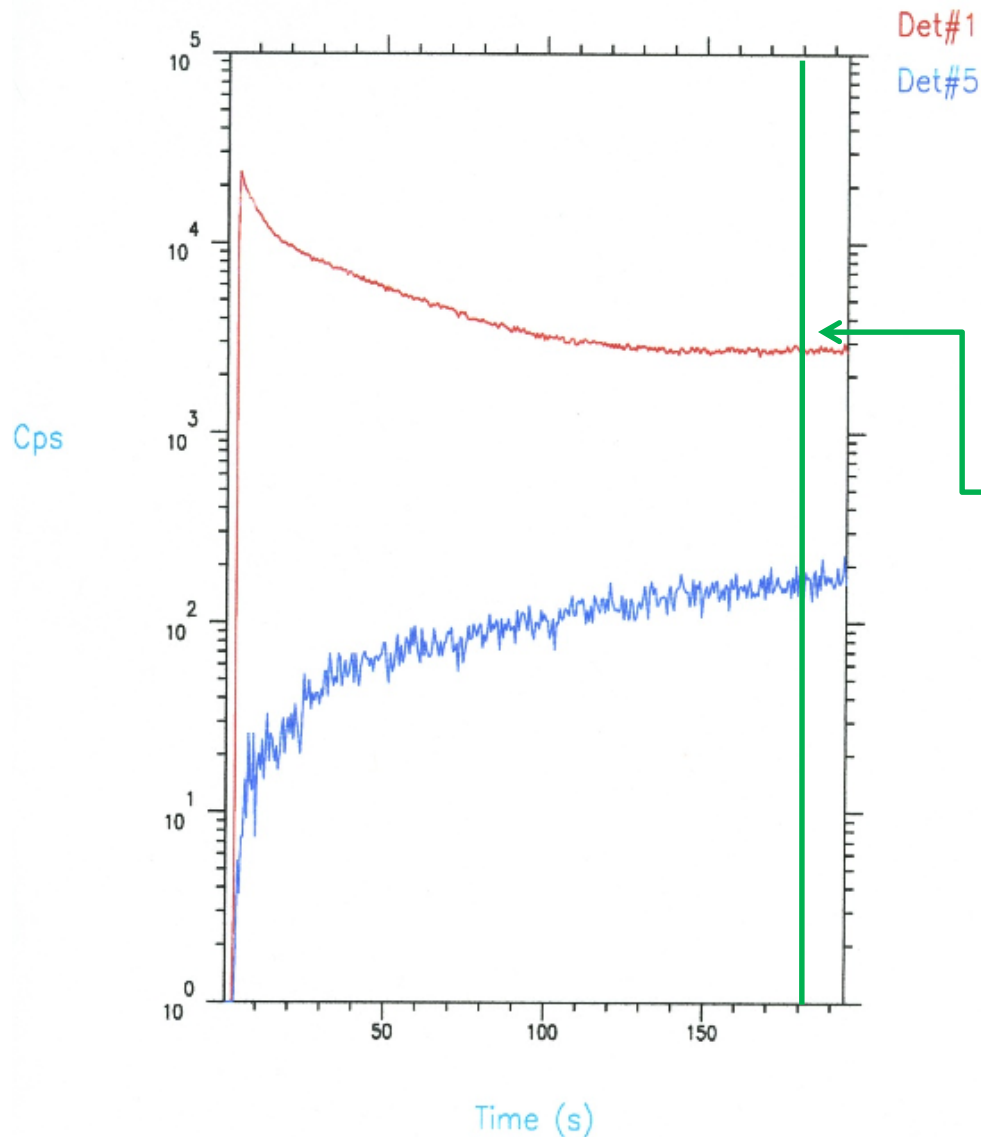
1. Create a prespinner image file
2. Setup and run grain mode image
3. Start IDL & test the grain mode image
4. Run at least 1 grain mode isotope measurement on a defined particle
5. Load both the prespinner image file and the isotope measurement file into chain mode
6. Setup up Chain Mode and pray it works

Create presputter image file:

1. Get high beam current: Larger D1; increase L0 and L1; or some combination

Create prespitter image file:

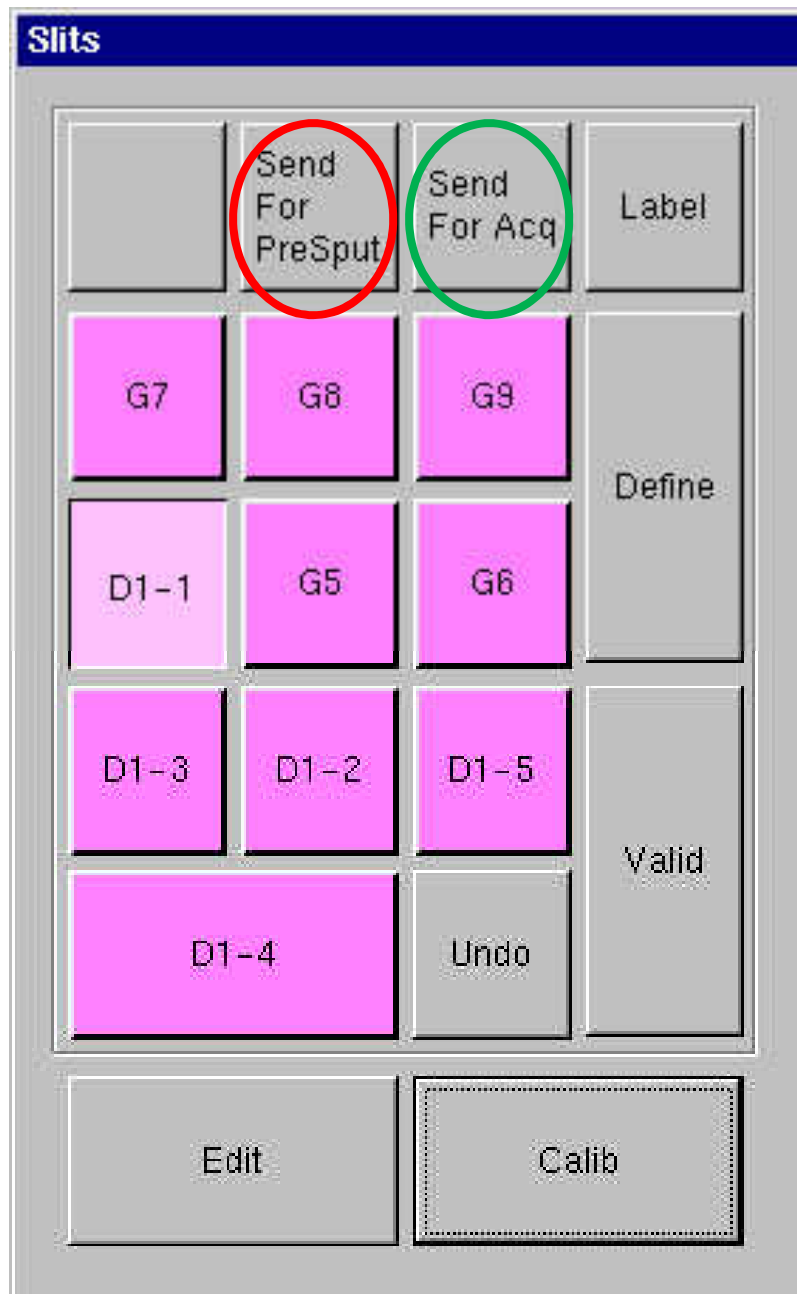
1. Get high beam current: Larger D1; increase L0 and L1; or some combination
2. Run **Beam Stability** on pristine area similar to actual measurement place till signal stabilizes



Presputter with
high beam for
about this long
(~180s in this case)

Create prespitter image file:

1. Get high beam current: Larger D1; increase L0 and L1; or some combination
2. Run **Beam Stability** on pristine area similar to actual measurement place till signal stabilizes
3. Setup presets for prespitter and acquisition



Presets

1. **Presputter**: Should contain both lens & slit settings for your high beam. Set ALL EM HVs to ZERO (add them by clicking *Define* if not available)
2. **Acquisition**: Should contain actual measurement settings for the grain mode image and isotope files. Set all EM HVs back to original values.

Create presputter image file:

1. Get high beam current: Larger D1; increase L0 and L1; or some combination
2. Run **Beam Stability** on pristine area similar to actual measurement place till signal stabilizes
3. Setup presets for presputter and acquisition
4. Setup typical image measurement: 256x256, **100 μ s/pix** (or something similar), turn on presputtering & adjust # of cycles to match amount you want to presputter

Load... Save Save as... New Data inc.: No

Sample ID :
Matrix ID :

Total analysis time: 0s Time finished : 14:02

Meas. number: 1

Lens preset : None
Slit preset : None

Pre-sputtering: No Yes

Nb cycles: 1 Raster size (um): 20.0
Time: 65.5 s
Lens preset : ☐ rrent [125pA] ☒ More...
Slit preset : None ☐ More...

Raster size (um): 20.0
Real size (um): 20.0

Comment :

GO
acquisition

Analysis
type
selection

Working Frame
Width : 256 Height : 256

Scanning frame
Start Col : 1 Start Row : 1
Width : 256 Height : 256

Magnetic Field List
B1 1331.065

Ct/px (us) : 1000 Ct/fr (s) : 65.536
Offset (V) : 0.00

☐ Print results after acquisition

Centering

Base Detector List

Line	N	Id	Species Symbol	a.m.u.	Radius
			FC	15.231	377.560
		Tr1	16O	16.000	386.972
		Tr2	18O	17.999	410.435
		Tr3	28Si	28.001	511.922
		Tr4	29Si	29.001	520.983
		Tr5	30Si	30.001	529.886
		ES	Electron Scanning Image		

Working Frame
256 x 256
Scanning Frame
256 x 256

Change to:
~100μs/pix

Adjust to be your
presputter time

Make sure it has your
presets!

Setup Grain Mode image file:

RIMS-ORG1d-2-OSI-redone_47.im

Load... Save Save as... New Data inc: No

Sample ID :
Matrix ID :
Total analysis time: 0s Time finished : 14:02
Meas. number: 1

Lens preset: None
Slit preset: None
Pre-sputtering: No Yes

Raster size (um): 20.0
Real size (um): 20.0
Comment :

GO Analysis type selection

Nanosims 50 - GRAIN MODE - IMAGE

Working Frame
Width: 256 Height: 256
Scanning frame
Start Col: 1 Start Row: 1
Width: 256 Height: 256

Magnetic Field List

B1 1331.065

Ct/px (u s) : 1000 Ct/fr (s) : 65.536
Offset (V) : 0.00

Print result after acquisition

Centering

Base Line	N	Id	Species Symbol	a.m.u.	Radius
FC				15.231	377.560
Tr1	160			16.000	386.972
Tr2	180			17.999	410.435
Tr3	285i			28.001	511.922
Tr4	295i			29.001	520.983
Tr5	305i			30.001	529.886
ES			Electron Scanning Image		

Adjust for total time of image acquisition you want. **NOTE:** in grain mode you can't increase the # of frames!

Make sure it has your presets!

Start & run IDL:

1. Right click on desktop & click on:
Files -> Programs -> Shell Tool
2. Type: `idl -vm=/space/ims/frankg/autograin.sav`

Start & run IDL:

A terminal window titled "shelltool - /bin/csh" showing a command being executed. The command is "idl -vm=/space/ims/frankg/autograin.sav" and it is preceded by the prompt "laotzu.wustl.edu:~/space/ims>".

```
shelltool - /bin/csh
laotzu.wustl.edu:~/space/ims>idl -vm=/space/ims/frankg/autograin.sav
```

Start & run IDL:

1. Right click on desktop& click on:
Files -> Programs -> Shell Tool
2. Type: `idl -vm =/space/ims/frankg/autograin.sav`
3. Click anywhere on Splash Screen

IDL^{VM}

The IDL Virtual Machine™

Distribution Platform for IDL Applications

[click to continue](#)

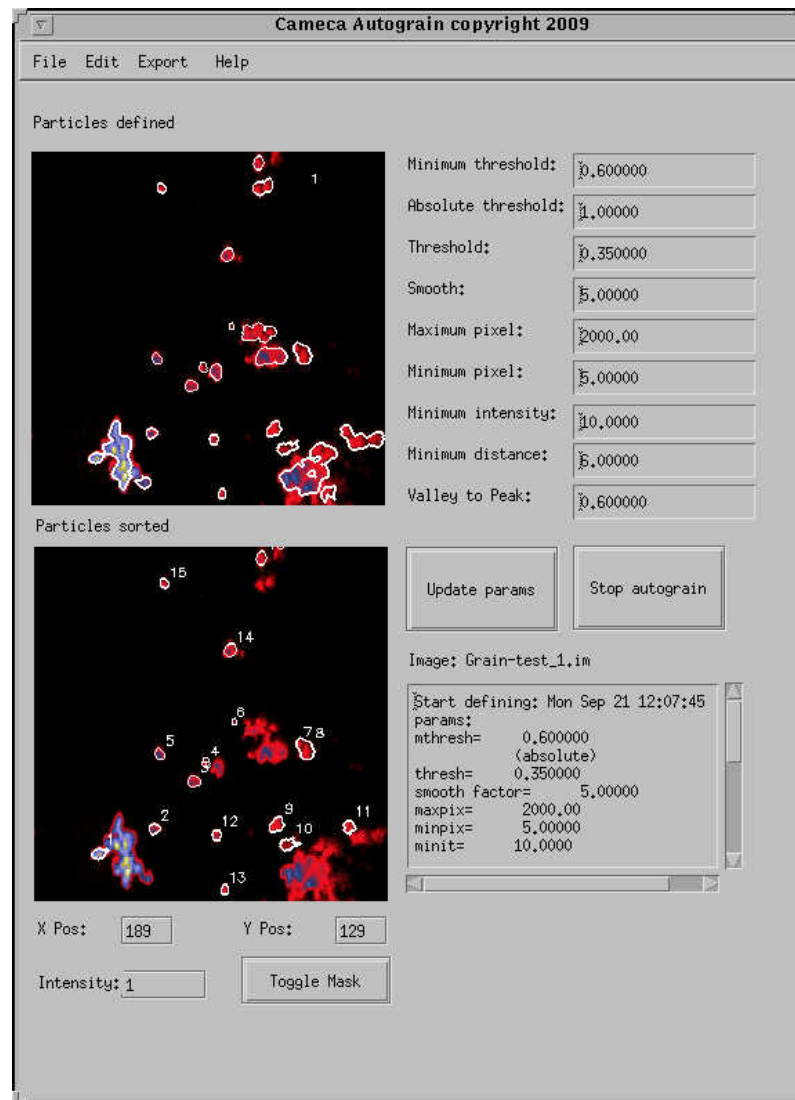
Upgrade to a development version of IDL and:

- interactively explore your data in the IDL environment
- develop cross-platform applications for distribution
- test custom data analysis algorithms

Find out more at www.rsinc.com/IDL

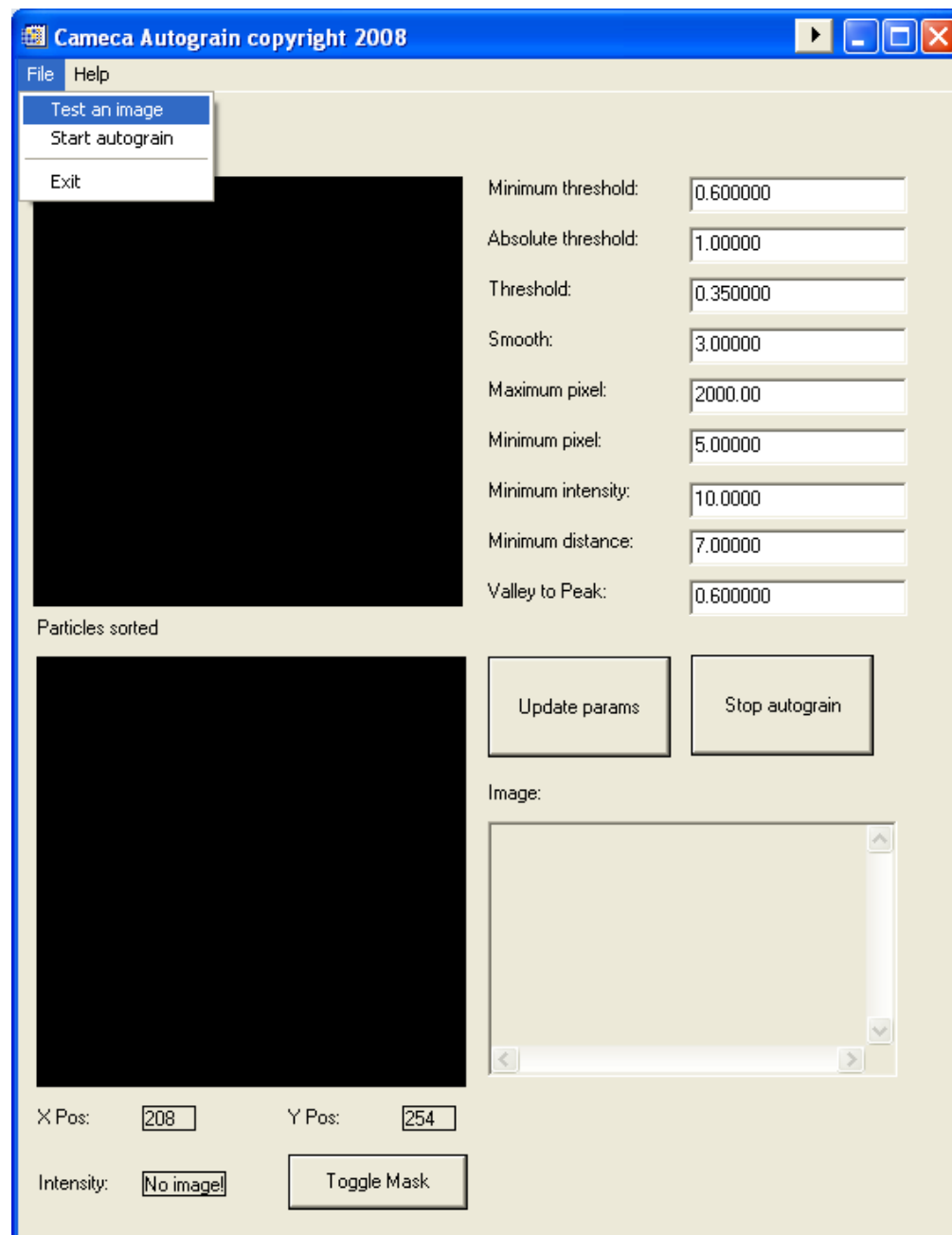
RSI

Start & run IDL:



Start & run IDL:

1. Right click on desktop& click on:
Files -> Programs -> Shell Tool
2. Type: `idl -vm =/space/ims/frankg/autograin.sav`
3. Click on Splash Screen
4. Once the Grain Mode image has finished, test it in the autograin program:
File -> Test an image



Start & run IDL:

1. Right click on desktop& click on:
Files -> Programs -> Shell Tool
2. Type: `idl -vm =/space/ims/frankg/autograin.sav`
3. Click on Splash Screen
4. Once the Grain Mode image has finished, test it in the autograin program:
File -> Test an image
6. Once finished, start autograin by going to:
File -> Start autograin

Setup Grain Mode isotope file:

The screenshot shows the Nanosims 50 - GRAIN MODE - ISOTOPES interface. The left panel, titled 'Measurement Conditions - NSIMS: 11 Feb08_52_1.is', contains various settings for the simulation. The right panel, titled 'Nanosims 50 - GRAIN MODE - ISOTOPES', shows the 'Mode' set to 'Auto Grain' (circled in purple) and the 'Magnetic Field List' with 'B1 1331.065'. The 'Detector List' table is visible at the bottom right. A red circle highlights the 'Ct/px (us)' and 'Offset (V)' fields, with a red arrow pointing to them from a text box. A red 'X' is drawn over the 'Pre-sputtering' section in the left panel.

Measurement Conditions - NSIMS: 11 Feb08_52_1.is

Load... Save Save as... New Data inc.: No

Sample ID :
Matrix ID :

Meas. nb: 100

Block number: 10
Meas. per block: 10
Rejection at (sigma): 2

Lens preset : None
Slit preset : None

Pre-sputtering: No Yes

Nb cycles: Raster size (um): 20.0
Time: 65.5 s
Lens preset : [125pA] More...
Slit preset : None

Raster size (um): 20.0

Comment :

Analysis type selection

Nanosims 50 - GRAIN MODE - ISOTOPES

Scanning mode : No Yes Mode : Graphic Semi Graphic Auto Grain

Magnetic Field List

B1 1331.065

Ct/px (us): 1000
Offset (V): 0.00

Print results after acquisition

Centering

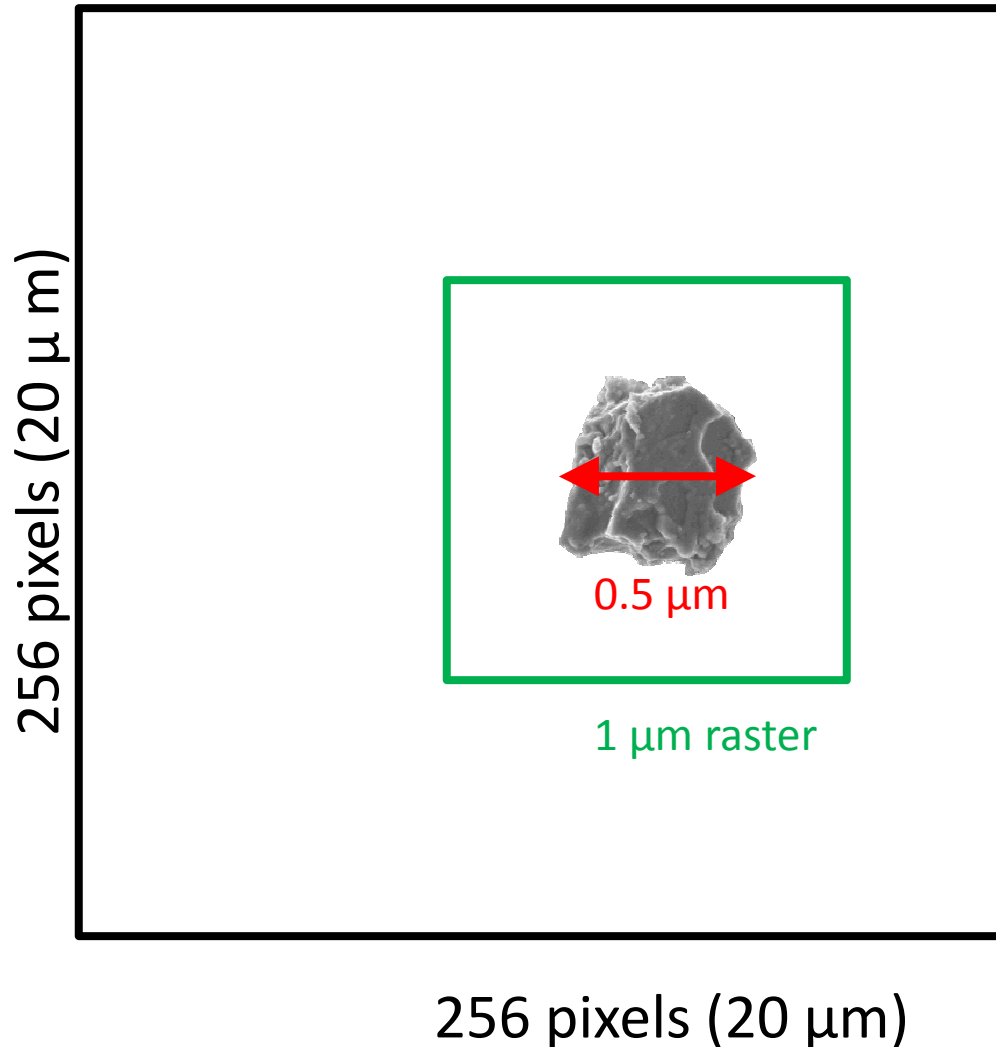
SIBC

Detector List

Base Line	N	Id	Species Symbol	a.m.u.	Radius	Peak Num.	Ref. Peak Num.
FC				15.231	377.560		
Tr1	16O			16.000	386.972		
Tr2	18O			17.999	410.435		
Tr3	28Si			28.001	511.922		
Tr4	29Si			29.001	520.983		
Tr5	30Si			30.001	529.886		

Adjust for approximate amount of total measurement time you want. **NOTE:** actual time will depend on size (in pixels) of grain defined

How many $\mu\text{s}/\text{pix}$?



The software calculates a raster size roughly twice the grain diameter.

For a 0.5 μm grain, this leads to a raster size of 1 μm (12.8 pixels in this example).

Total number of pixels = $12.8^2 = 164$.




For counting time of 1000 $\mu\text{s}/\text{pixel}$, acquisition time per cycle = 164 ms

For 10 blocks of 10 cycles = 16.4s.

Probably way too short.

NOTE: Some grains may be smaller, some may larger. Optimize counting time per pixel to achieve sufficient statistics for the size of the average grain.

Setup Chain Mode:

1. Click *Add...* to make a second line.
2. With first line selected, click  and select your prespinner file (e.g., prespinner.im)
3. With second line selected, click  and select your grain mode isotope file ONLY (e.g., grain_mode.is). The grain mode image file associated with it will be automatically loaded too
4. Click on the snake () movement scheme and click *Chain all* button and put in parameters

Setup Chain Mode:


Chained Analysis – new4.cha,dir:/morespace/data/frankg/11Feb08

Load... Save Save as... New file lon : Cs+

#	Sample name	Matrix	Stage pos	Analysis type	File name	Time schedule	Status
1	pregrid1		200 : 4470	Image nano	pregrid1@2.im	02'10''	edited
2	grid1		200 : 4470	Grain Mode	grid1@2.im	05'33''	edited
3	grid1		200 : 4470	Grain Mode	grid1@2_mg_y.is	01'46''	edited

Total chained analysis time (mn) : 09'29"


Sample name : pregrid1 Matrix :

Stage Move : 


File name : pregrid1@2

Measurement conditions : dir : /morespace/data/frankg/11Feb08

START STOP ABORT

SHOW ACQ  Analysis type selection

Delete all Delete Add Chain All

Nb : 1 

Edit MC Load... presputter-125pA.im Snap

1

4

2 - 3

Setup Chain Mode:

Chained Analysis – new4.cha.dir/morespace/data/frankg/11Feb08 (edited)

Ion : Cs+

#	Sample name	Matrix	Stage pos	Analysis type	File name	Time schedule	Status
1: 4	pregrid1		200 : -4470	Image nano	pregrid1@_...im	08'40 "	edited
2	grid1		200 : -4470	Grain Mode	grid1#2.im	05'33 "	edited
3	grid1		200 : -4470	Grain Mode	grid1#2_eq_y.is	01'46 "	edited

Total chained analysis time (mn) : 15'59"

Chain All

Stage Move :

dX : 25 x 1
dY : -25 x 5

Nb : 1

Future Improvements: IDL

1. Increase general software stability
2. Add ability to define grains to measure based on isotopic ratios
3. Add a log file that records/exports everything: all variables, file names, actions taken, etc
4. Add export of images with raster boxes overlaid
5. Better optimize the sorting algorithm for grains that are too close to each other.
6. Enhance cross-platform compatibility

Future Improvements: Cameca

1. Allow dynamic measurement termination
2. Allow multiple frames in the grain mode image
3. Create a more streamlined/integrated incorporation of grain mode into chain mode
4. Fix the quirkiness of the measurement presets

Technical stuff

DIRECTORY AND FILE INFORMATION

Here is a list of the directory and files used for communication:

/space/ims/data/raw_ima/	Directory for communication files
.AutoGrainIsOn	File saying IDL software is on and running
.AutoGrainImage	2 line text file: 1st line flag (0 or 1) whether image is done being acquired, 2 nd line is full path of image for IDL to analyze
.AutoGrainList	Text file list of grains to analyze
.AutoGrainDPPARS	Text file list of particle definition parameters
.AutoGrainResults	Text results file that is displayed in the result window
.AutoGrainCompleted	Text file IDL creates when it is done creating the grainlist file

GRAIN DEFINITION PARAMETERS

The following is a table of what the particle definition parameters mean. It is best to just play around with them for a given image to see what effect they have.

Minimum threshold	minimum intensity pixel must have to be considered a center of a particle
Absolute threshold	if equal 1 then minimum threshold is absolute value, otherwise it is fraction of maximum image intensity
Threshold	pixels > threshold*maximum intensity are included in particle
Smooth	images smoothed by this amount before defining
Maximum Pixel	maximum number of pixels allowed in a particle
Minimum Pixel	minimum number of pixels allowed in a particle
Minimum Intensity	minimum intensity for pixel to be included in particle
Minimum Distance	minimum radius between adjacent grains
Valley to peak	valley to peak intensity ratio allowed of adjacent grains