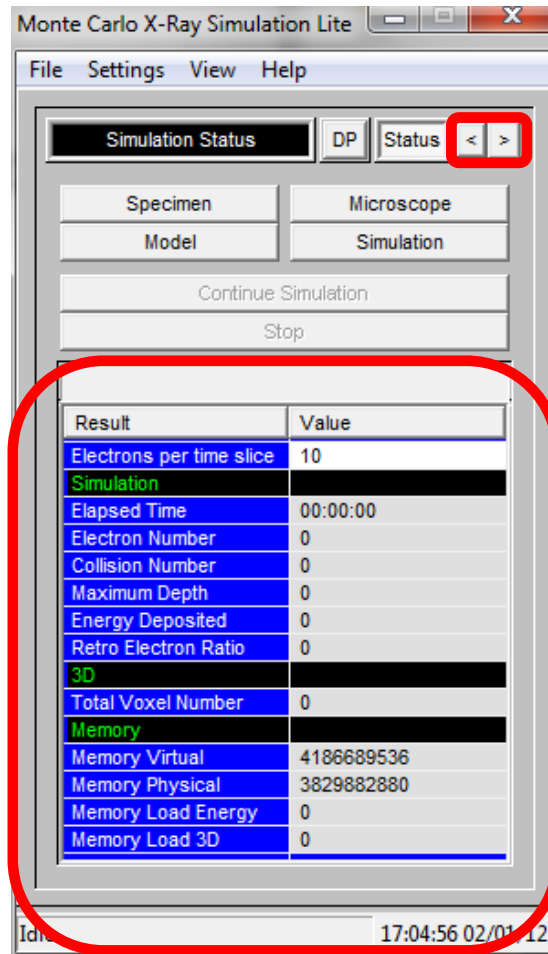


MC X-Ray Lite User Manual

Version 1.2

August 2012

MC X-Ray Lite



Navigate between main and spectrum simulation dialogs

Information about the simulation progress

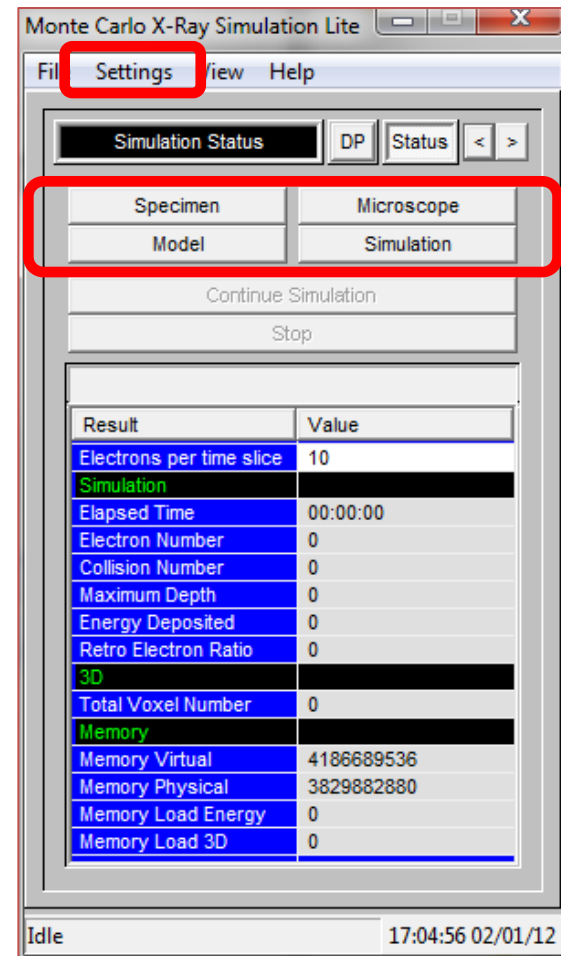
Examples Used

- `AlMgBulk5keV.sim`
 - AlMg Alloy (bulk) at 5keV.
 - Al 50% weight fraction, Mg 50%.
- `AuParticleInC20keV.sim`
 - Au nanoparticle (NP) in C substrate at 20 keV.
 - NP diameter 20 nm just below the surface.
- `CarbonNanotube_0nm.sim`
 - Carbon nanotube at 5 keV.
 - Outer radius 10 nm, inner radius 5 nm, center vacuum.

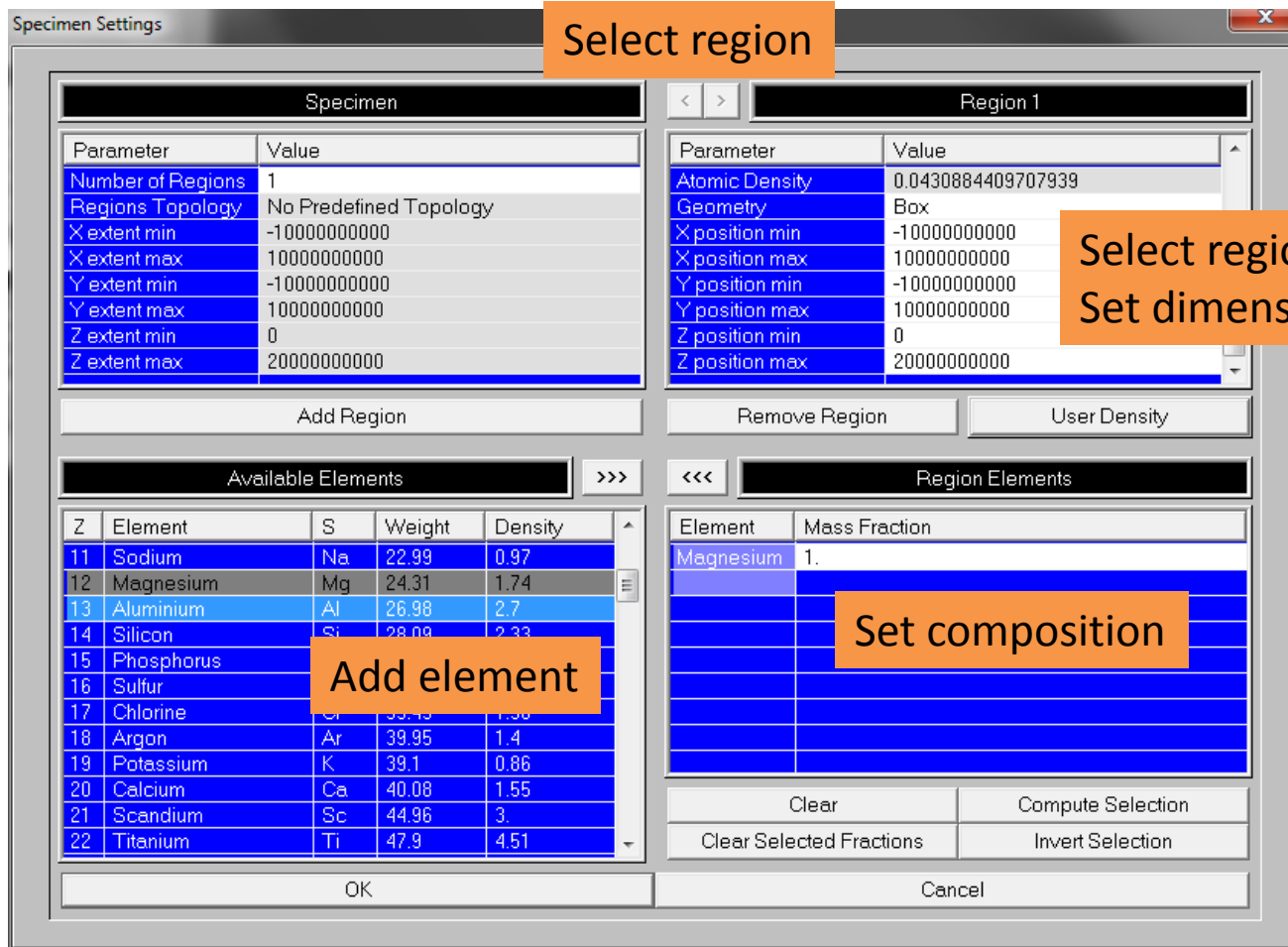
Settings

- Specimen
- Microscope
- Models
- Simulation Parameters

Can be access either by the buttons or the menu



Specimen Settings



The first region have to be a box and no region with $z < 0$.

Specimen Settings

Specimen

Parameter	Value
Number of Regions	1
Regions Topology	No Predefined Topology
X extent min	-100000000000
X extent max	100000000000
Y extent min	-100000000000
Y extent max	100000000000
Z extent min	0
Z extent max	200000000000

Add Region

Available Elements >>>

Z	Element	S	Weight	Density
11	Sodium	Na	22.99	0.97
12	Magnesium	Mg	24.31	1.74
13	Aluminium	Al	26.98	2.7
14	Silicon	Si	28.09	2.33
15	Phosphorus	P	30.97	1.82
16	Sulfur	S	32.06	2.07
17	Chlorine	Cl	35.45	1.56
18	Argon	Ar	39.95	1.4
19	Potassium	K	39.1	0.86
20	Calcium	Ca	40.08	1.55
21	Scandium	Sc	44.96	3.
22	Titanium	Ti	47.9	4.51

OK

Region 1

Parameter	Value
Atomic Density	0.0430884409707939
Geometry	Box
X position min	-100000000000
X position max	100000000000
Y position min	-100000000000
Y position max	100000000000
Z position min	0
Z position max	200000000000

Remove Region

<<< **Region Elements**

Element	Mass Fraction
Magnesium	1.

Clear Compute Selection

Clear Selected Fractions Invert Selection

Cancel

Box X, Y, Z in Angstroms

Electron travel toward Z position - specimen bottom area

Electron travel
toward Z positive

- specimen surface at 0
- bottom at 200 Å

Region Sphere

Specimen Settings

Specimen

Parameter	Value
Number of Regions	2
Regions Topology	No Predefined Topology
X extent min	-10000000000
X extent max	10000000000
Y extent min	-10000000000
Y extent max	10000000000
Z extent min	0
Z extent max	20000000000

Add Region

Region 2

Parameter	Value
Mean Atomic Weight	196.97
Mass Density	19.3
Atomic Density	0.0589866477128497
Geometry	Sphere
X position	0
Y position	0
Z position	101
Radius	100

Remove Region

Available Elements

Z	Element	S	Weight	Density
1	Hydrogen	H	1.008	7.1e-002
2	Helium	He	4.003	0.126
3	Lithium	Li	6.94	0.53
4	Beryllium	Be	9.01	1.85
5	Boron	B	10.81	2.34
6	Carbon	C	12.01	2.26
7	Nitrogen	N	14.01	0.81
8	Oxygen	O	16.	1.14
9	Fluorine	F	19.	1.505
10	Neon	Ne	20.18	1.2
11	Sodium	Na	22.99	0.97
12	Magnesium	Mg	24.31	1.74

Region Elements

Element	Mass Fraction
Gold	1.

Clear

Clear Selected Fractions

Compute Selection

Invert Selection

OK

Cancel

Sphere:

- center position (X, Y, Z)
- radius

All in Angstrom

Specimen Settings

Specimen	
Parameter	Value
Number of Regions	2
Regions Topology	No Predefined Topology
X extent min	-100
X extent max	100
Y extent min	-5000
Y extent max	5000
Z extent min	-100
Z extent max	100

Add Region

Region 1	
Parameter	Value
X position	0
Y position	-5000
Z position	0
X direction	0
Y direction	1
Z direction	0
Length	10000
Radius	100

Remove Region

Available Elements				
Z	Element	S	Weight	Density
1	Hydrogen	H	1.008	7.1e-002
2	Helium	He	4.003	0.126
3	Lithium	Li	6.94	0.53
4	Beryllium	Be	9.01	1.85
5	Boron	B	10.81	2.34
6	Carbon	C	12.01	2.26
7	Nitrogen	N	14.01	0.81
8	Oxygen	O	16	1.14
9	Fluorine	F	19	1.505
10	Neon	Ne	20.18	1.2
11	Sodium	Na	22.99	0.97
12	Magnesium	Mg	24.31	1.74

>>>

Region Elements	
Element	Mass Fraction
Carbon	1.

<<<

Clear	Compute Selection
Clear Selected Fractions	Invert Selection

OK Cancel

Cylinder:

- top position
- direction
- length
- radius

All in Angstroms

- top position (X, Y, Z)
- direction (X, Y, Z)
- length
- radius

All in Angstrom

Region User Density

Specimen Settings

Specimen

Parameter	Value
Number of Regions	1
Regions Topology	No Predefined Topology
X extent min	-10000000000
X extent max	10000000000
Y extent min	-10000000000
Y extent max	10000000000
Z extent min	0
Z extent max	20000000000

Add Region

Region 1

Parameter	Value
Number of Elements	2
Mean Atomic Number	12.4739715344122
Mean Atomic Weight	25.5755000000005
Mass Density	0
Atomic Density	0.0249039039209100
Geometry	Box
X position min	-10000000000
X position max	10000000000

Remove Region

User Density

Available Elements

Z	Element	S	Weight	Density
11	Sodium	Na	22.99	0.97
12	Magnesium	Mg	24.31	1.74
13	Aluminium	Al	26.98	2.7
14	Silicon	Si	28.09	2.33
15	Phosphorus	P	30.97	1.82
16	Sulfur	S	32.06	2.07
17	Chlorine	Cl	35.45	1.56
18	Argon	Ar	39.95	1.4
19	Potassium	K	39.1	0.86
20	Calcium	Ca	40.08	1.55
21	Scandium	Sc	44.96	3.
22	Titanium	Ti	47.9	4.51

Region Elements

Element	Mass Fraction
Magnesium	0.5
Aluminium	0.5

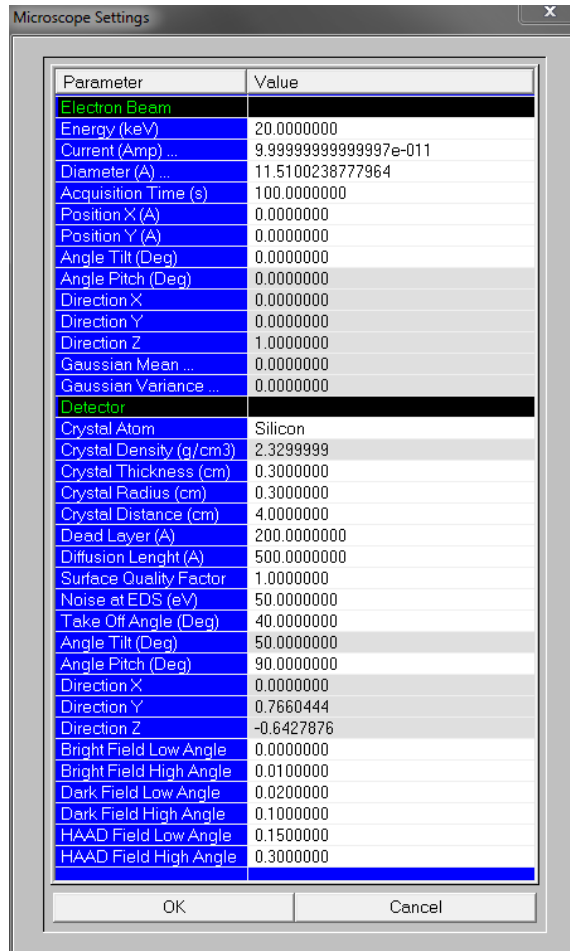
Clear Compute Selection

Clear Selected Fractions Invert Selection

OK Cancel

The mass density (g/cm³) can be set by the user by clicking the button and enter the value in the editbox

Microscope Settings



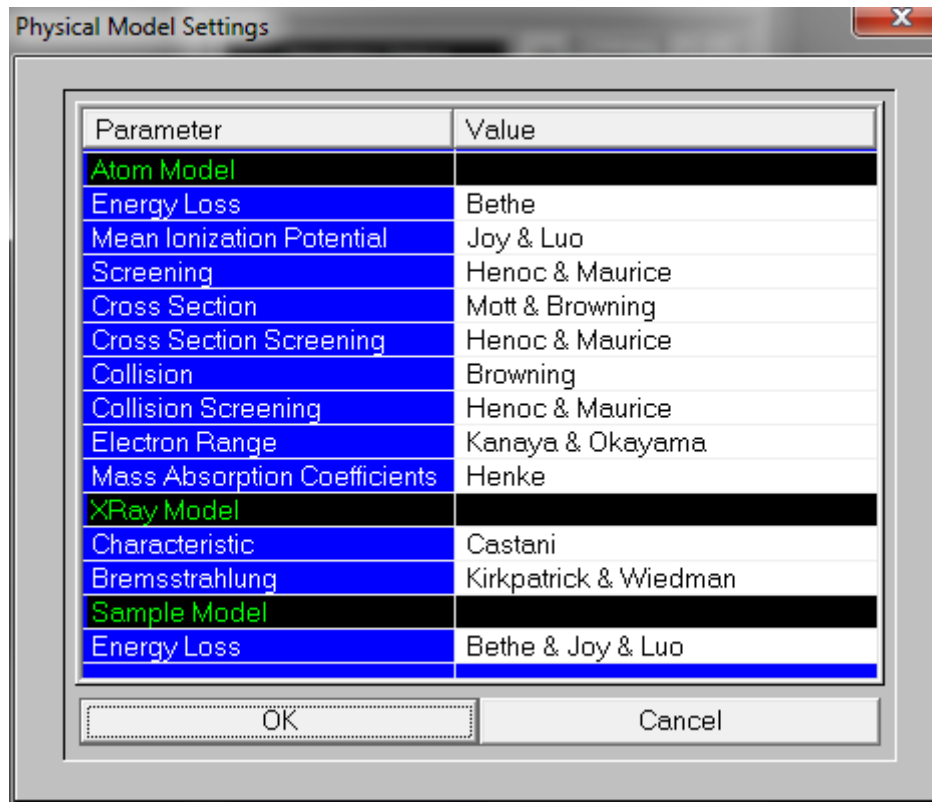
The screenshot shows a 'Microscope Settings' dialog box with a table of parameters. The 'Electron Beam' section is highlighted in green. The 'Detector' section is also highlighted in green. The table lists various parameters and their values, with some rows highlighted in blue.

Parameter	Value
Electron Beam	
Energy (keV)	20.0000000
Current (Amp) ...	9.99999999999997e-011
Diameter (A) ...	11.5100238777964
Acquisition Time (s)	100.0000000
Position X (A)	0.0000000
Position Y (A)	0.0000000
Angle Tilt (Deg)	0.0000000
Angle Pitch (Deg)	0.0000000
Direction X	0.0000000
Direction Y	0.0000000
Direction Z	1.0000000
Gaussian Mean ...	0.0000000
Gaussian Variance ...	0.0000000
Detector	
Crystal Atom	Silicon
Crystal Density (g/cm3)	2.3299999
Crystal Thickness (cm)	0.3000000
Crystal Radius (cm)	0.3000000
Crystal Distance (cm)	4.0000000
Dead Layer (A)	200.0000000
Diffusion Length (A)	500.0000000
Surface Quality Factor	1.0000000
Noise at EDS (eV)	50.0000000
Take Off Angle (Deg)	40.0000000
Angle Tilt (Deg)	50.0000000
Angle Pitch (Deg)	90.0000000
Direction X	0.0000000
Direction Y	0.7660444
Direction Z	-0.6427876
Bright Field Low Angle	0.0000000
Bright Field High Angle	0.0100000
Dark Field Low Angle	0.0200000
Dark Field High Angle	0.1000000
HAAD Field Low Angle	0.1500000
HAAD Field High Angle	0.3000000

OK Cancel

- Electron Beam
 - Incident energy in keV
 - Beam diameter in A
 - Beam X, Y positions in A
 - Beam tilt in degree
- X-ray Detector
 - Take off angle in degree
- Transmitted Electron Detectors
 - All angle in radian

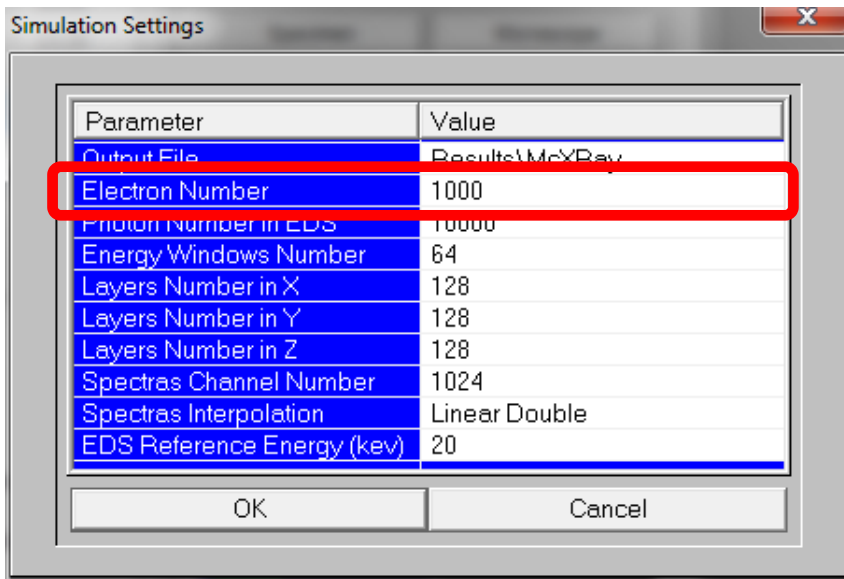
Models Settings



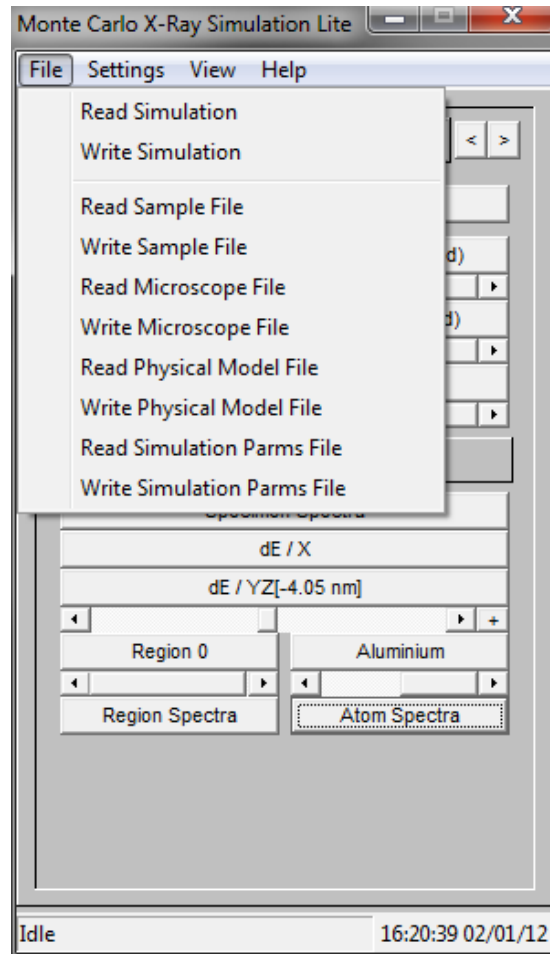
The default models are the best one to use in most simulation

Simulation Parameters

- Set the number of simulated electrons
- Other options are advanced feature, where the default values are good for most simulations

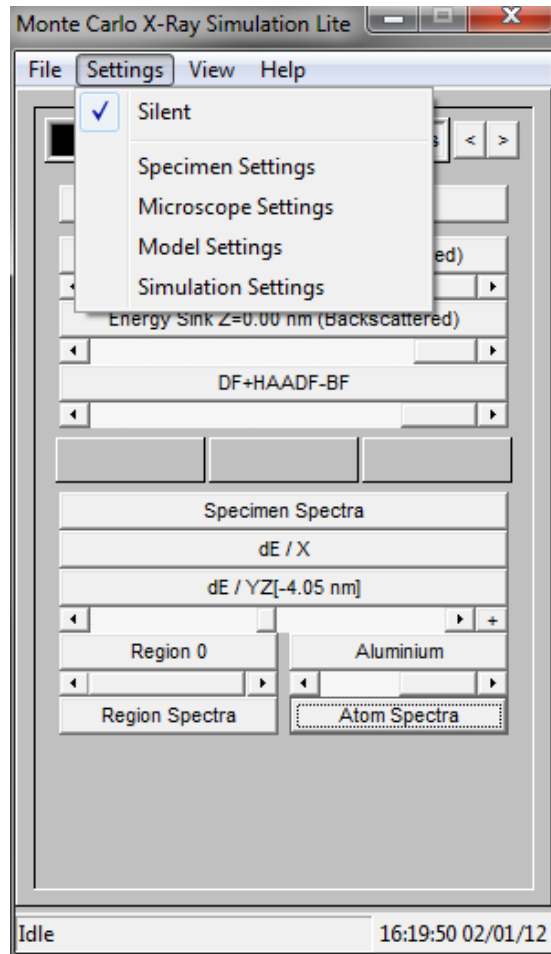


File Menu



Read and write all settings
in separate files

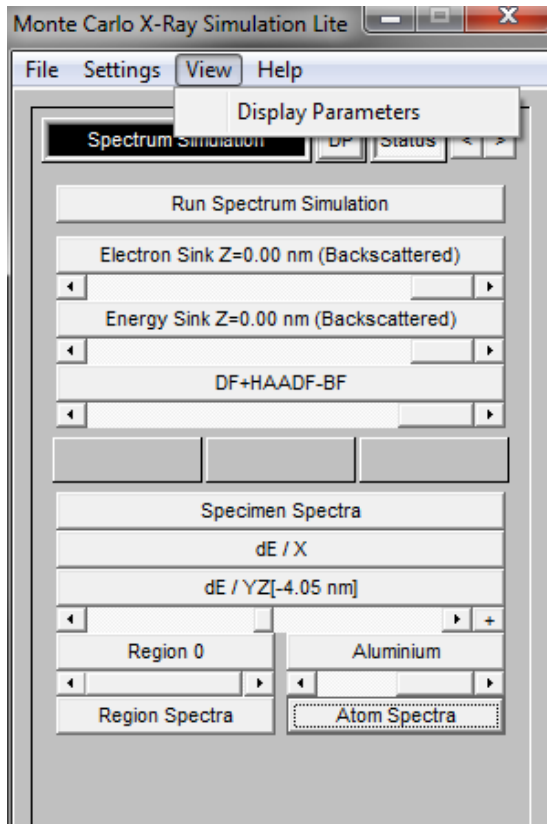
Settings Menu



Can access all settings from the menu

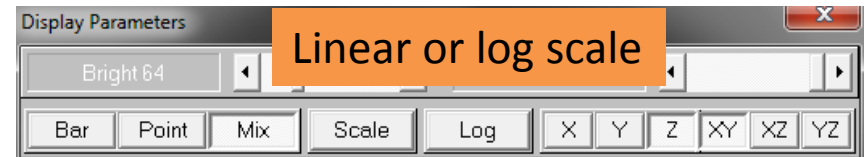
Uncheck Silent to hear a beep when the simulation is finished

View Menu



Open the Display Parameters dialog to adjust the displayed results

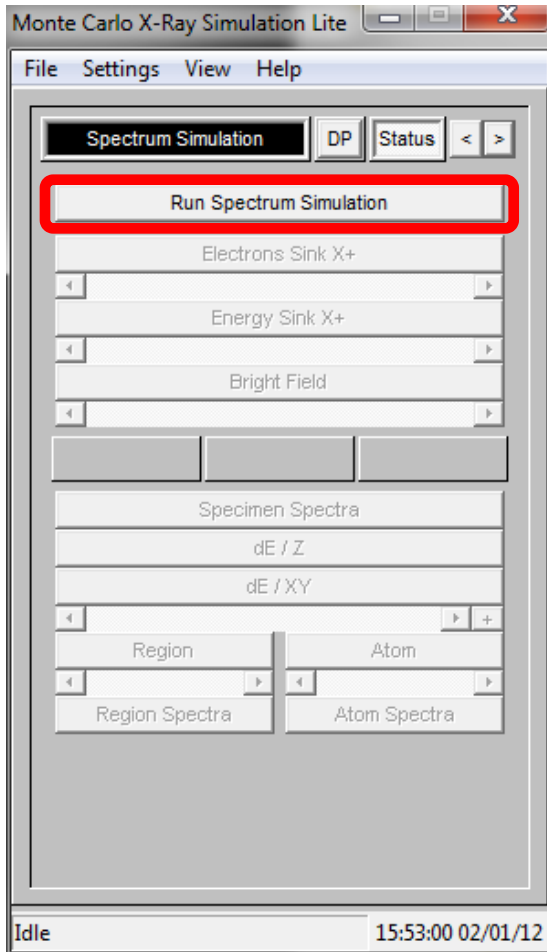
Display Parameters



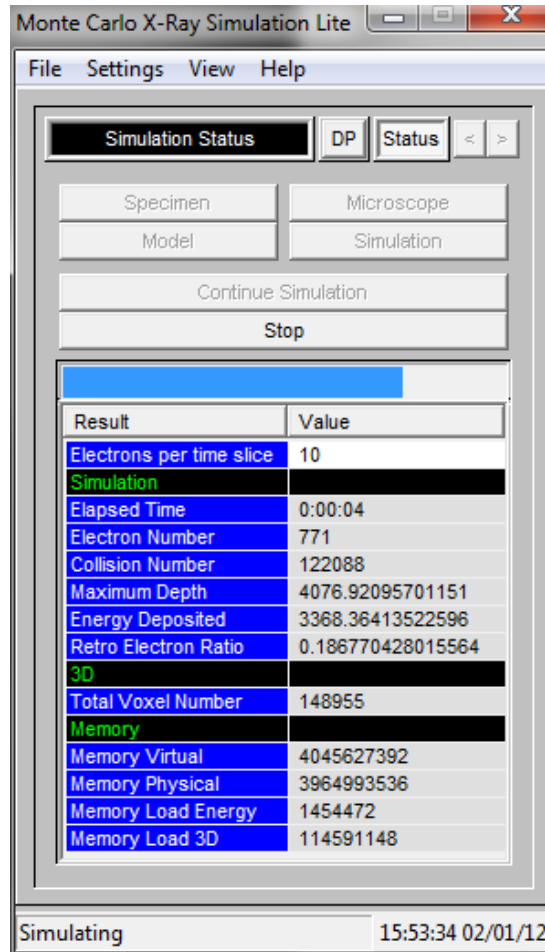
Line type in the graphic

Select the distribution dimension to display

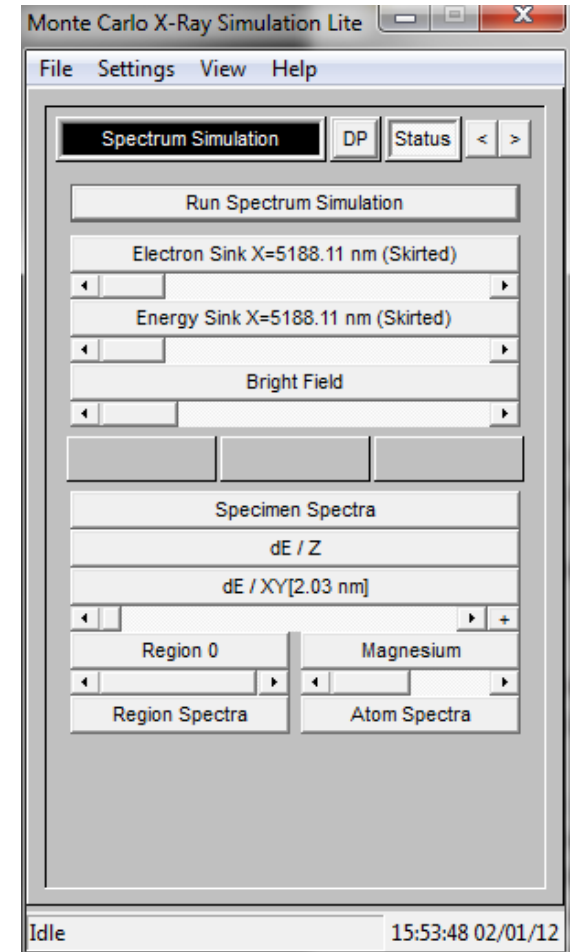
Spectrum Simulation



Start



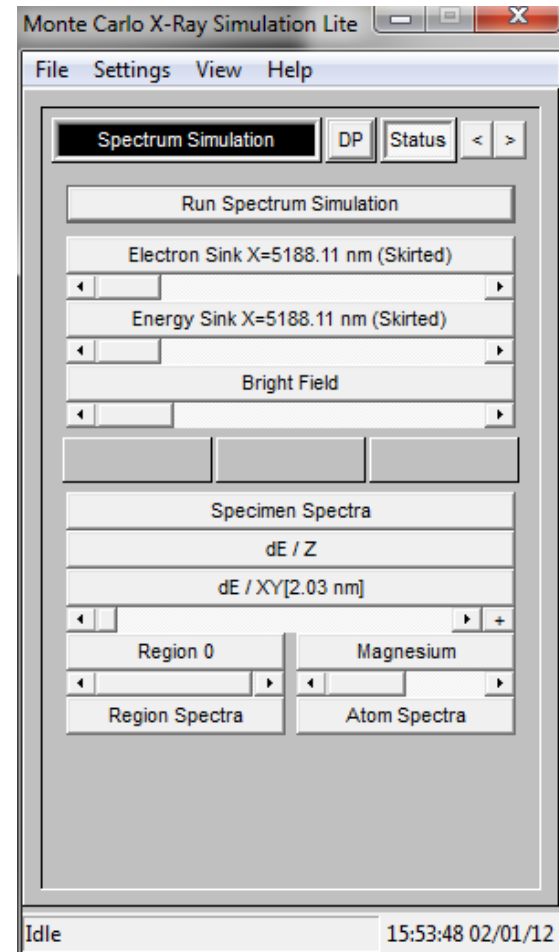
Simulating



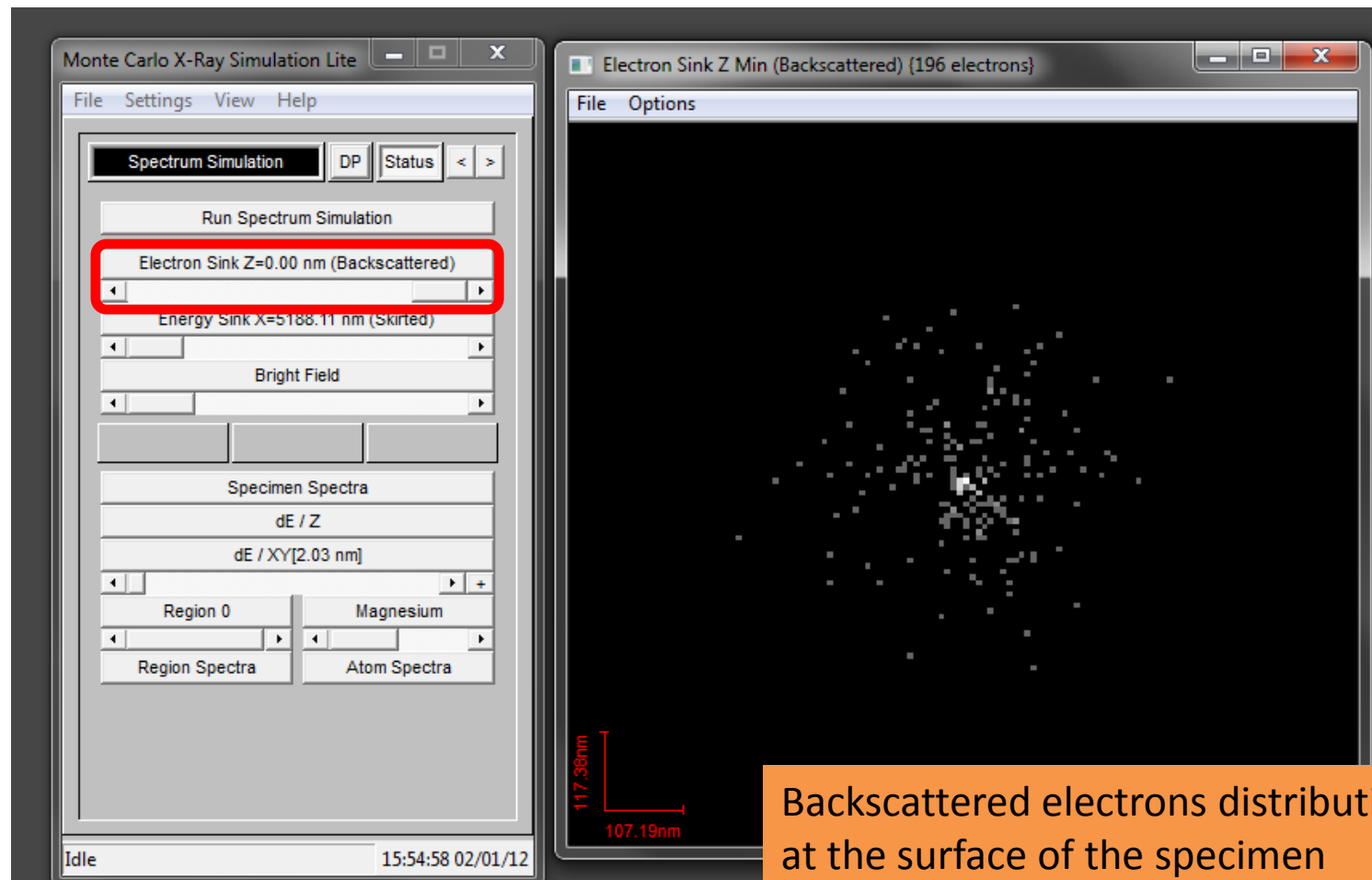
Done

Results

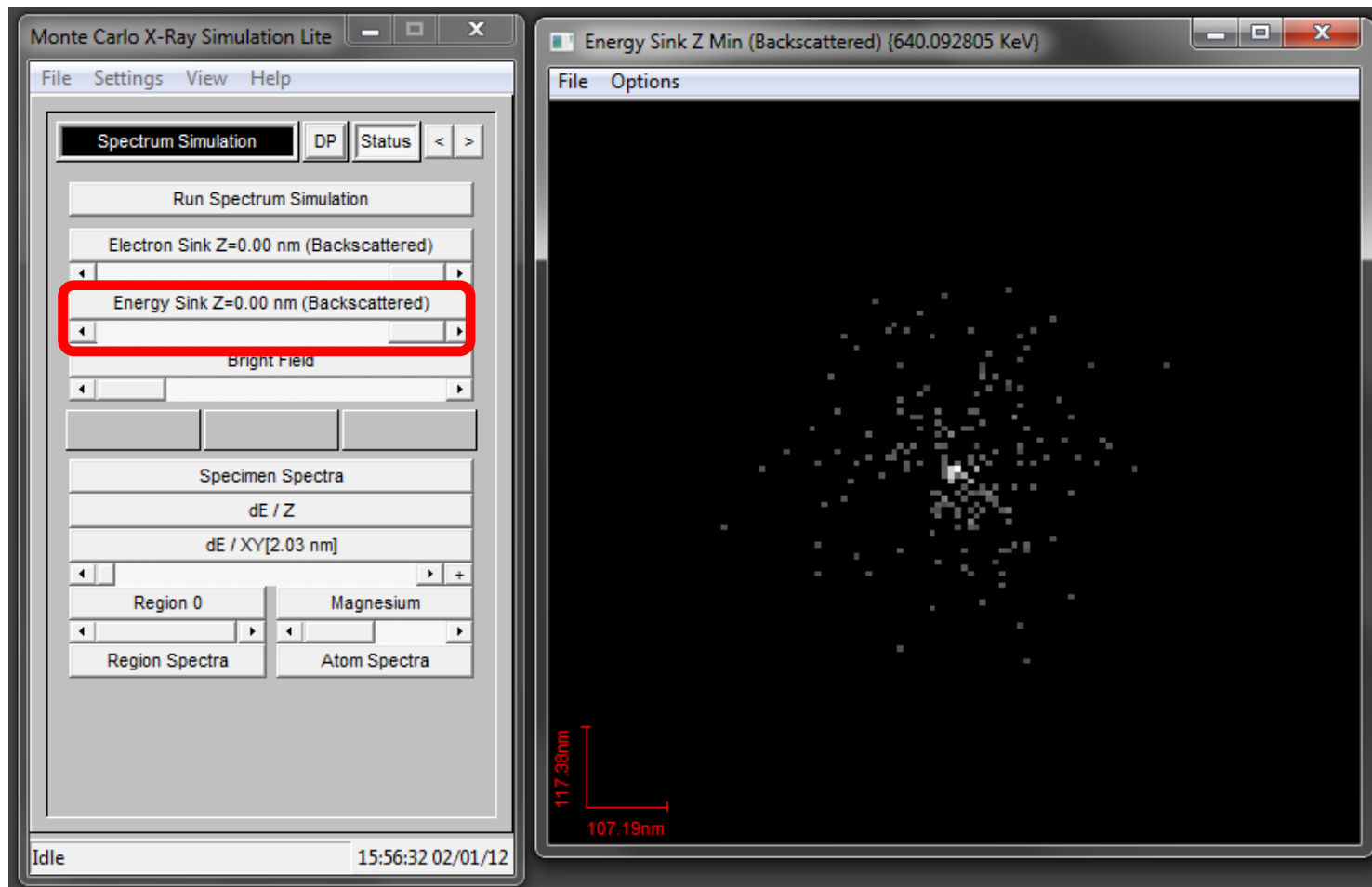
- Click on each label to display the results
- Electron and energy distribution at the specimen surfaces (6)
- Transmitted electrons distribution
- Energy loss distribution
- X-ray spectrum



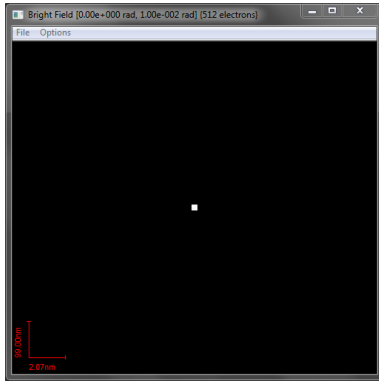
Electrons Sink



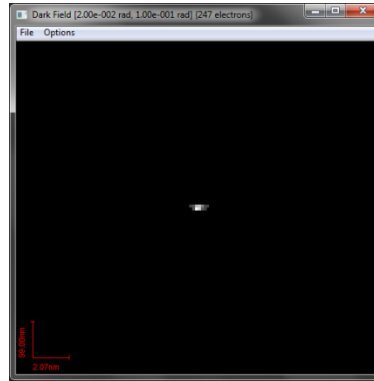
Energy Sink



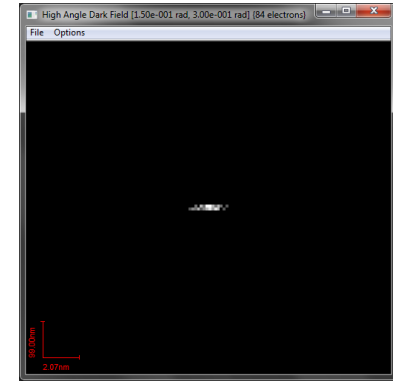
Transmitted Electrons



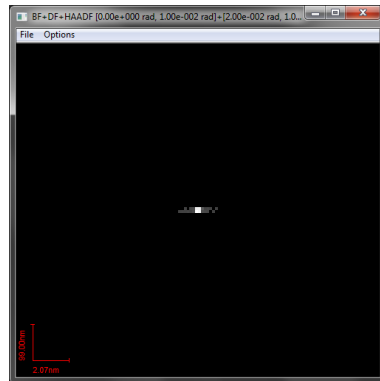
Bright Field



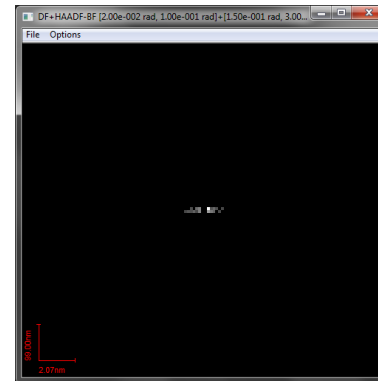
Dark Field



HAADF

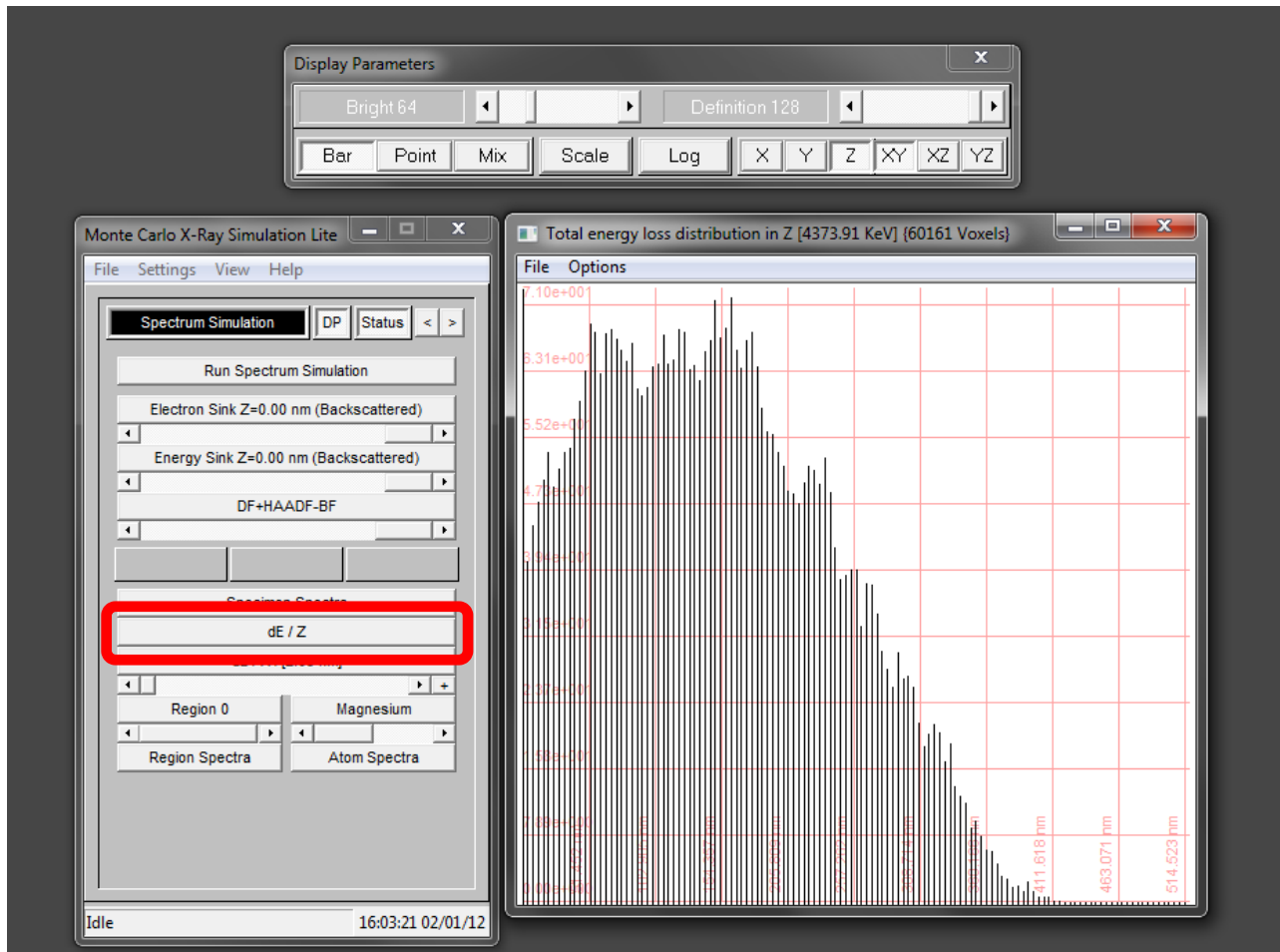


All detectors



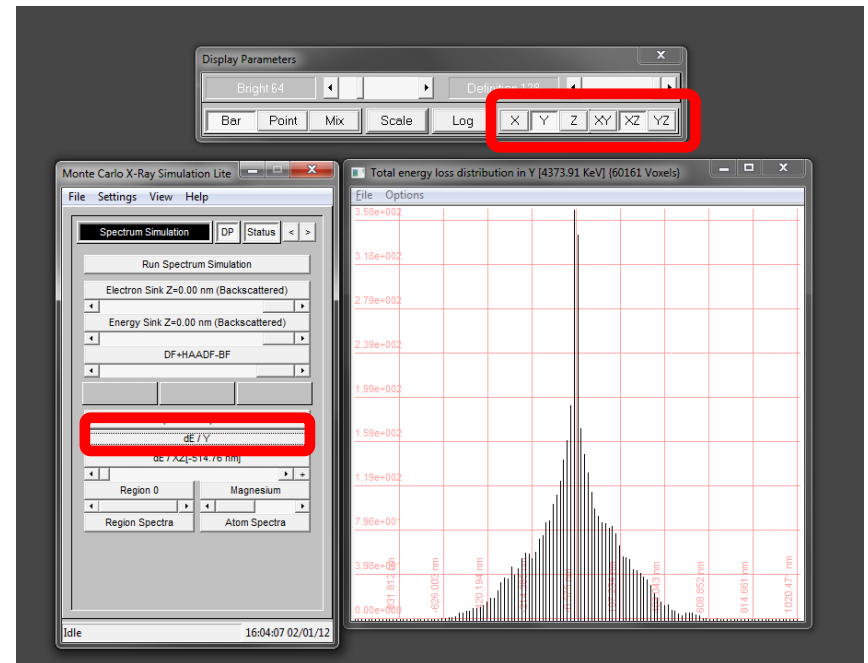
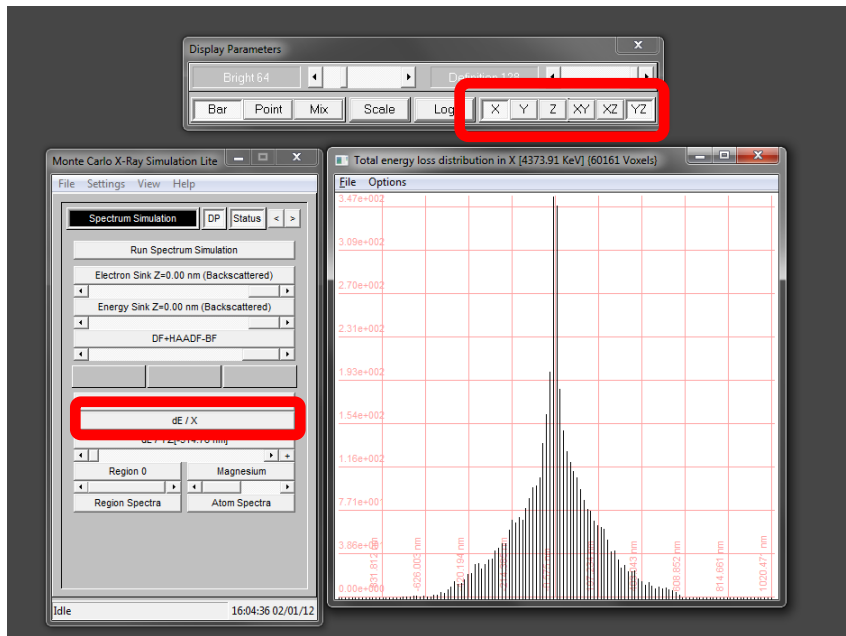
DF + HAADF - BF

Energy Loss Distribution 1D



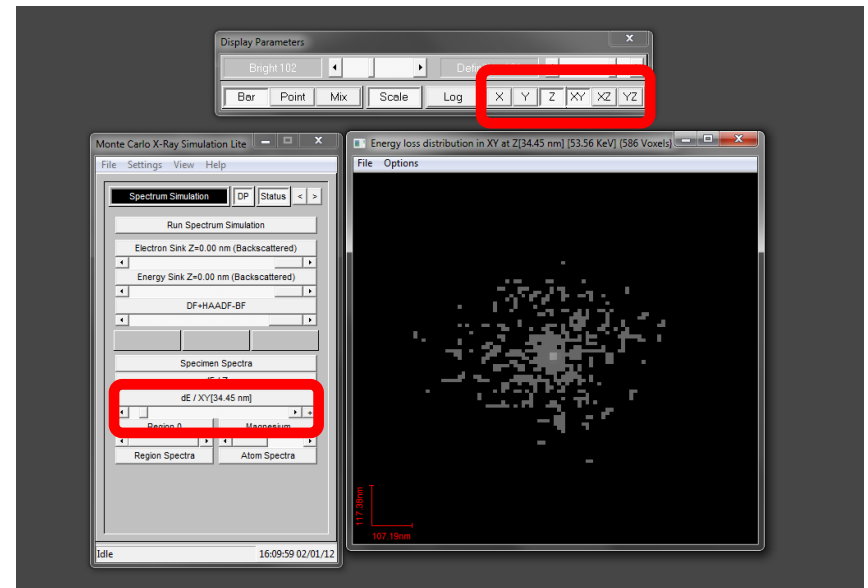
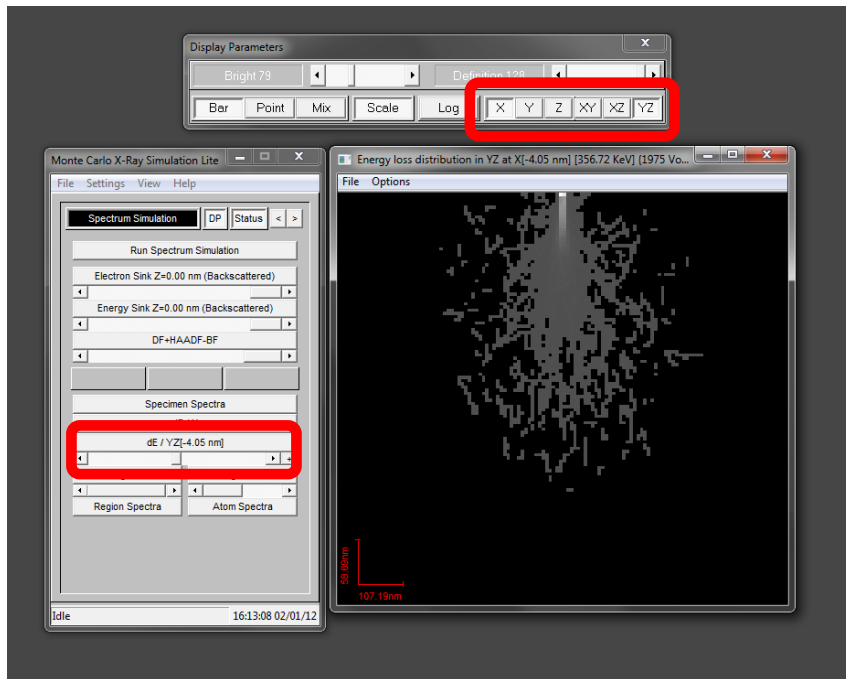
Energy loss depth distribution

Energy Loss Distribution 1D



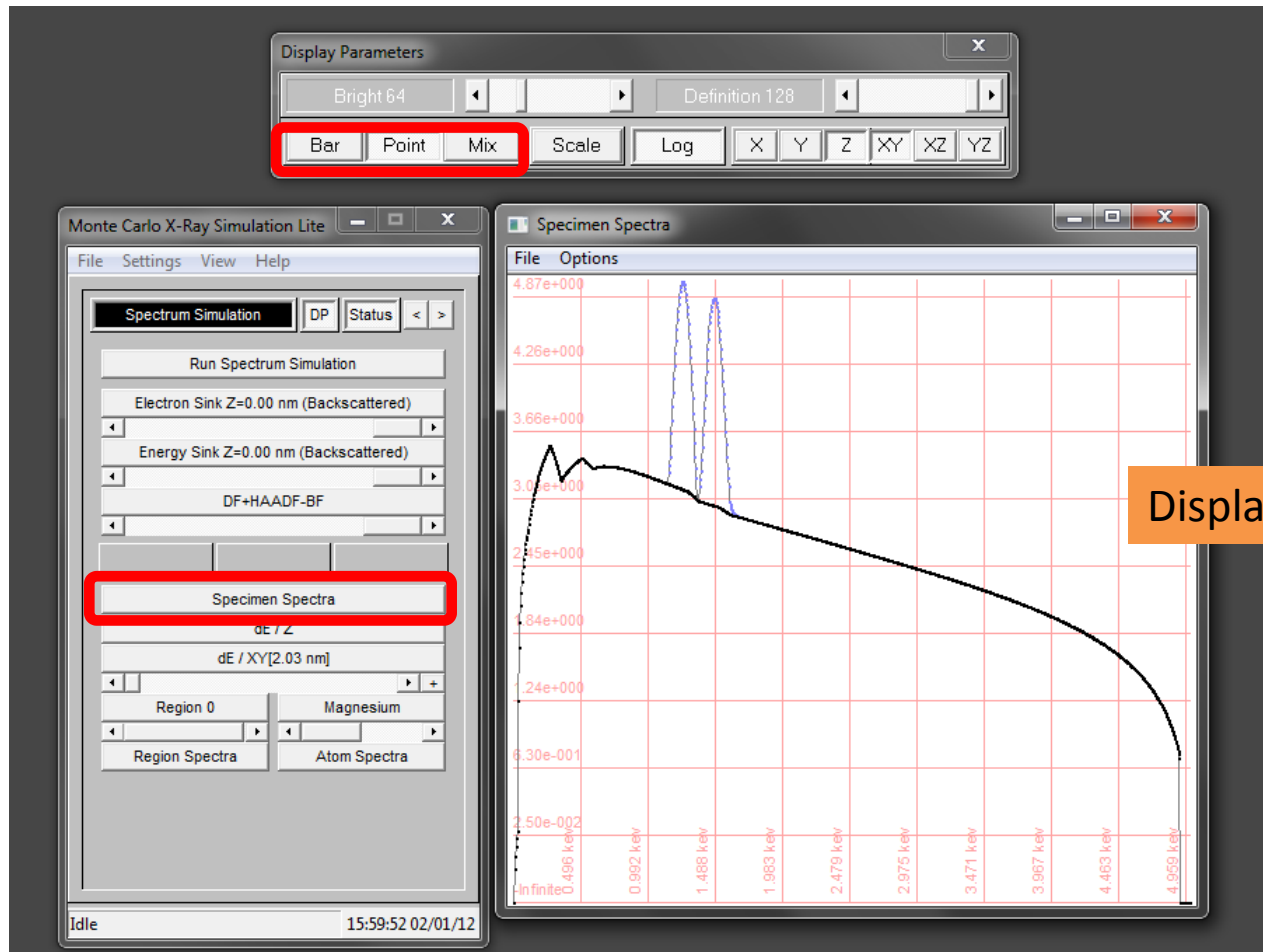
Energy loss lateral distribution

Energy Loss Distribution 2D



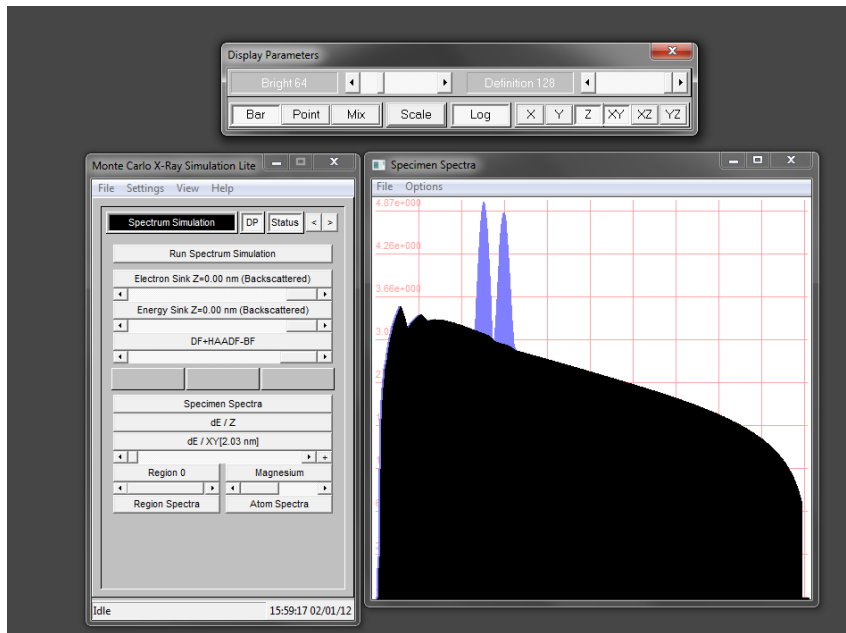
Energy loss 2D distribution

Specimen Spectrum

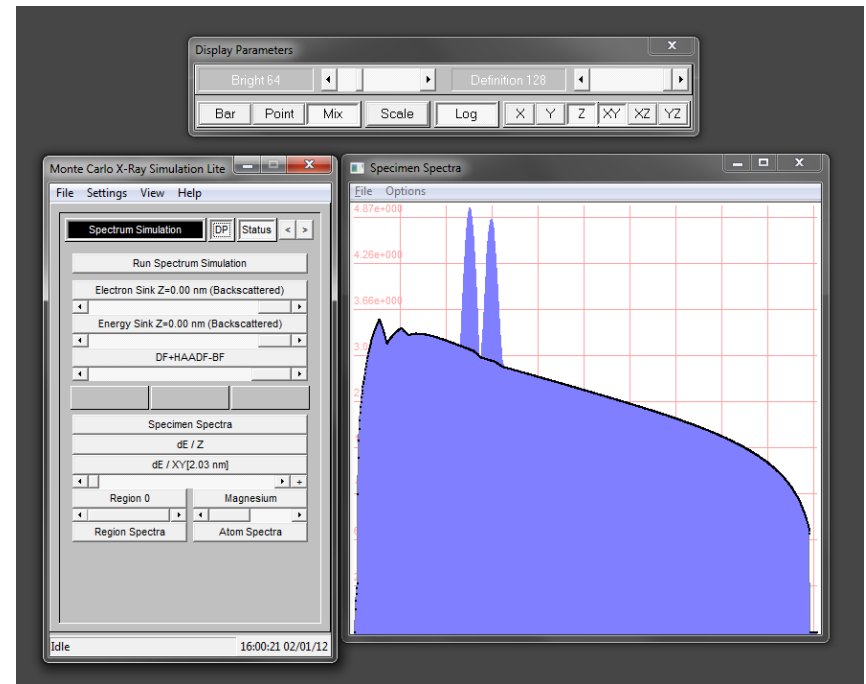


Complete x-ray spectrum for all elements in all regions
Show also the bremsstrahlung

Specimen Spectrum

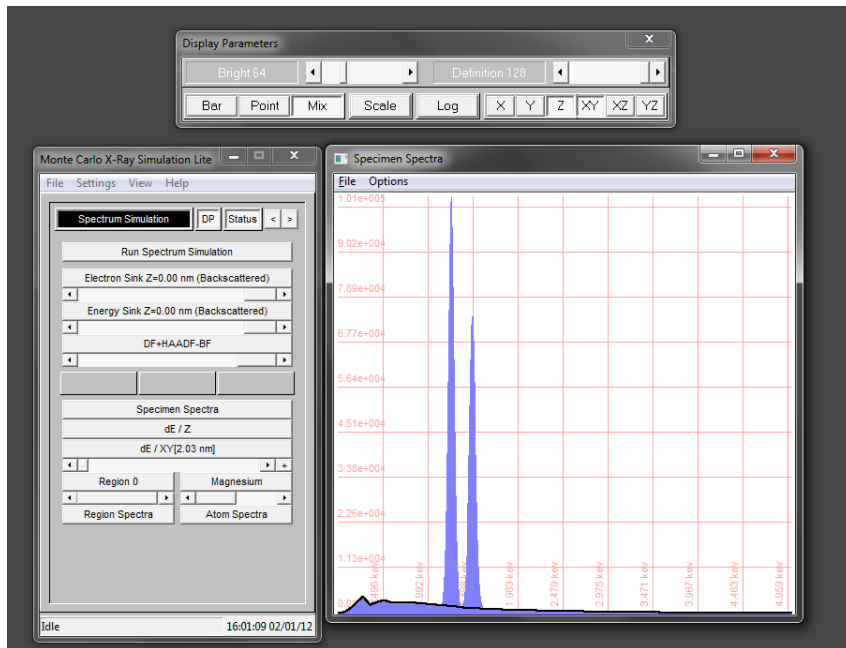


Displayed with bars

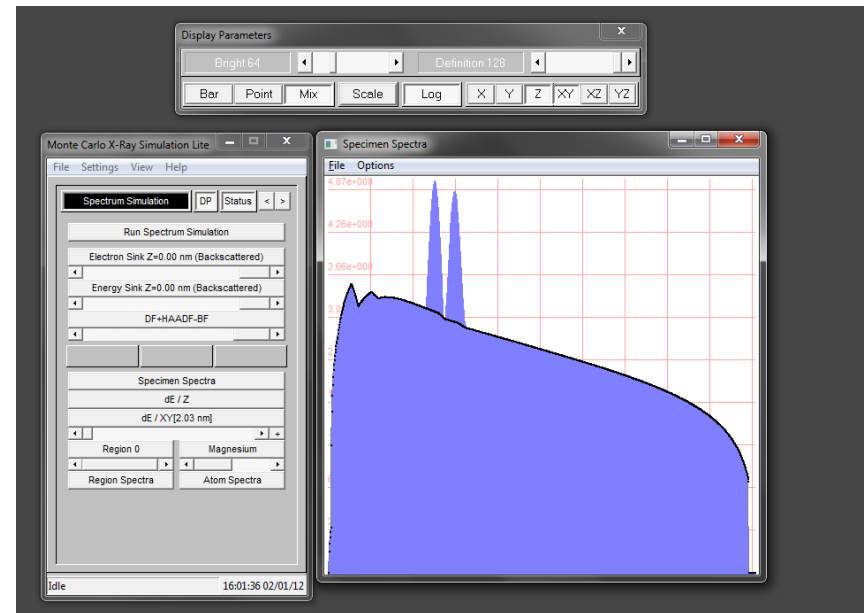


Displayed with points and bars

Specimen Spectrum

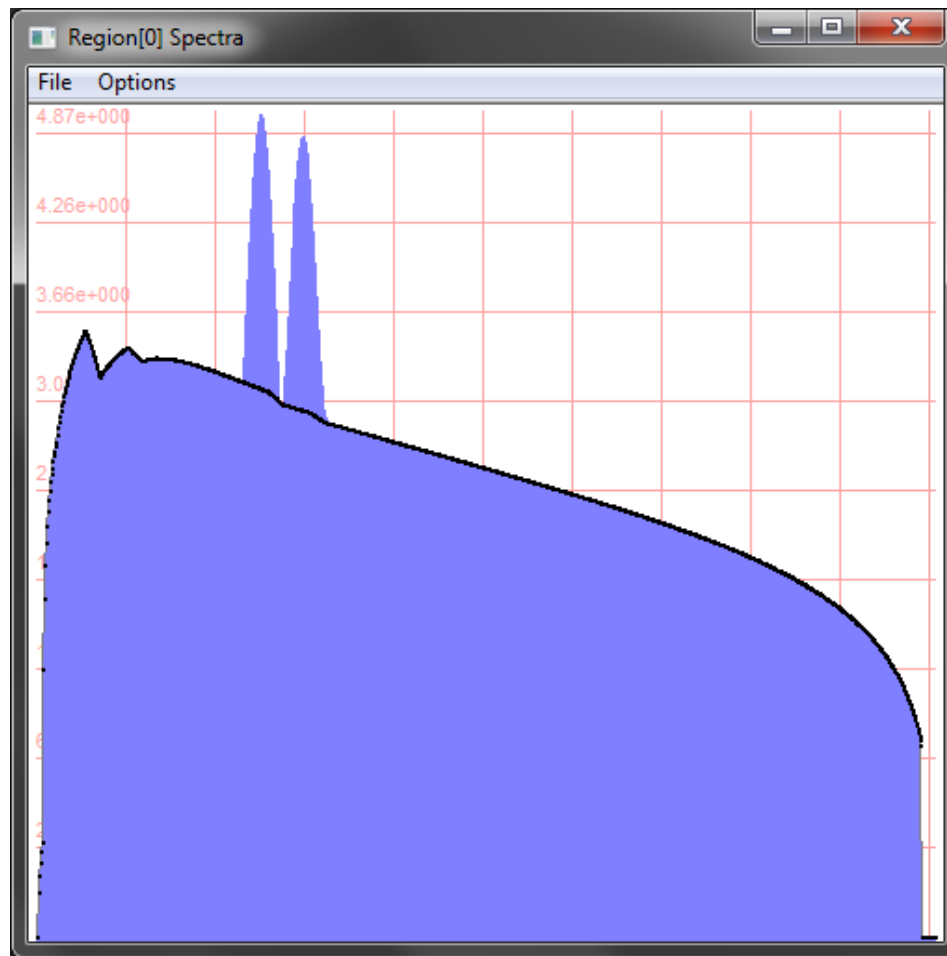


Linear scale



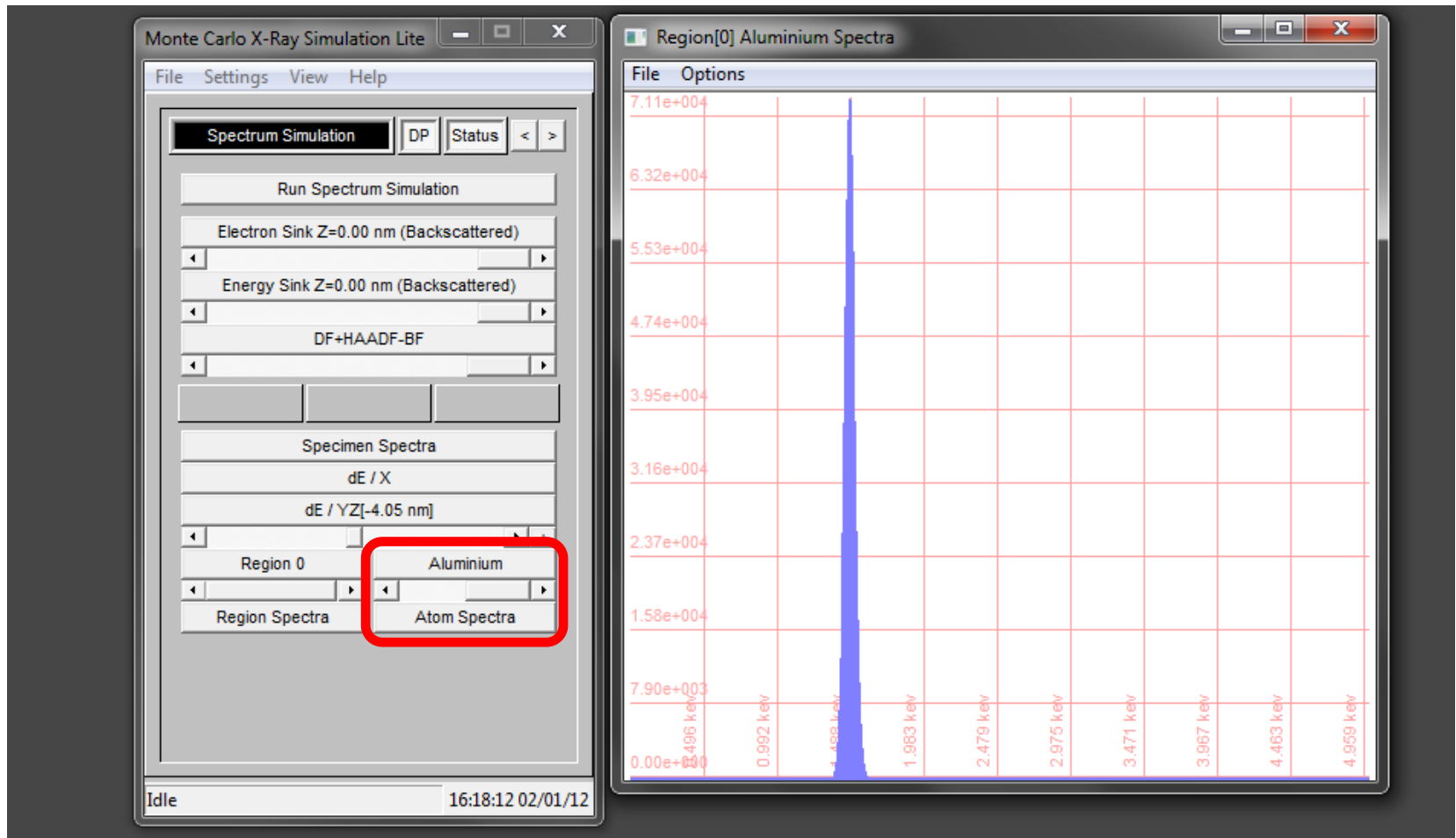
Logarithmic scale

Region Spectrum



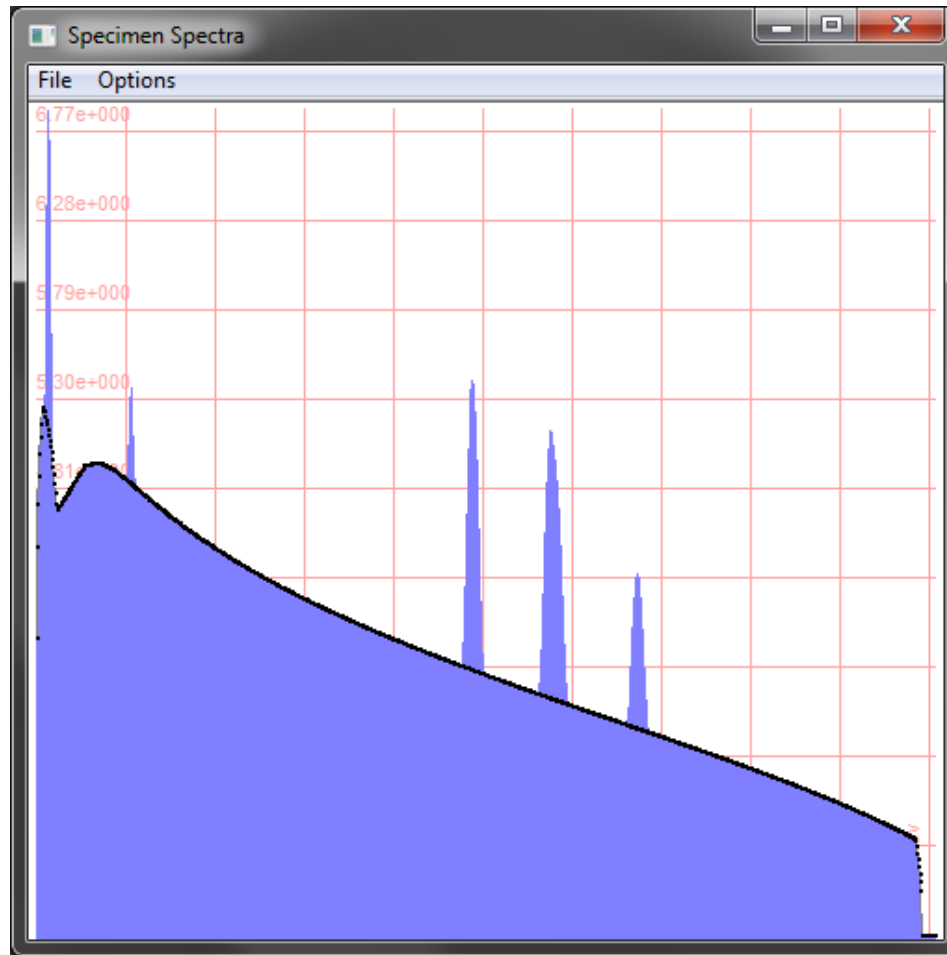
Display spectrum for each region

Atom Spectrum

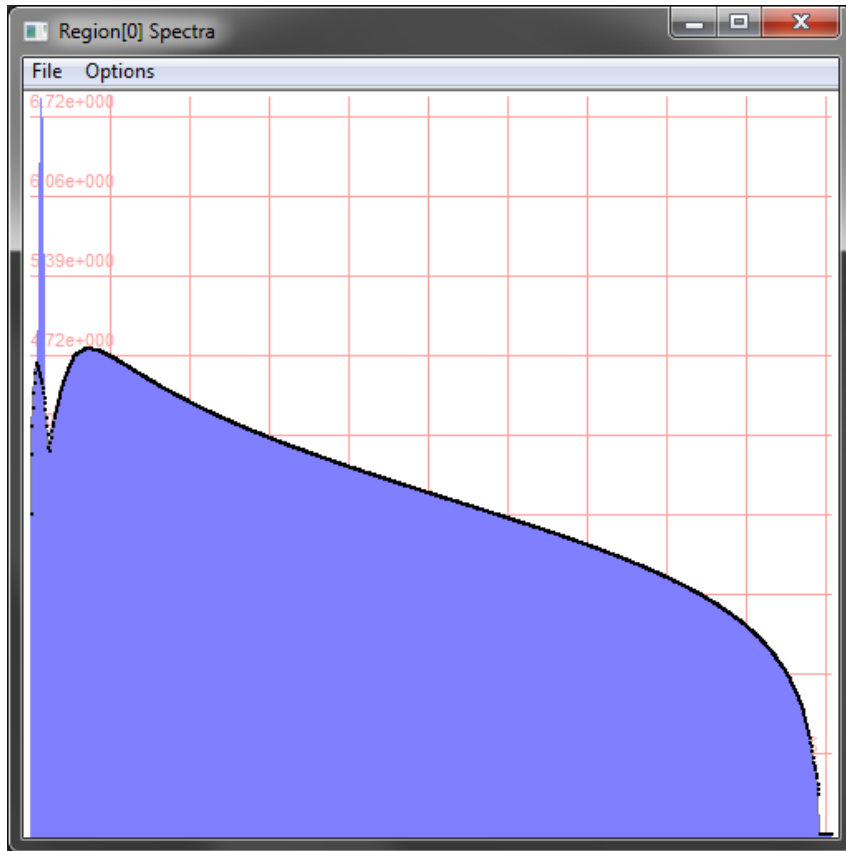


Display spectrum for each atom in a region

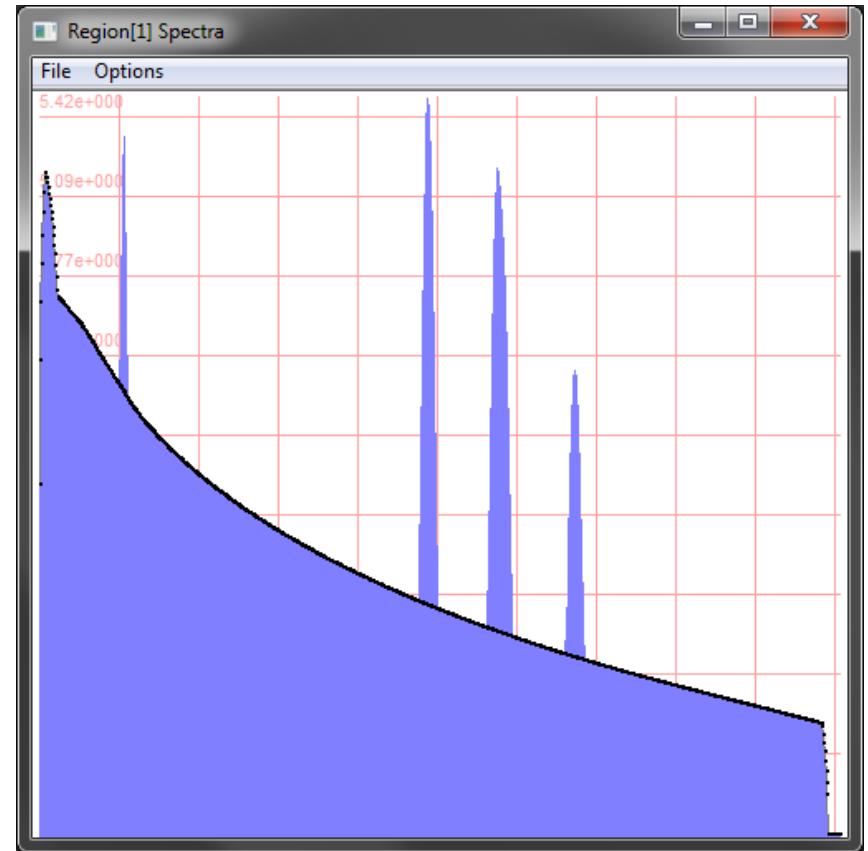
Au NP in C Specimen Spectrum



Au NP in C Region Spectrum

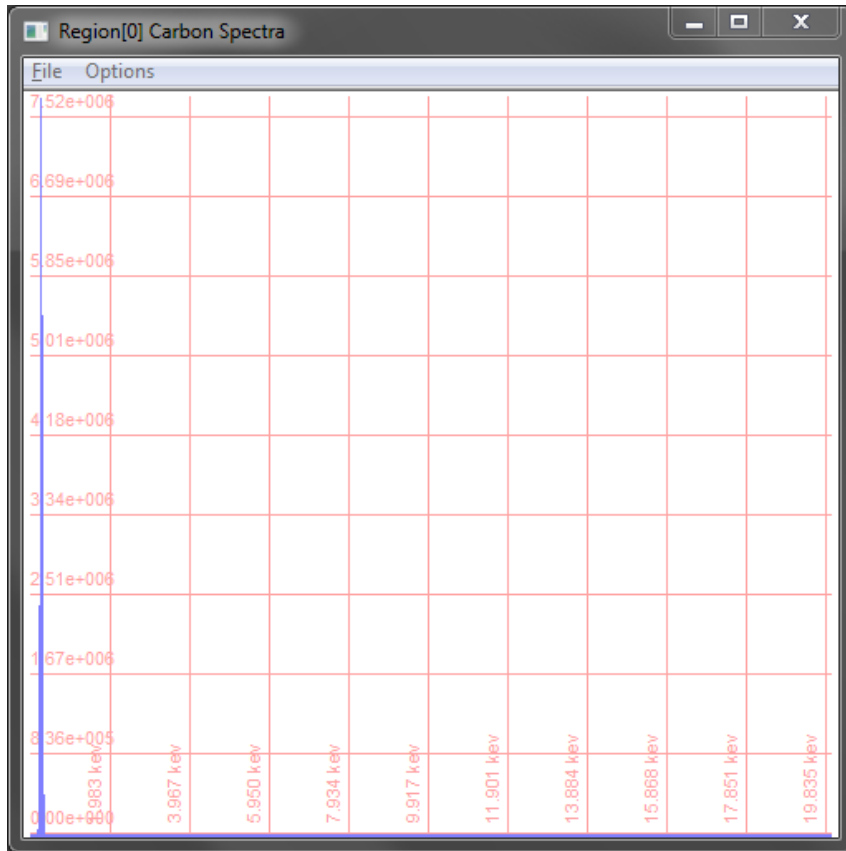


C Substrate

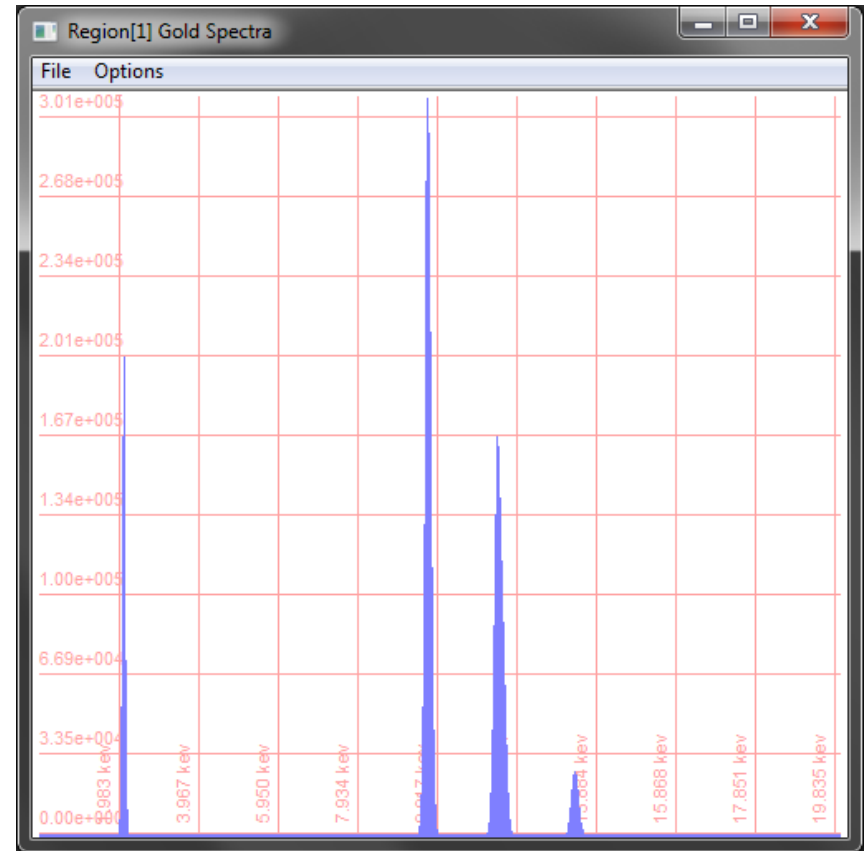


Au NP

Au NP in C Atom Spectrum



C Substrate

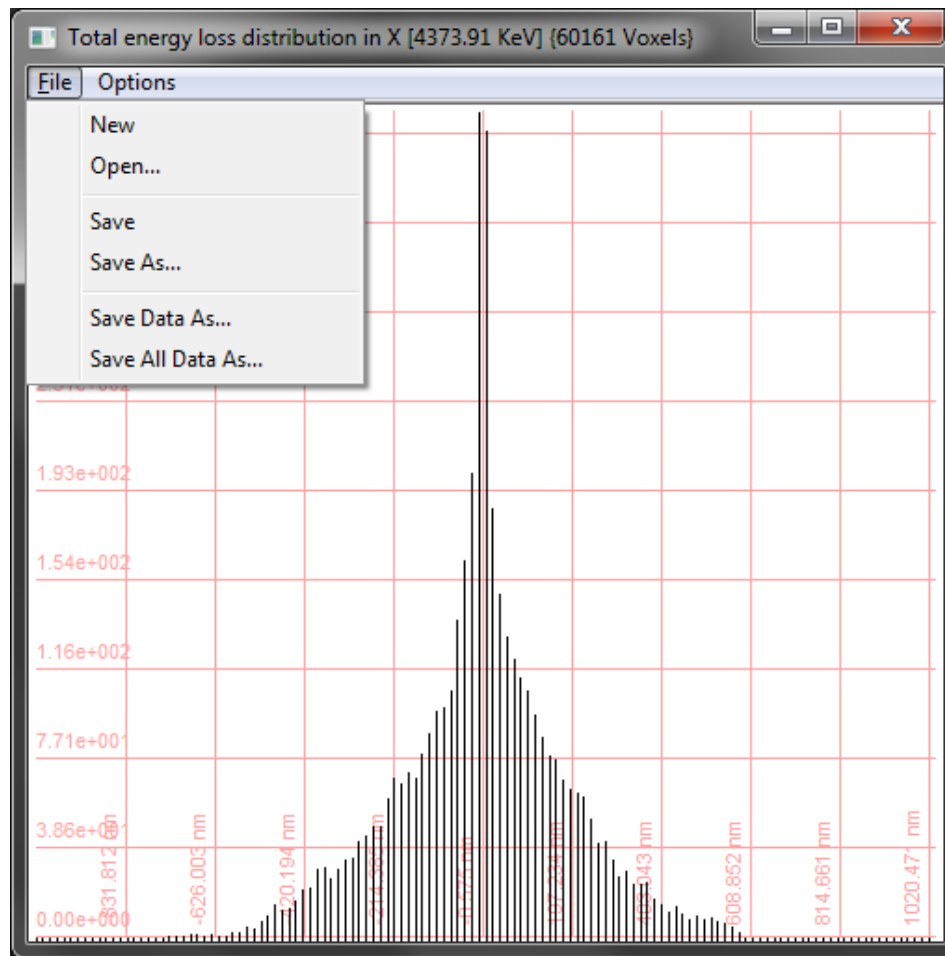


Au NP

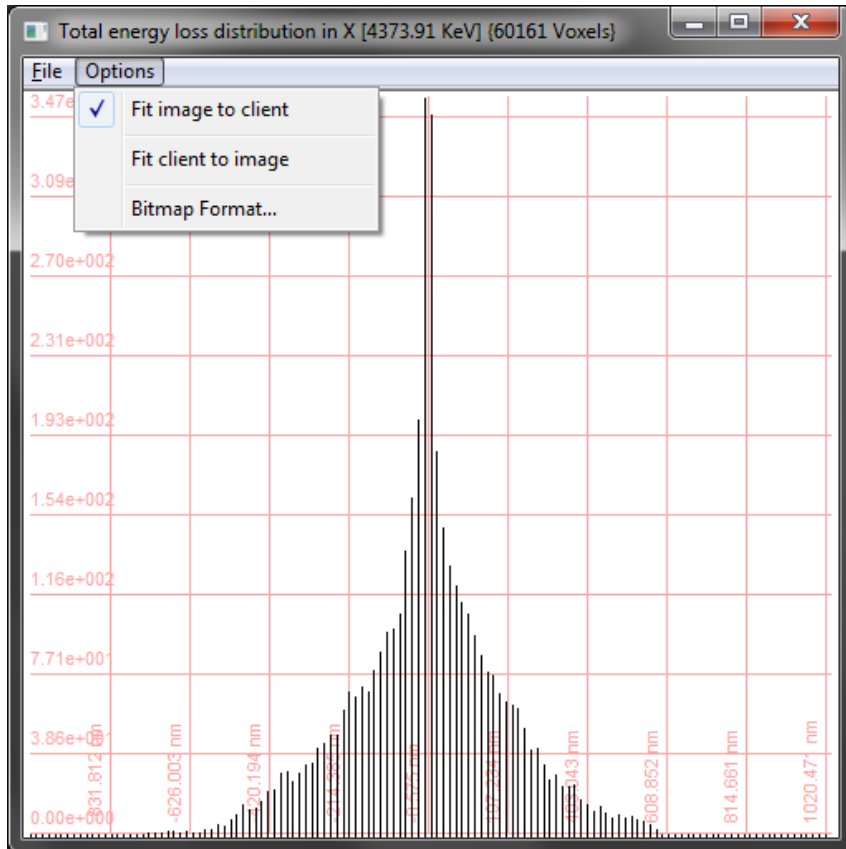
Display Results File Menu

Save the graphic
In a bitmap file

Save the data
in a text file



Display Results Options Menu



Bitmap Options

Width	492
Height	450
Bits per Pixel	32

OK Cancel