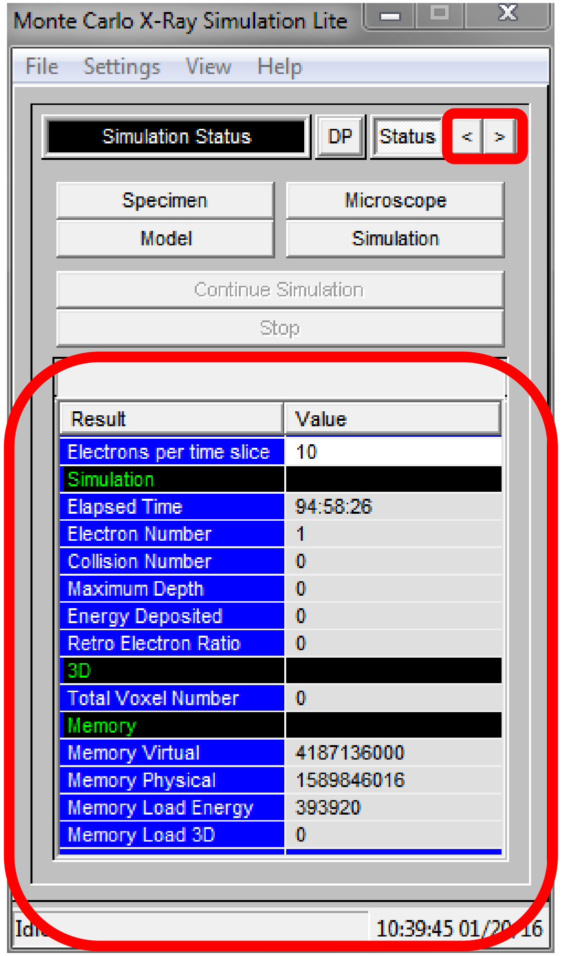
MC X-Ray Lite User Manual

Version 1.6

January 2016

MC X-Ray Lite



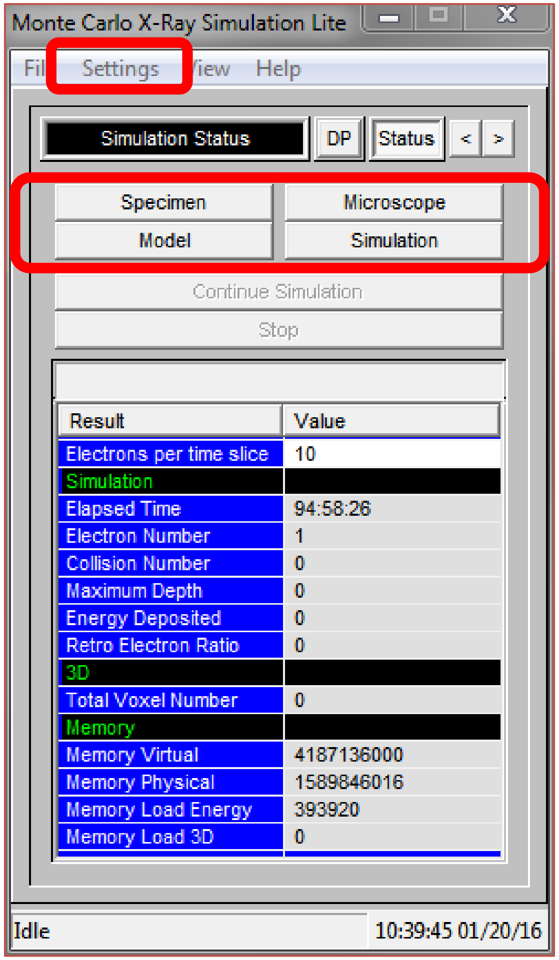
Navigate between main and spectrum simulation dialogs

Information about the simulation progress

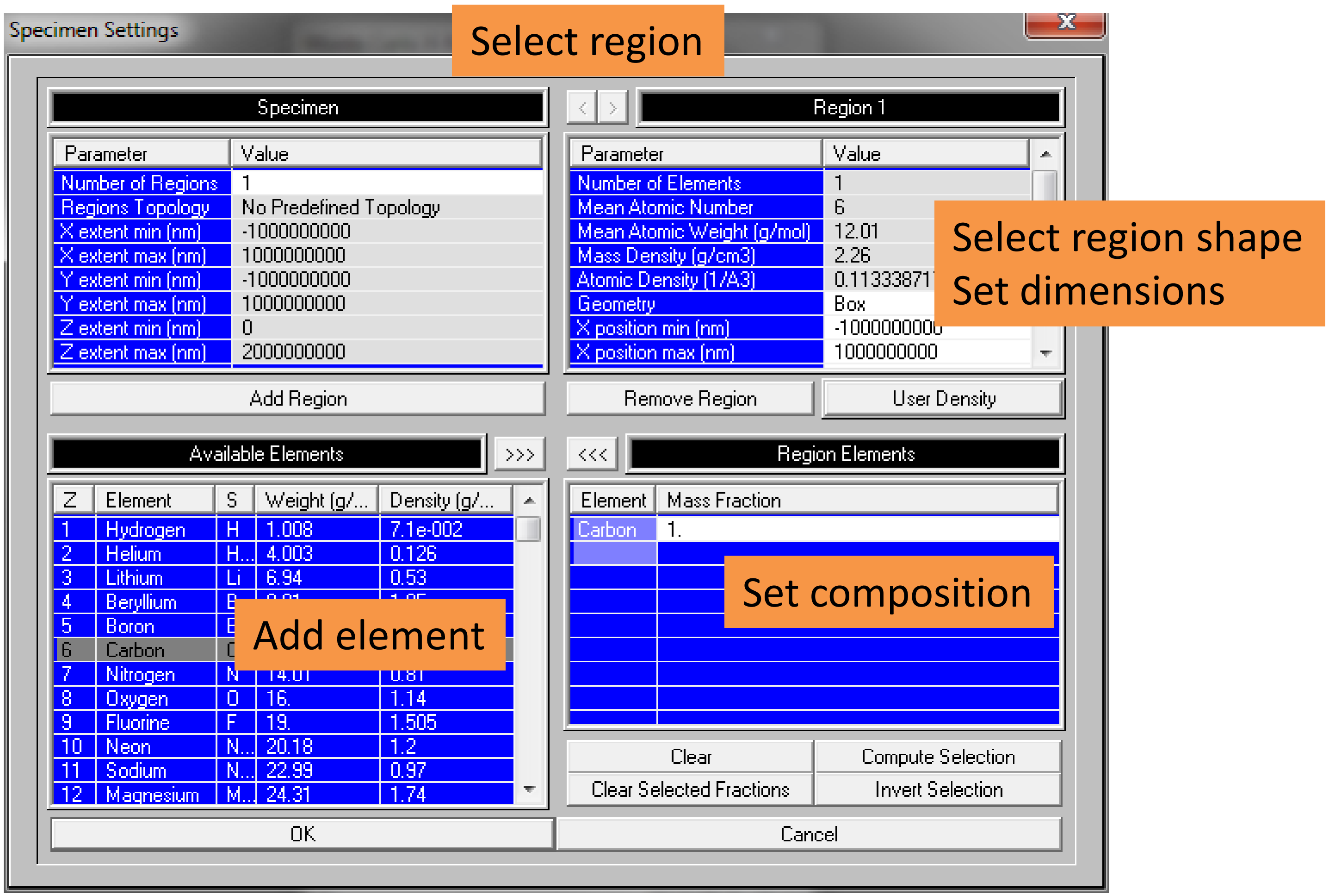
Settings

- Specimen
- Microscope
- Models
- Simulation Parameters

Can be access either by the buttons or the menu

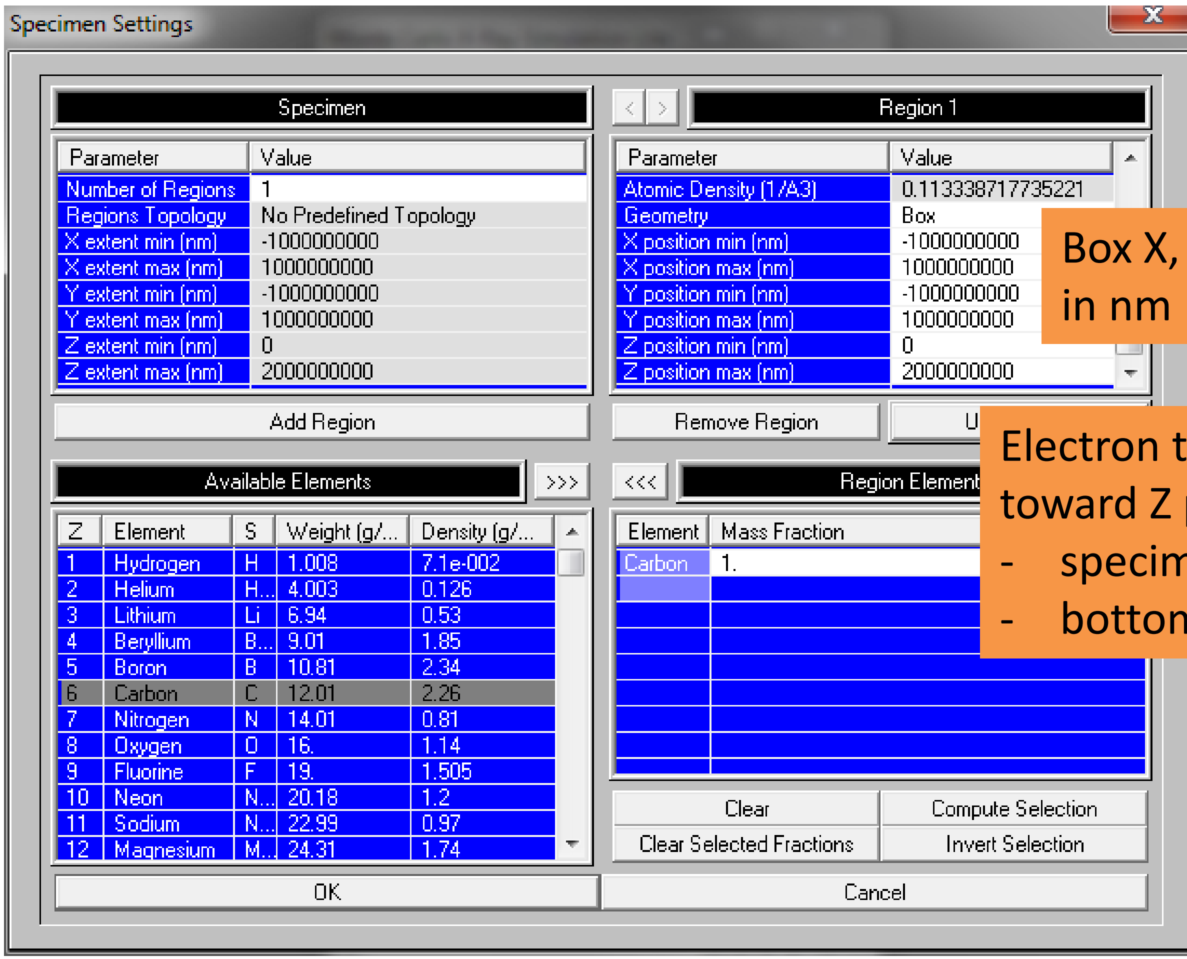


Specimen Settings



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

Region Box

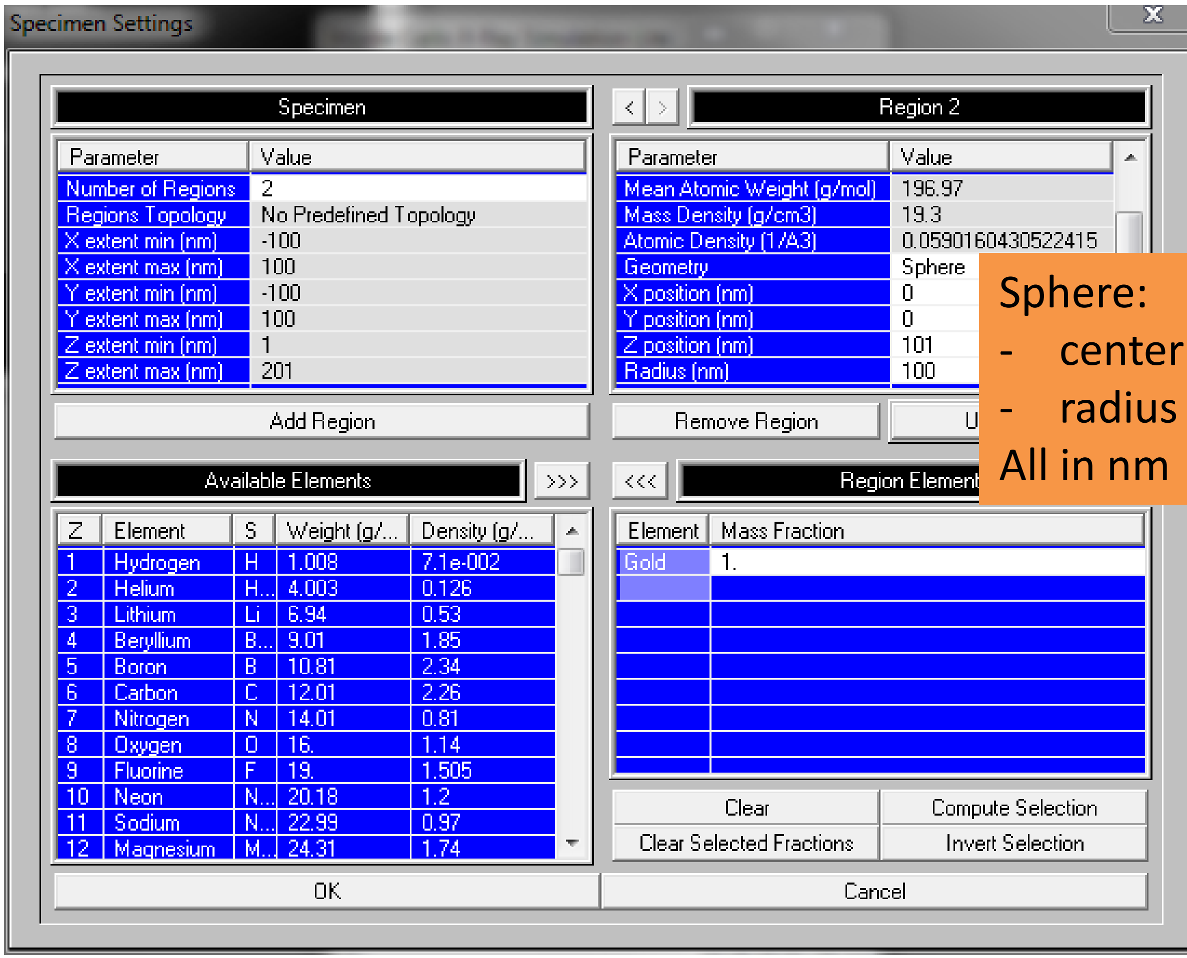


Box X, Y, Z dimensions in nm

Electron travel toward Z positive

- specimen surface at 0
- bottom at 2 m (2x10^9 nm)

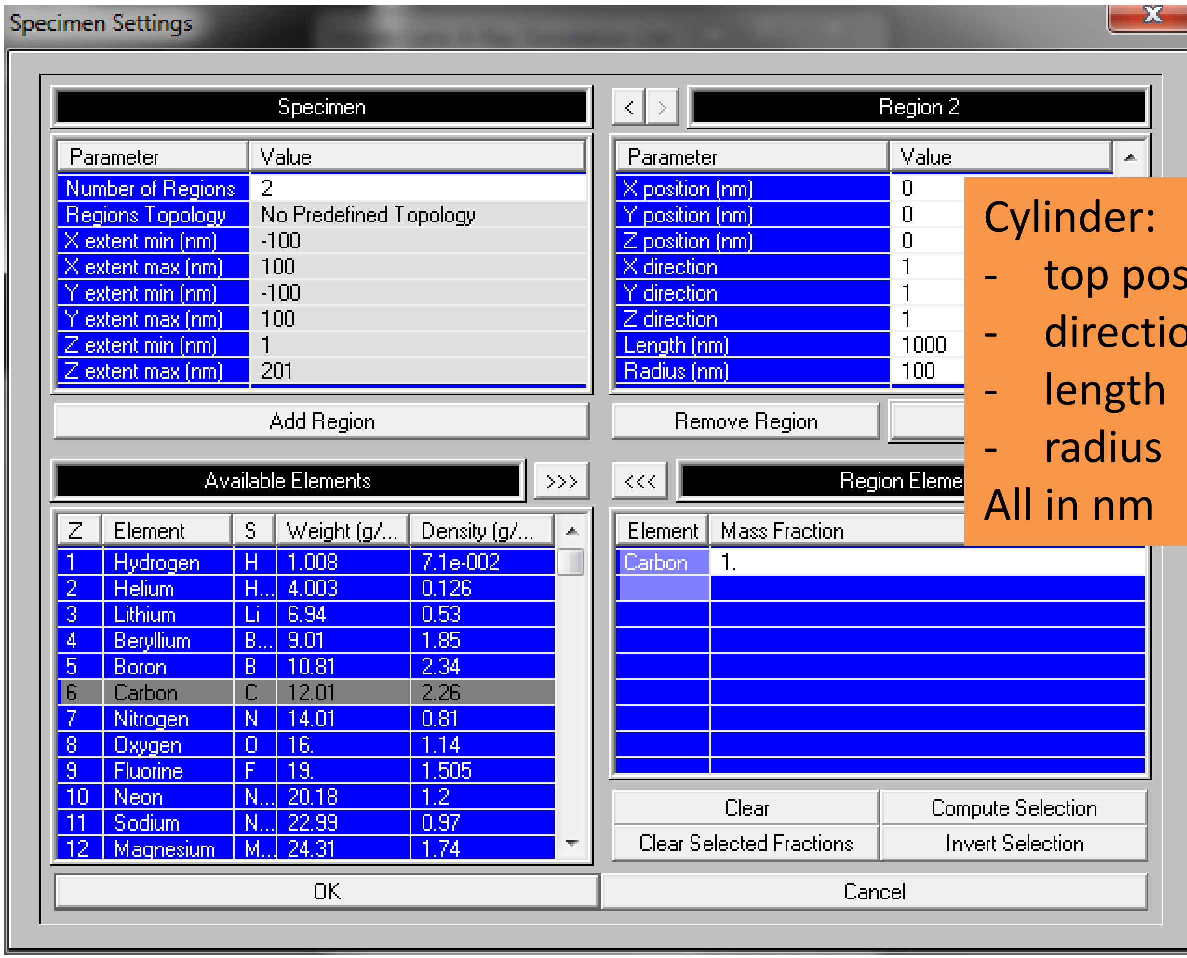
Region Sphere



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

All in nm

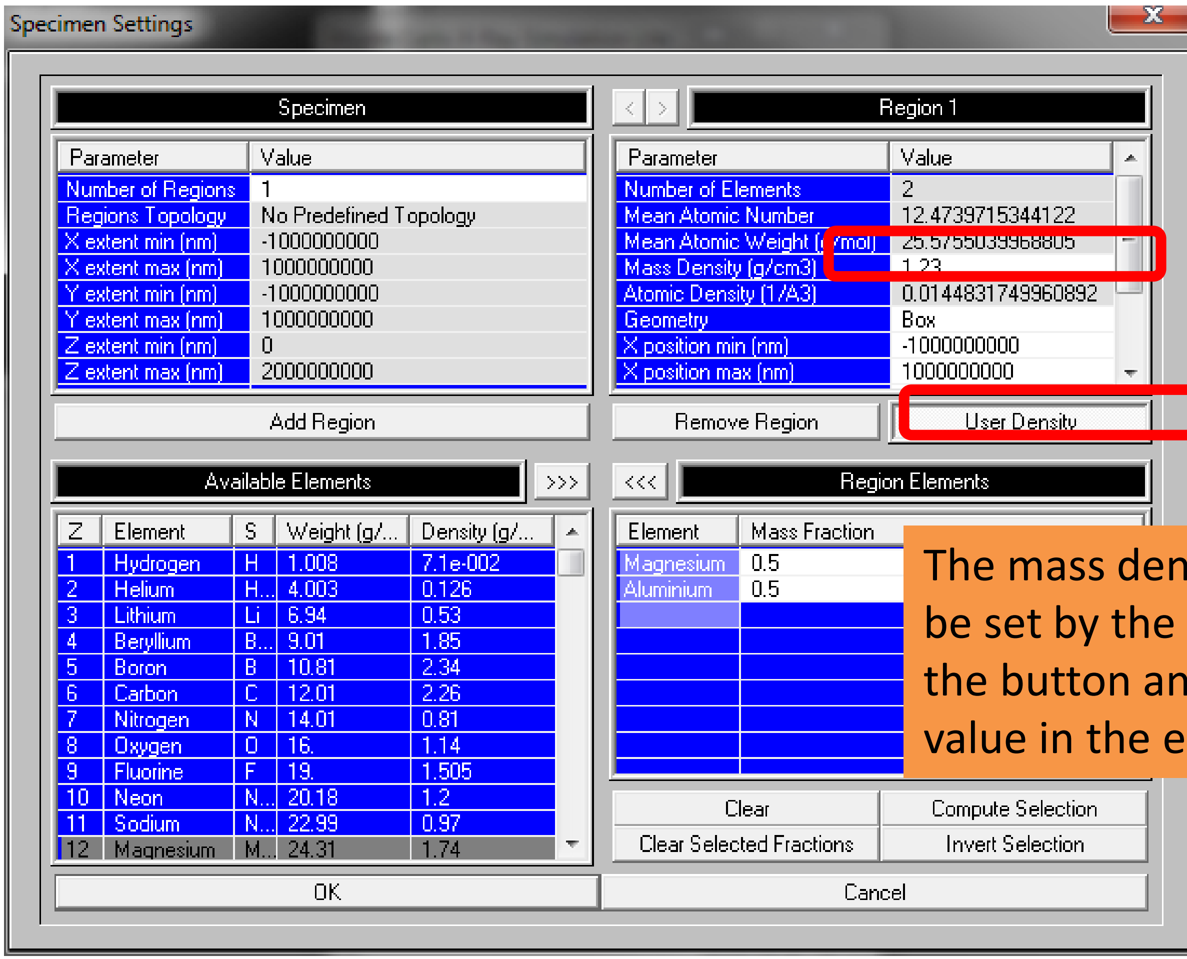
Region Cylinder



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

All in nm

Region User Density



The mass density (g/cm^3) can be set by the user by clicking the button and enter the value in the editbox

Microscope Settings

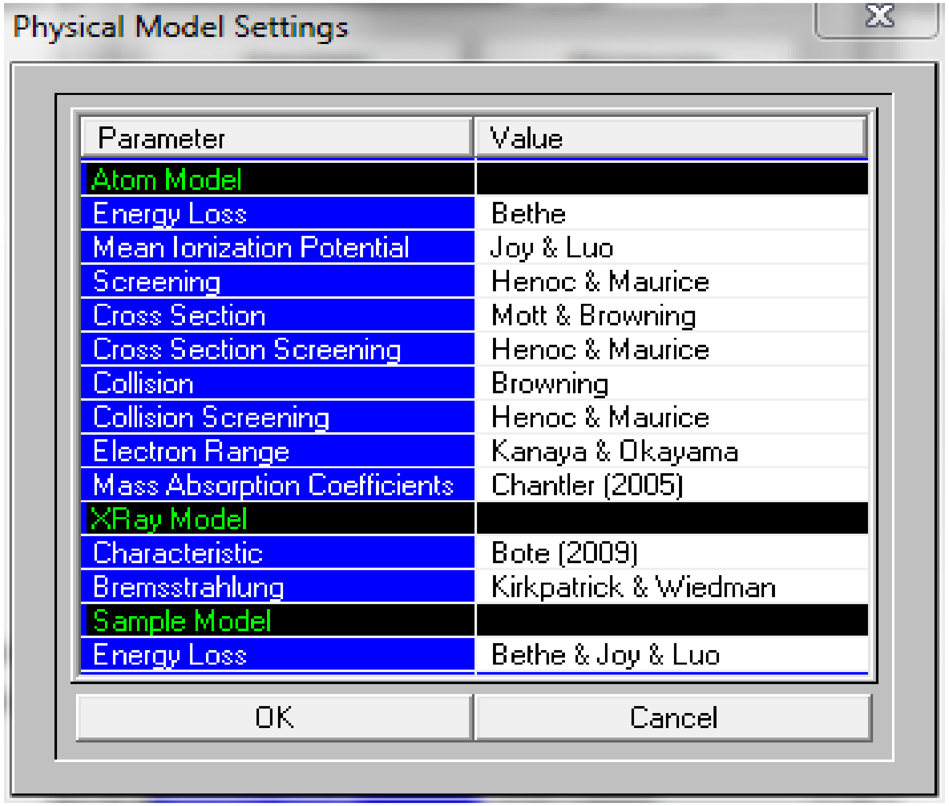
Microscope Settings

Parameter	Value
Electron Beam	
Energy (keV)	20.0000000
Current (A)	1e-009
Diameter (nm)	1
Acquisition Time (s)	100.0000000
Position X (nm)	0.0000000
Position Y (nm)	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	3.0303030
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)	2000.0000000
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)	50.0000000000274
Angle Pitch (deg)	90.0000000
Direction X	0.0000000
Direction Y	0.7660444
Direction Z	-0.6427876
Bright Field Low Angle (rad)	0.0000000
Bright Field High Angle (rad)	0.0100000
Dark Field Low Angle (rad)	0.0200000
Dark Field High Angle (rad)	0.1000000
HAAD Field Low Angle (rad)	0.1500000
HAAD Field High Angle (rad)	0.3000000

OK Cancel

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

Models Settings



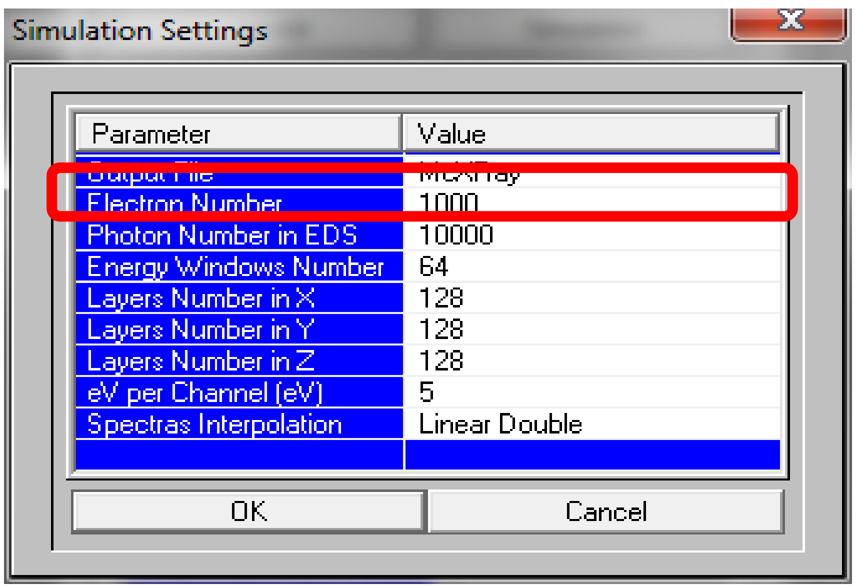
Physical Model Settings

Parameter	Value
Atom Model	
Energy Loss	Bethe
Mean Ionization Potential	Joy & Luo
Screening	Henoc & Maurice
Cross Section	Mott & Browning
Cross Section Screening	Henoc & Maurice
Collision	Browning
Collision Screening	Henoc & Maurice
Electron Range	Kanaya & Okayama
Mass Absorption Coefficients	Chantler (2005)
XRay Model	
Characteristic	Bote (2009)
Bremsstrahlung	Kirkpatrick & Wiedman
Sample Model	
Energy Loss	Bethe & Joy & Luo

OK Cancel

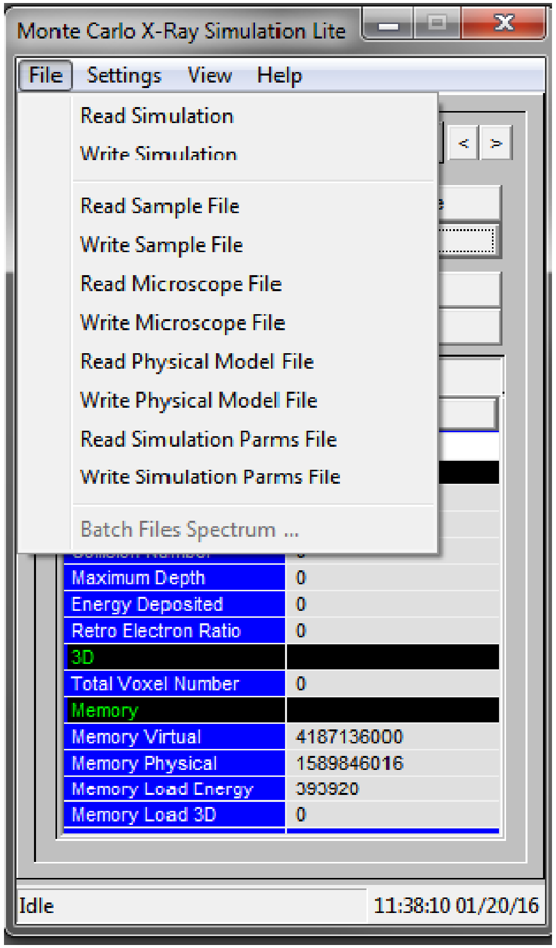
The default models are the best one to use in most simulation

Simulation Parameters



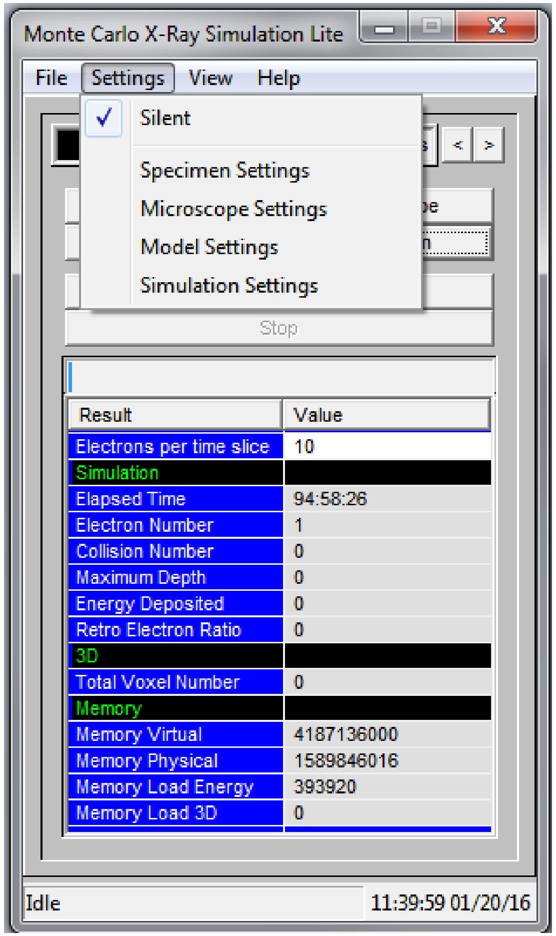
- Set the number of simulated electrons
- Other options are advanced feature, where the default values are good for most simulations

File Menu



Read and write all settings in separate files

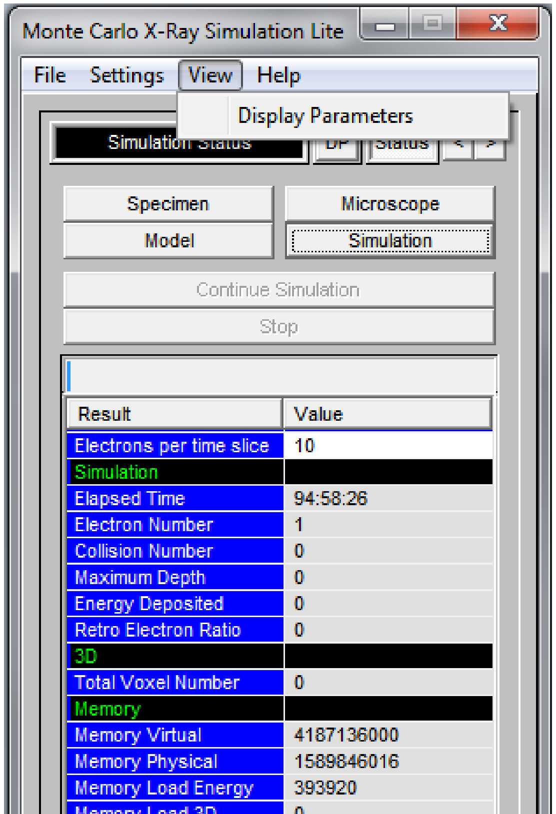
Settings Menu



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

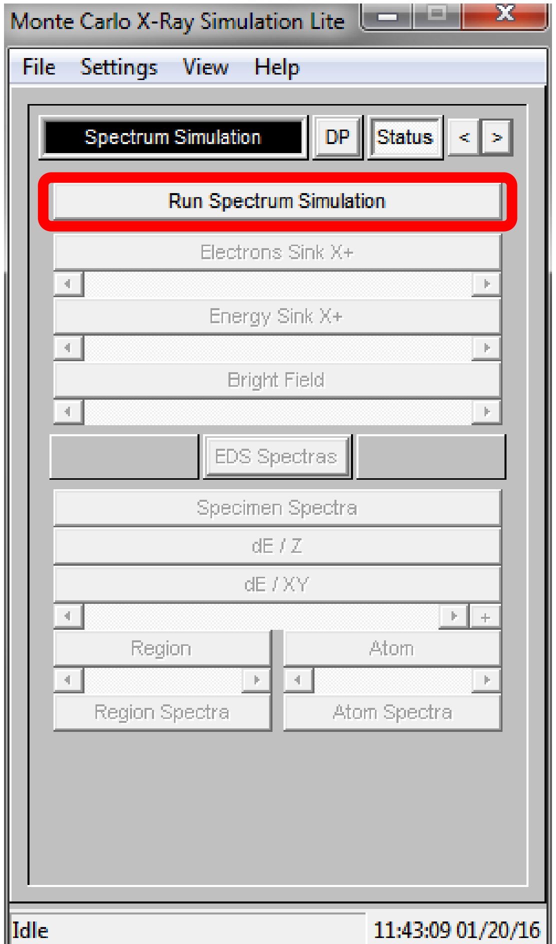
Display Parameters

Linear or log scale

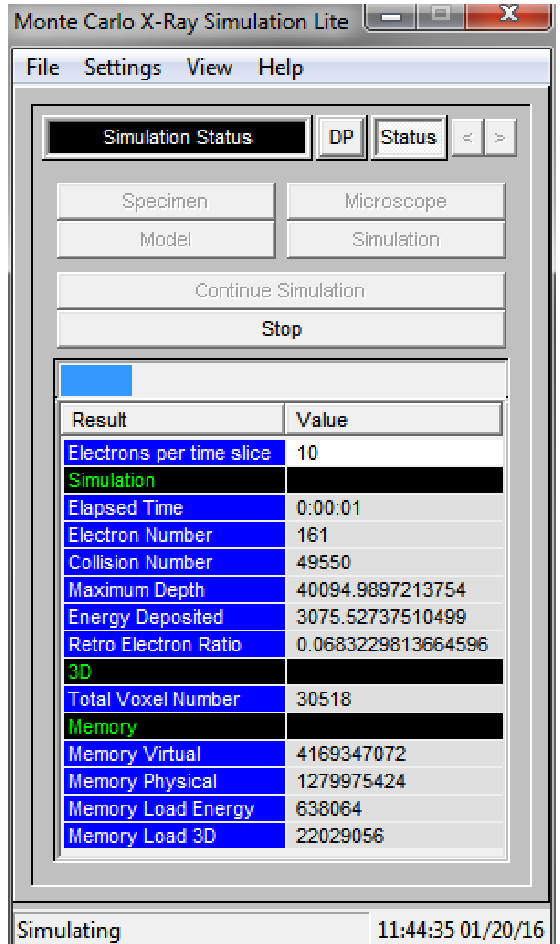
Line type in the graphic

Select the distribution dimension to display

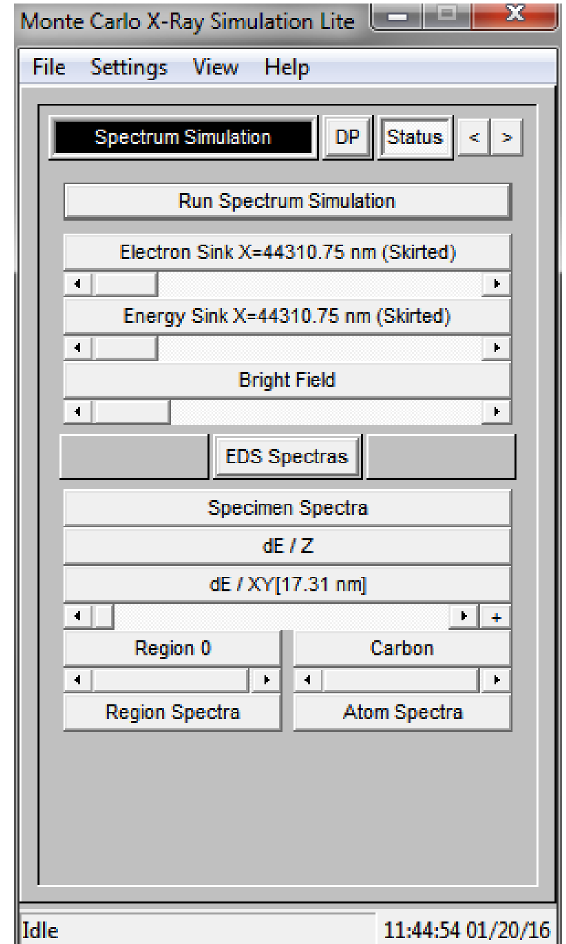
Spectrum Simulation



Start



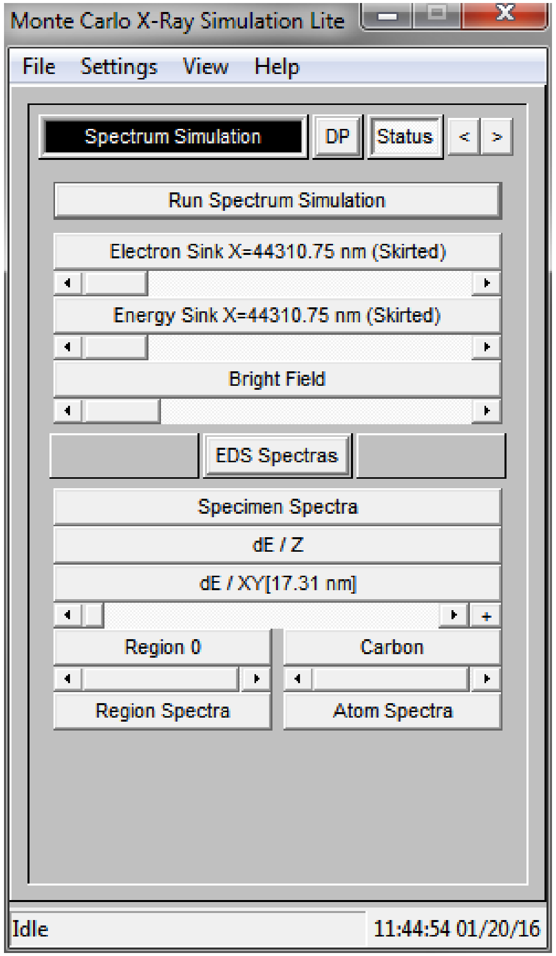
Simulating



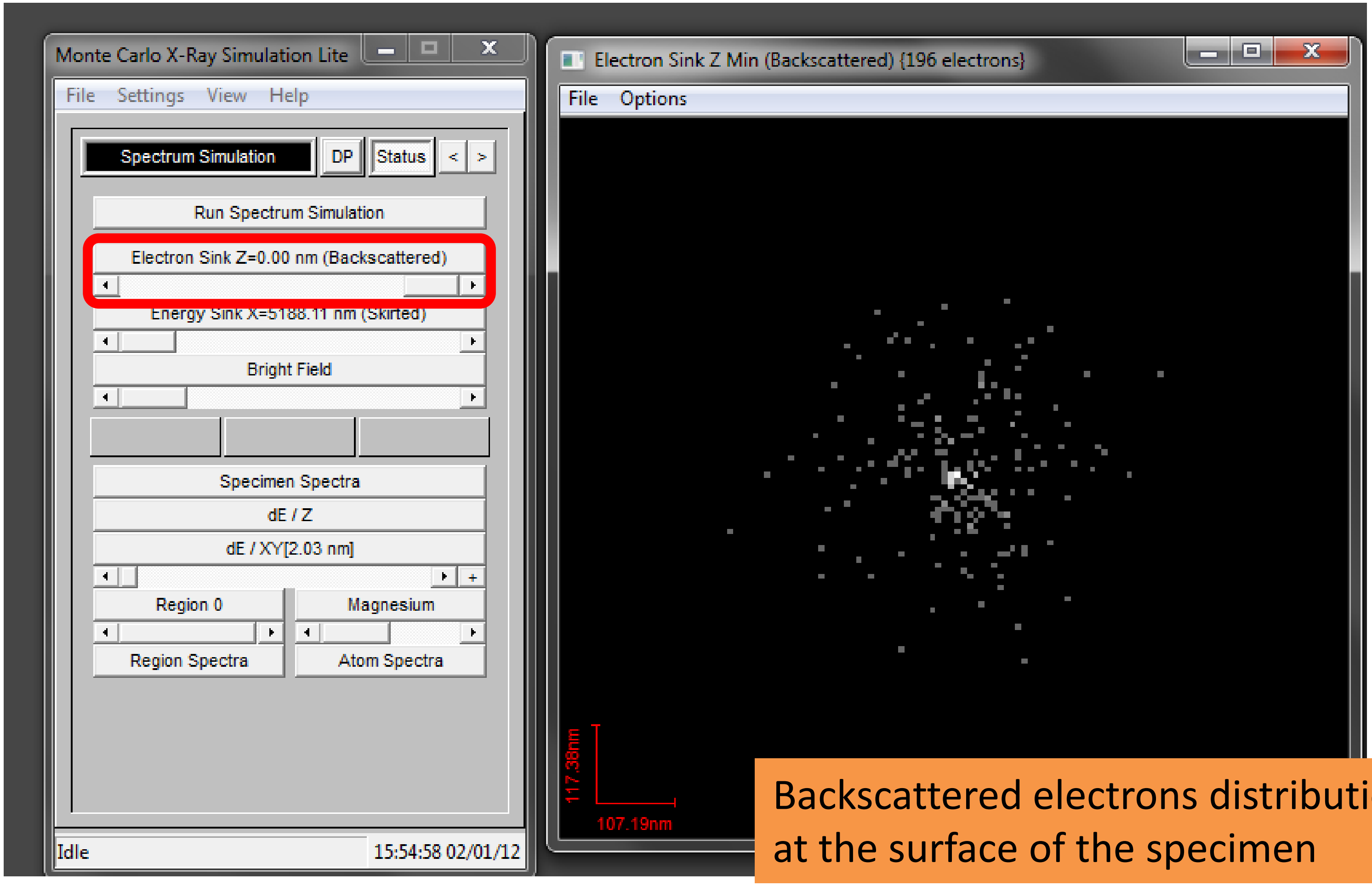
Done

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

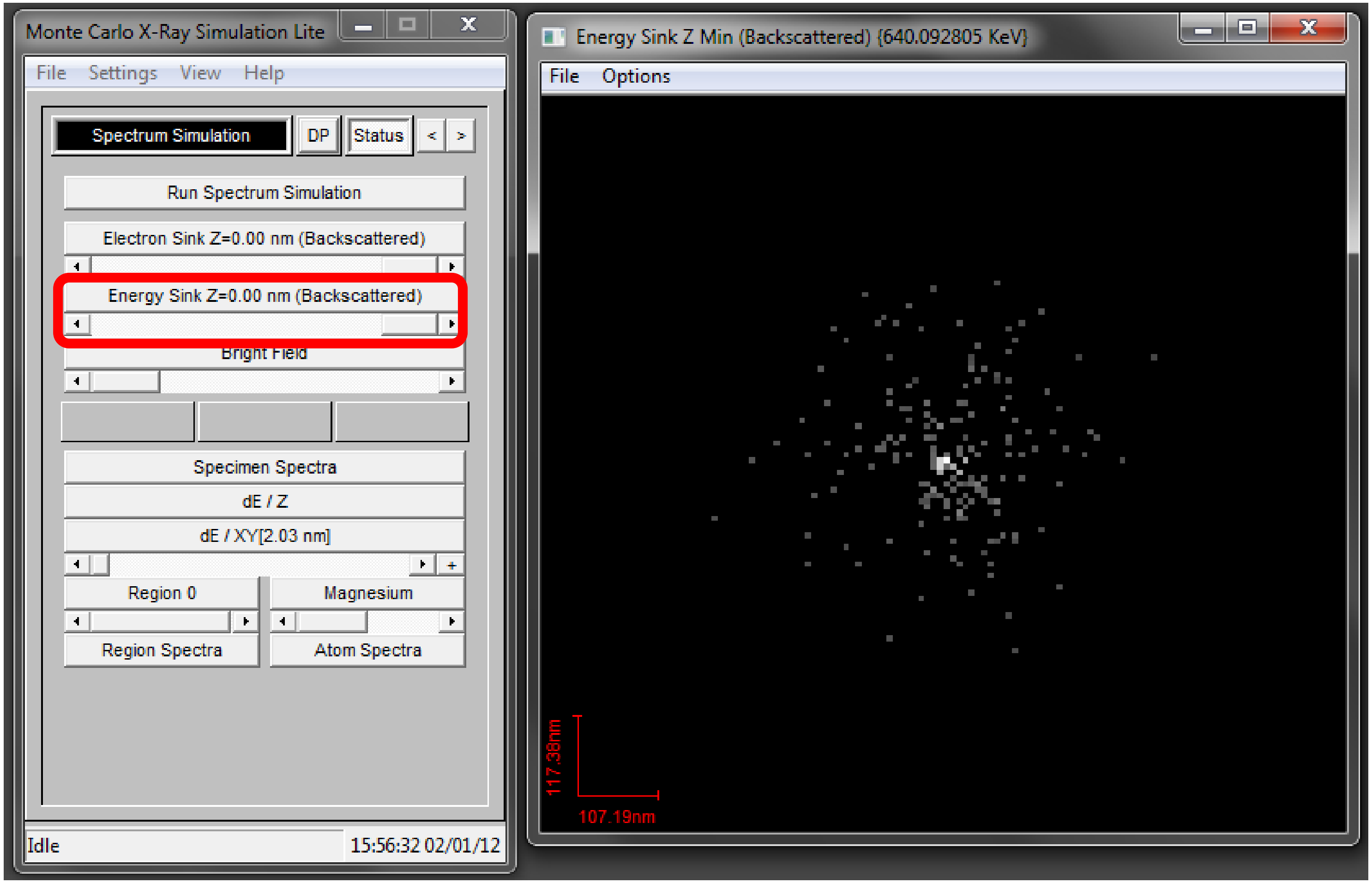


Electrons Sink

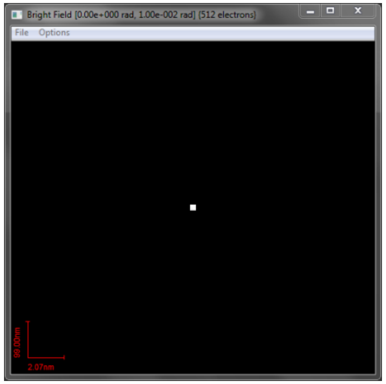


Backscattered electrons distribution at the surface of the specimen

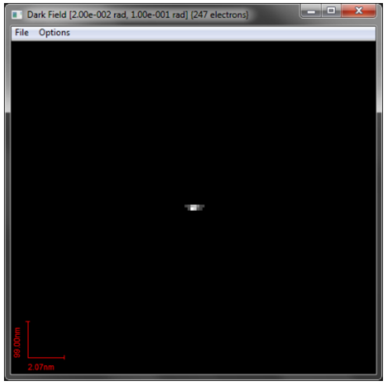
Energy Sink


Monte Carlo X-Ray Simulation Lite
File Settings View Help
Spectrum Simulation
DP
Status
Run Spectrum Simulation
Electron Sink Z=0.00 nm (Backscattered)
Energy Sink Z=0.00 nm (Backscattered)
Bright Field
Specimen Spectra
dE / Z
dE / XY[2.03 nm]
Region 0
Magnesium
Region Spectra
Atom Spectra
Idle
15:56:32 02/01/12
Energy Sink Z Min (Backscattered) {640.092805 KeV}
File Options
117.38nm
107.19nm

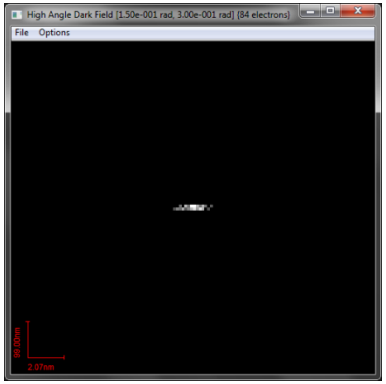
Transmitted Electrons



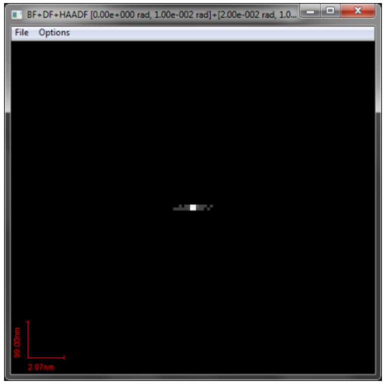
Bright Field



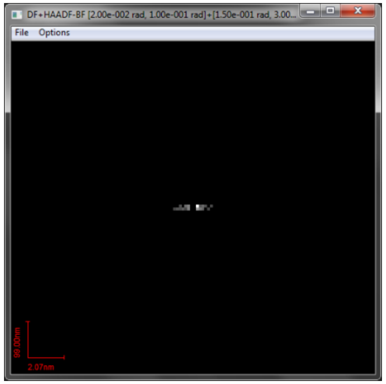
Dark Field



HAADF

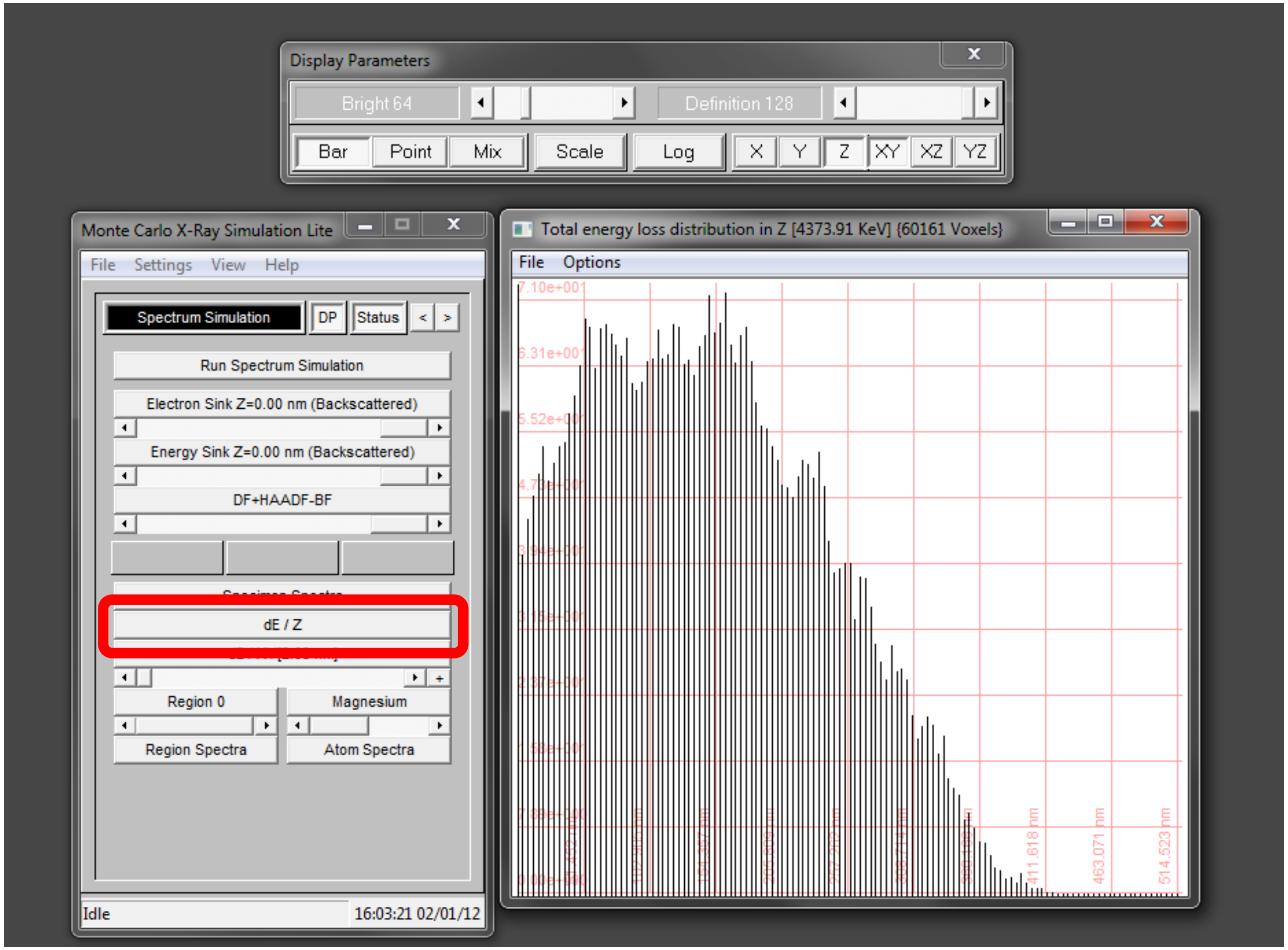


All detectors



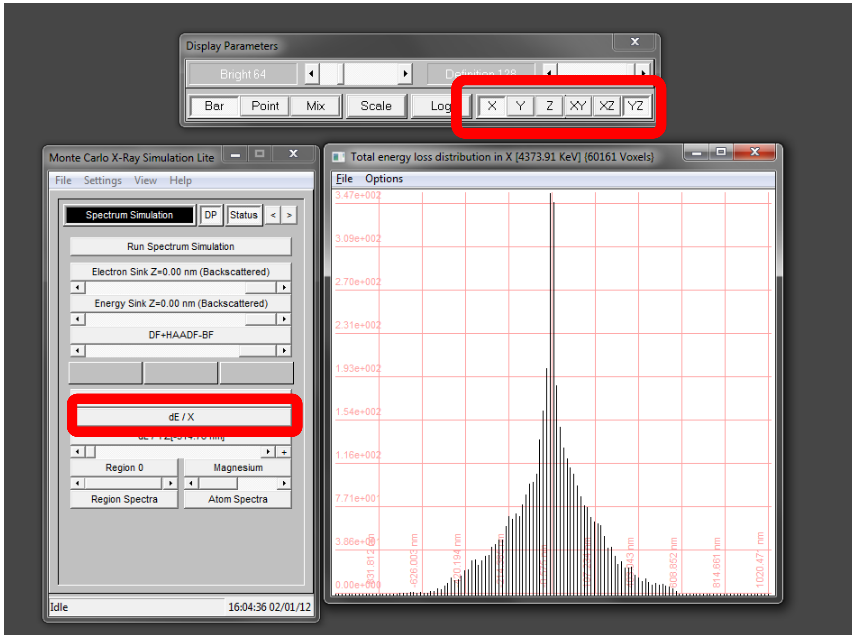
DF + HAADF - BF

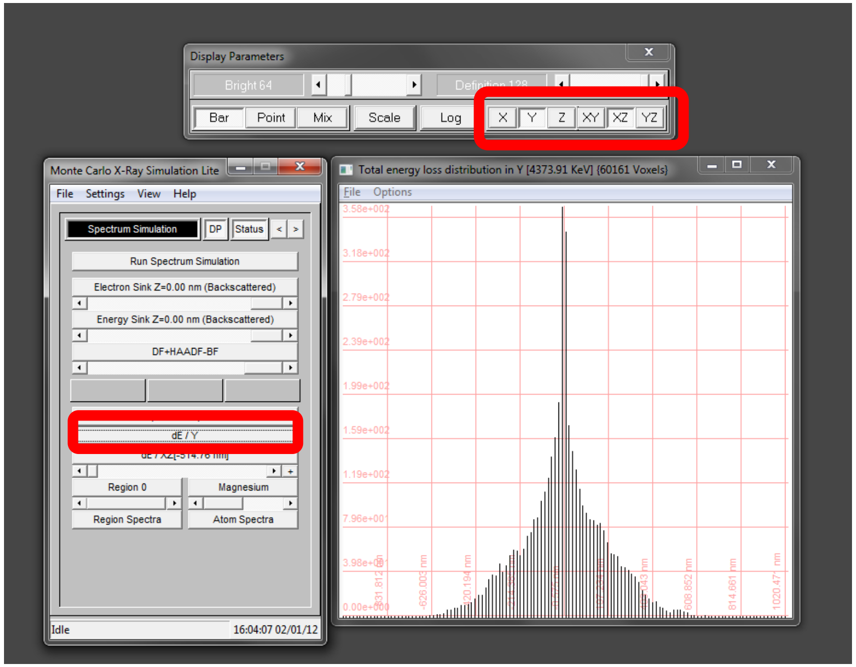
Energy Loss Distribution 1D



Energy loss depth distribution

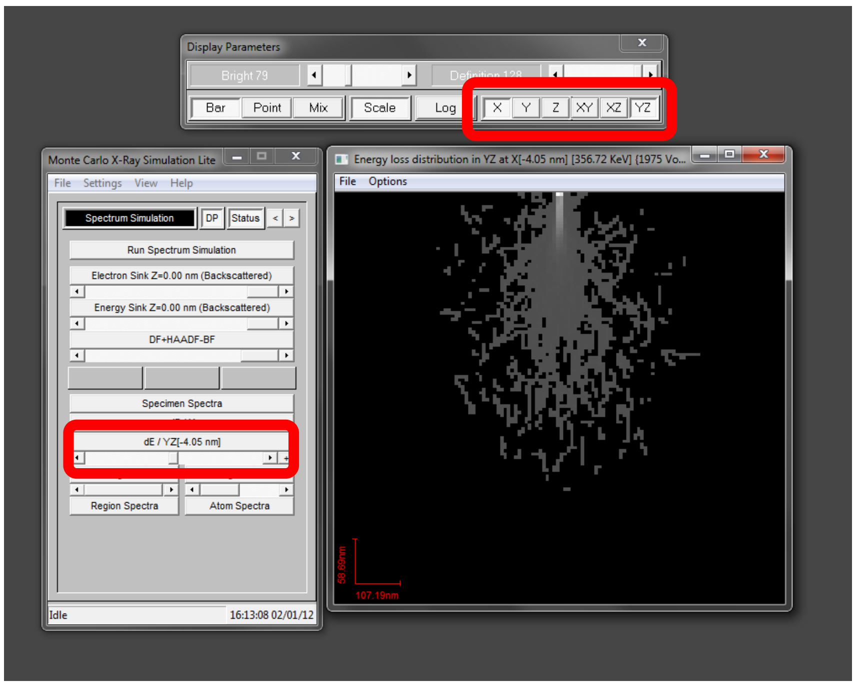
Energy Loss Distribution 1D

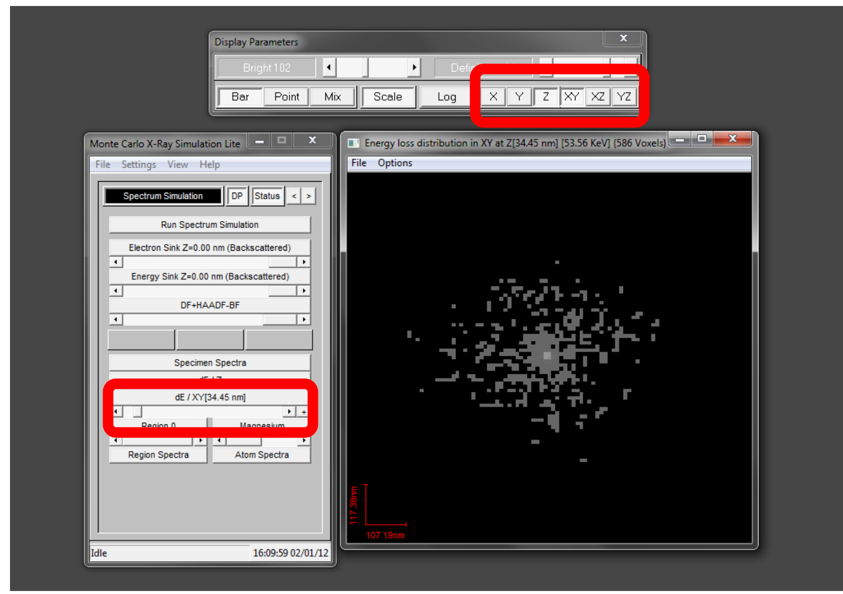




Energy loss lateral distribution

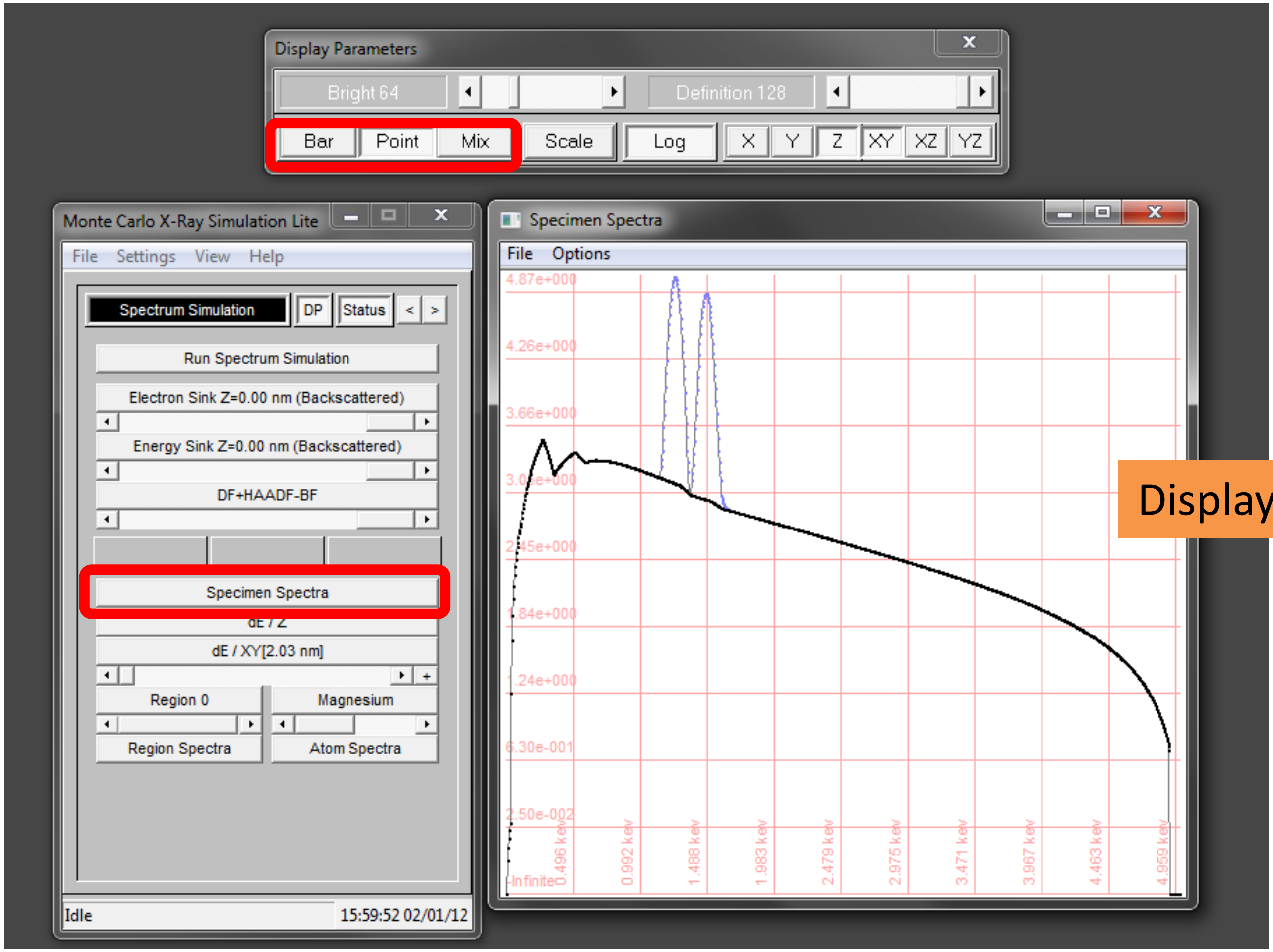
Energy Loss Distribution 2D





Energy loss 2D distribution

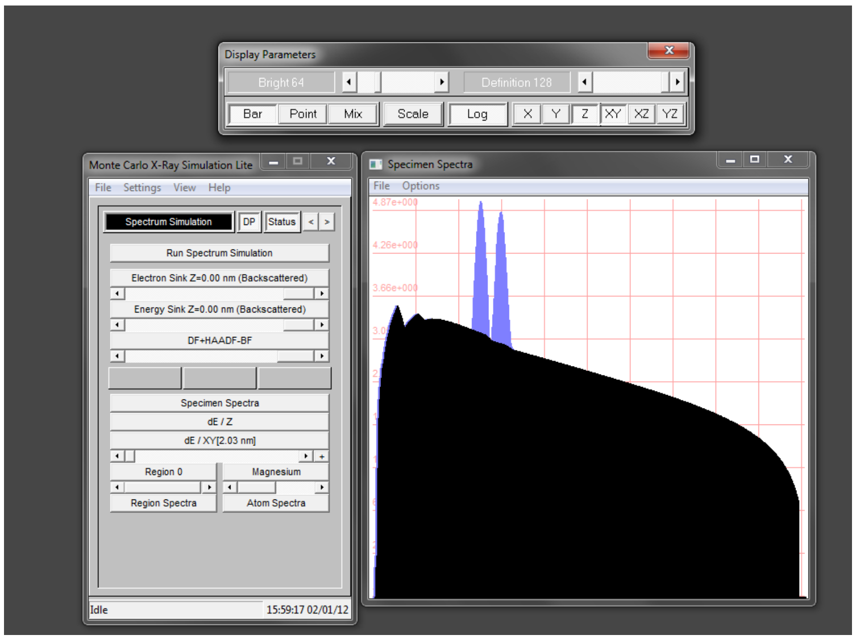
Specimen Spectrum



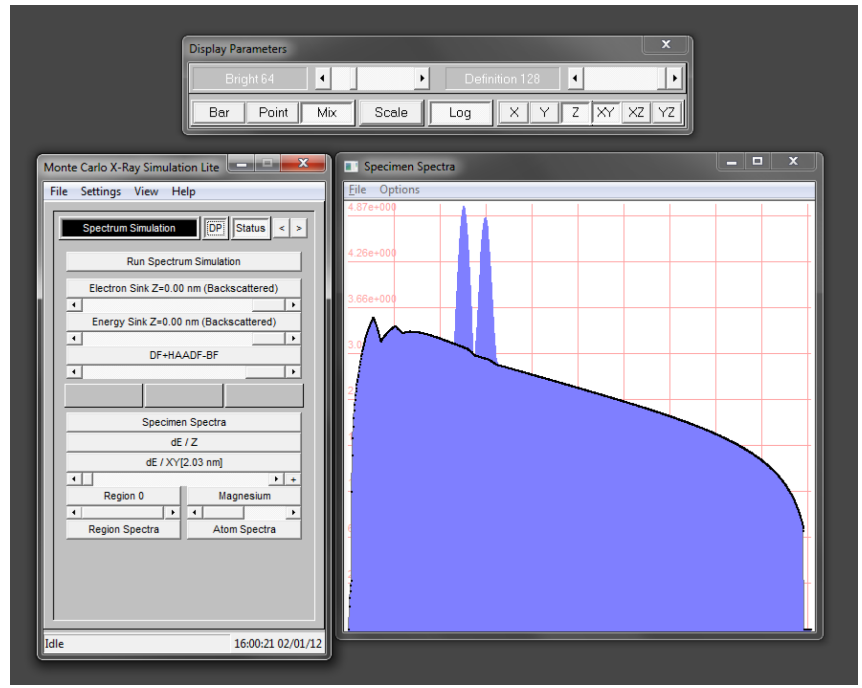
Displayed with points

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

Specimen Spectrum

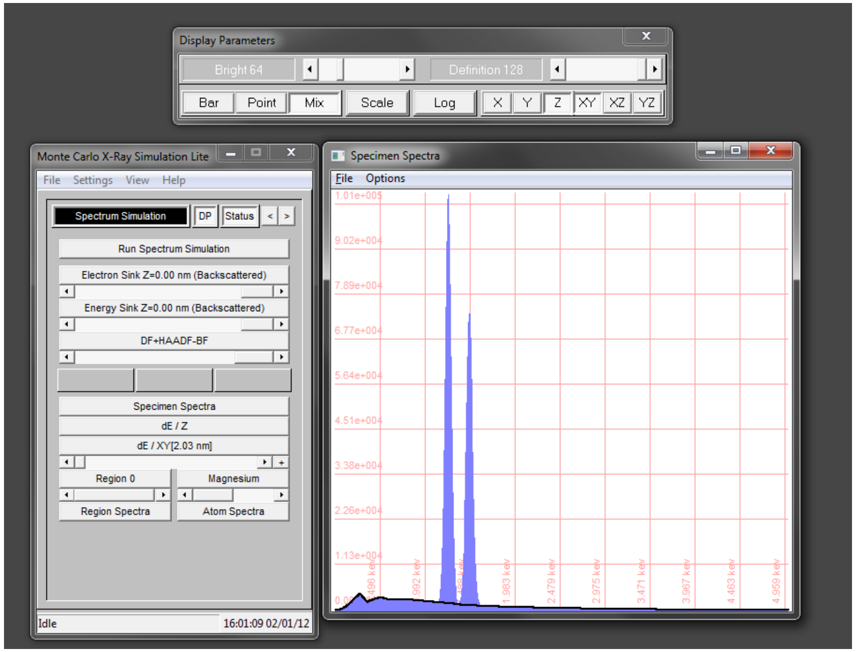


Displayed with bars

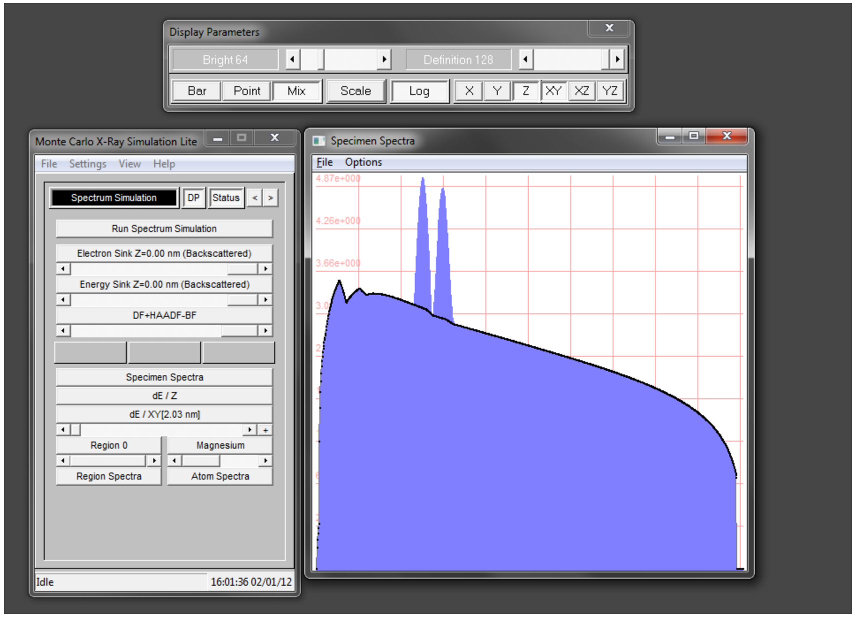


Displayed with points and bars

Specimen Spectrum

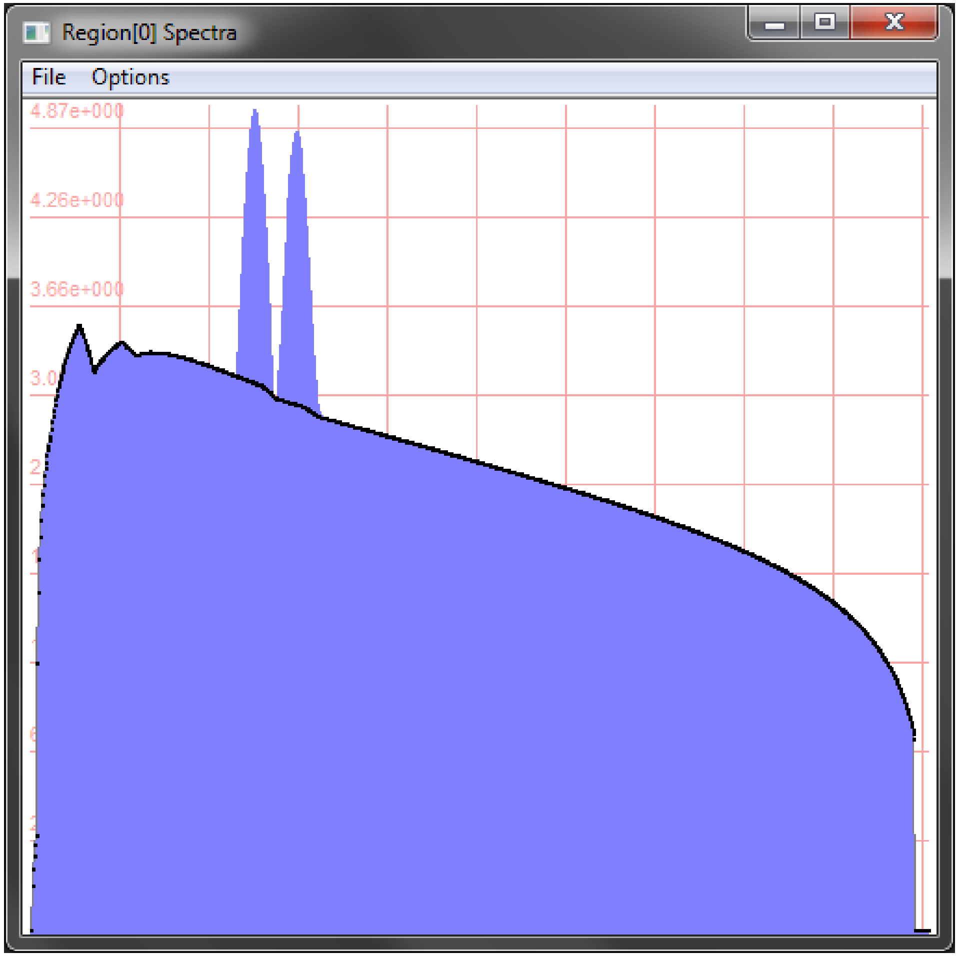


Linear scale



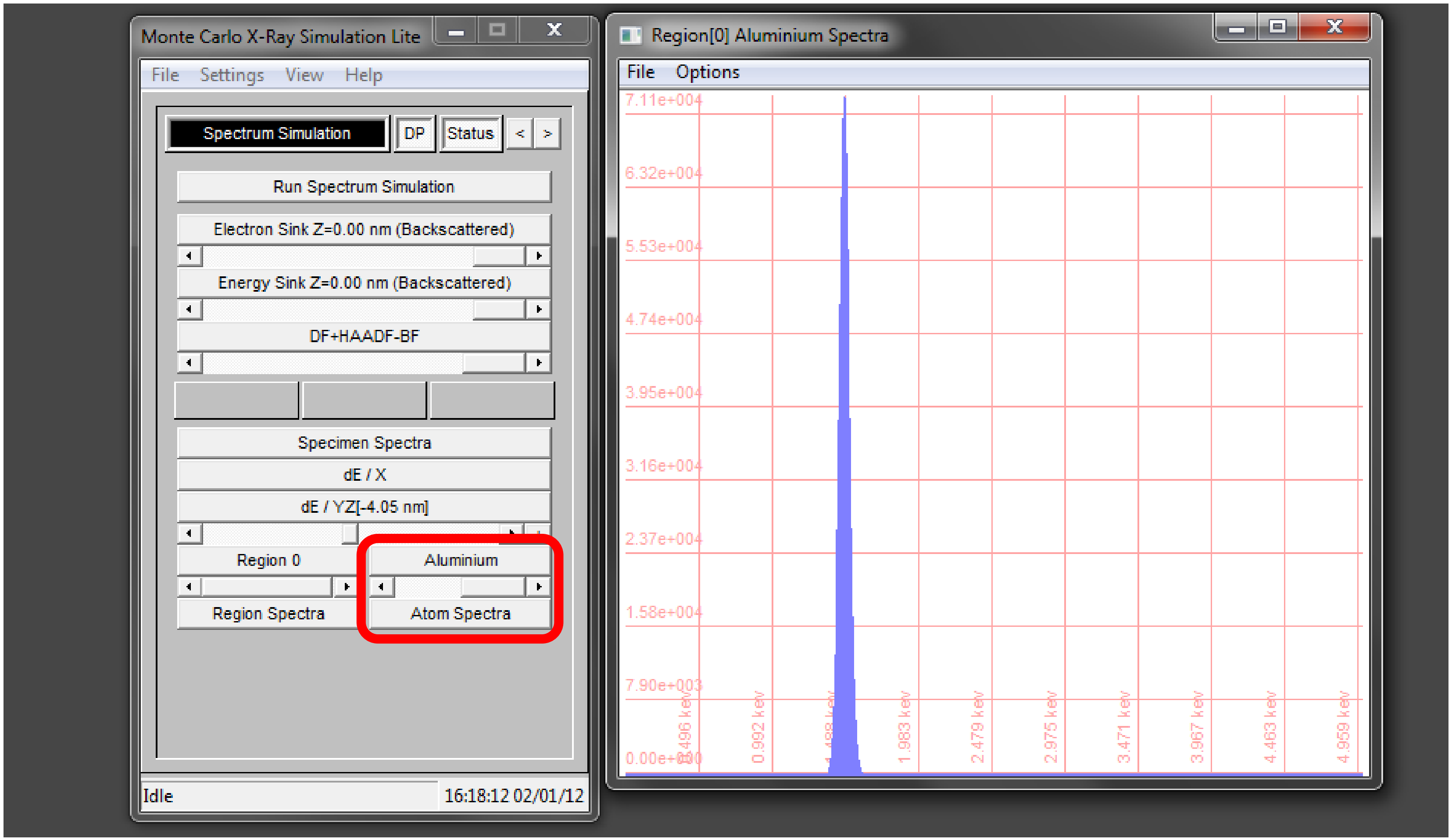
Logarithmic scale

Region Spectrum



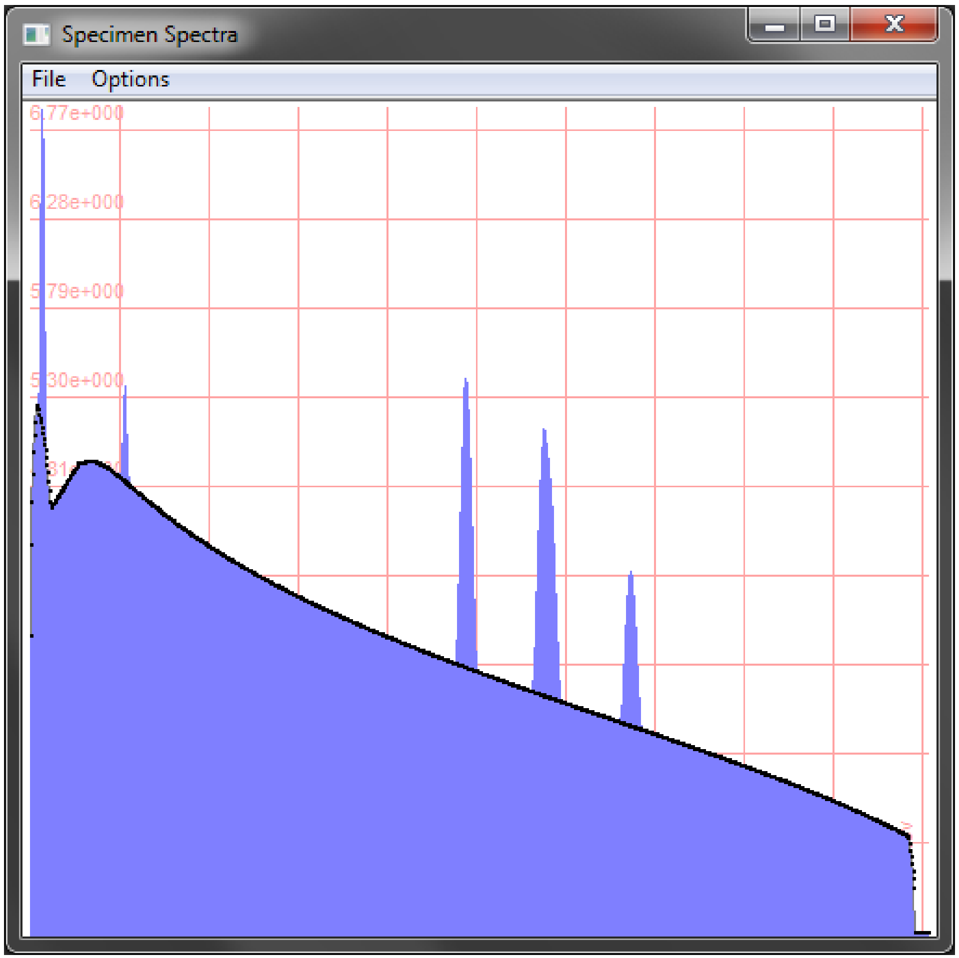
Display spectrum for each region

Atom Spectrum

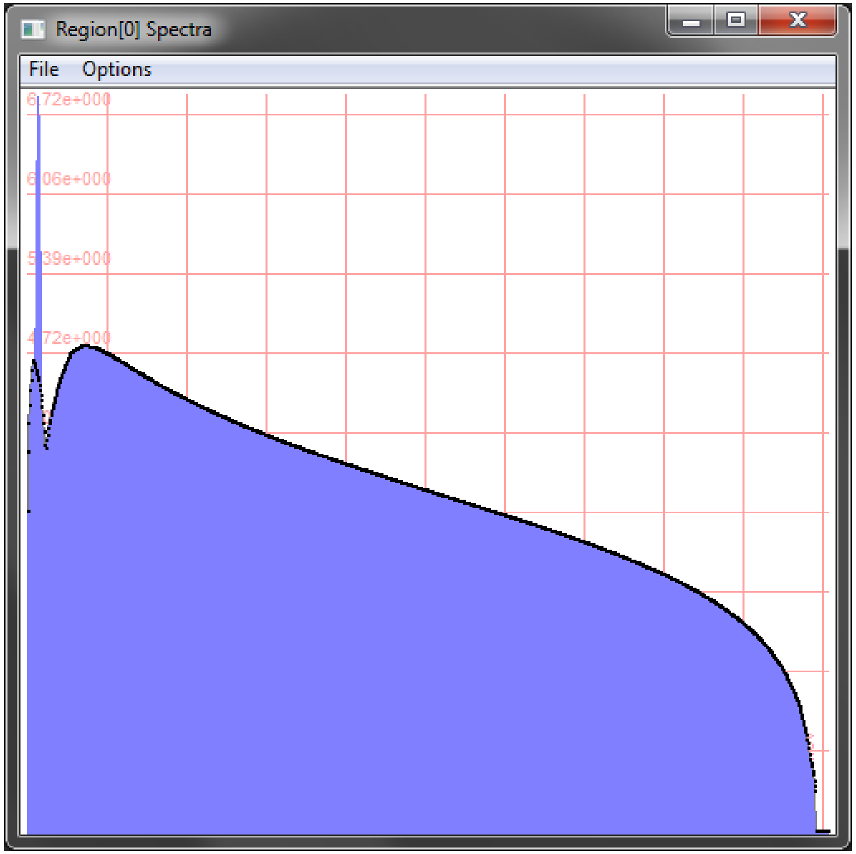


Display spectrum for each atom in a region

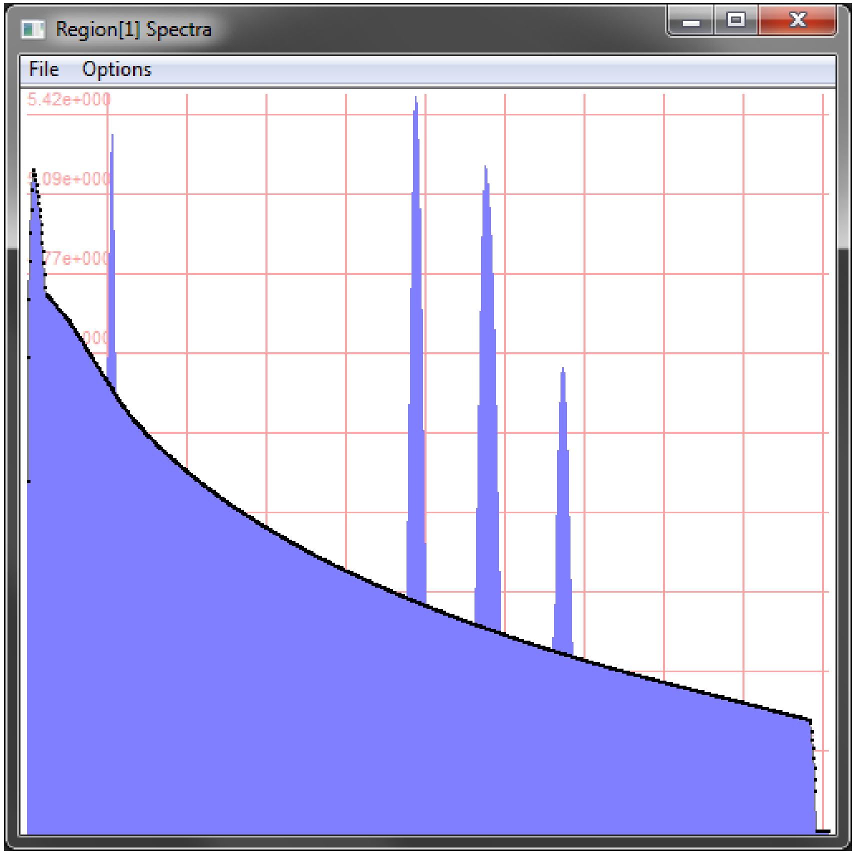
Au NP in C Specimen Spectrum



Au NP in C Region Spectrum

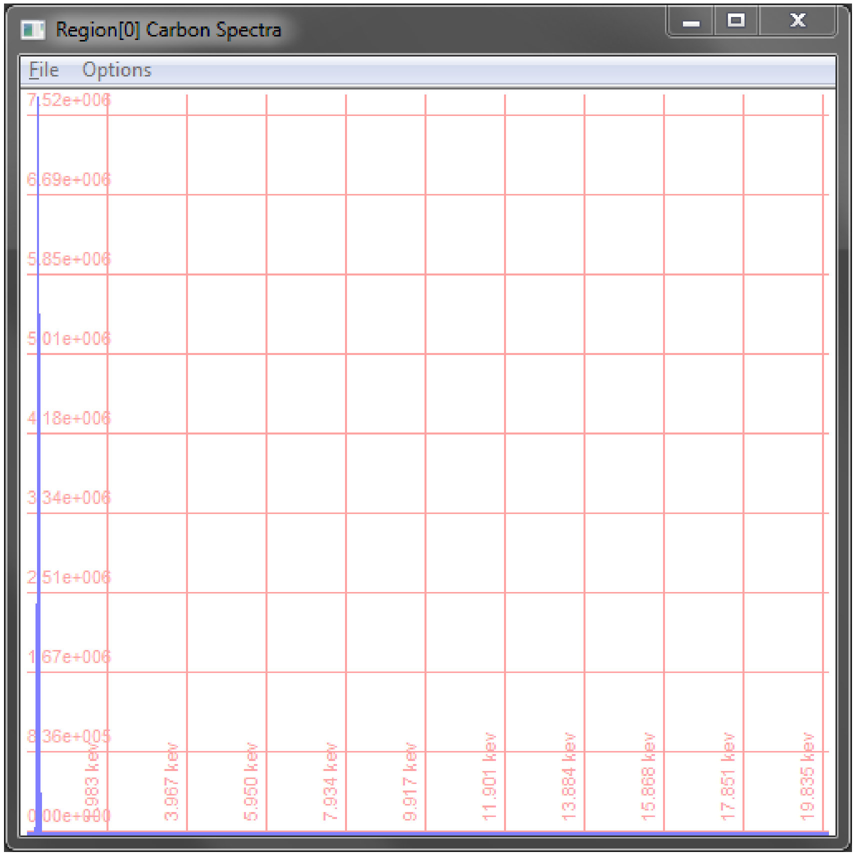


C Substrate

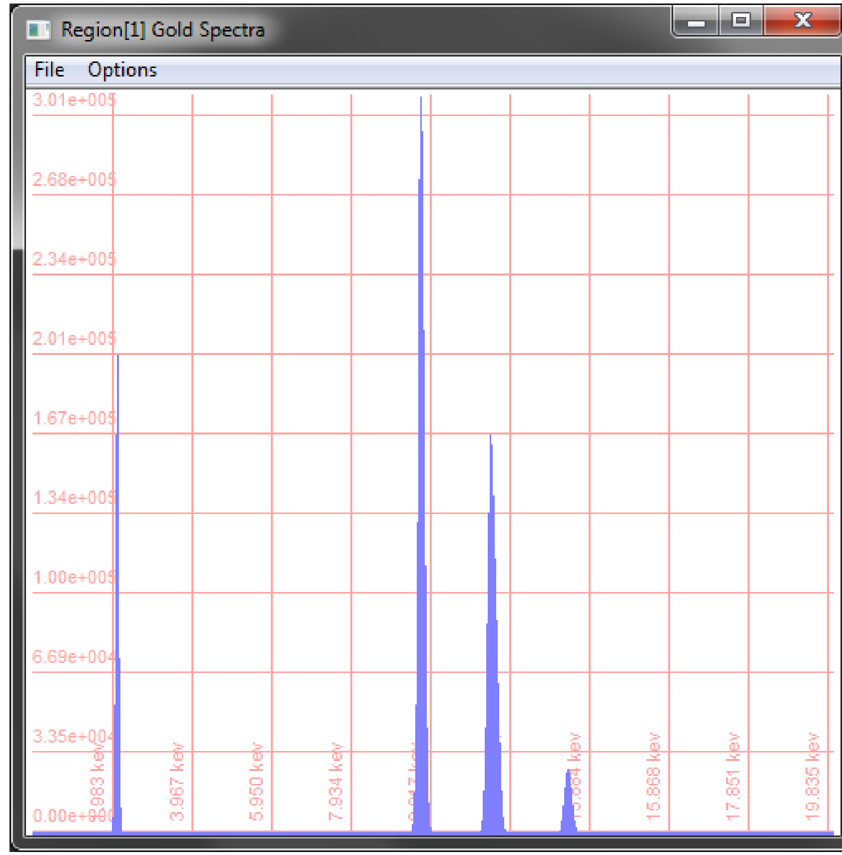


Au NP

Au NP in C Atom Spectrum



C Substrate

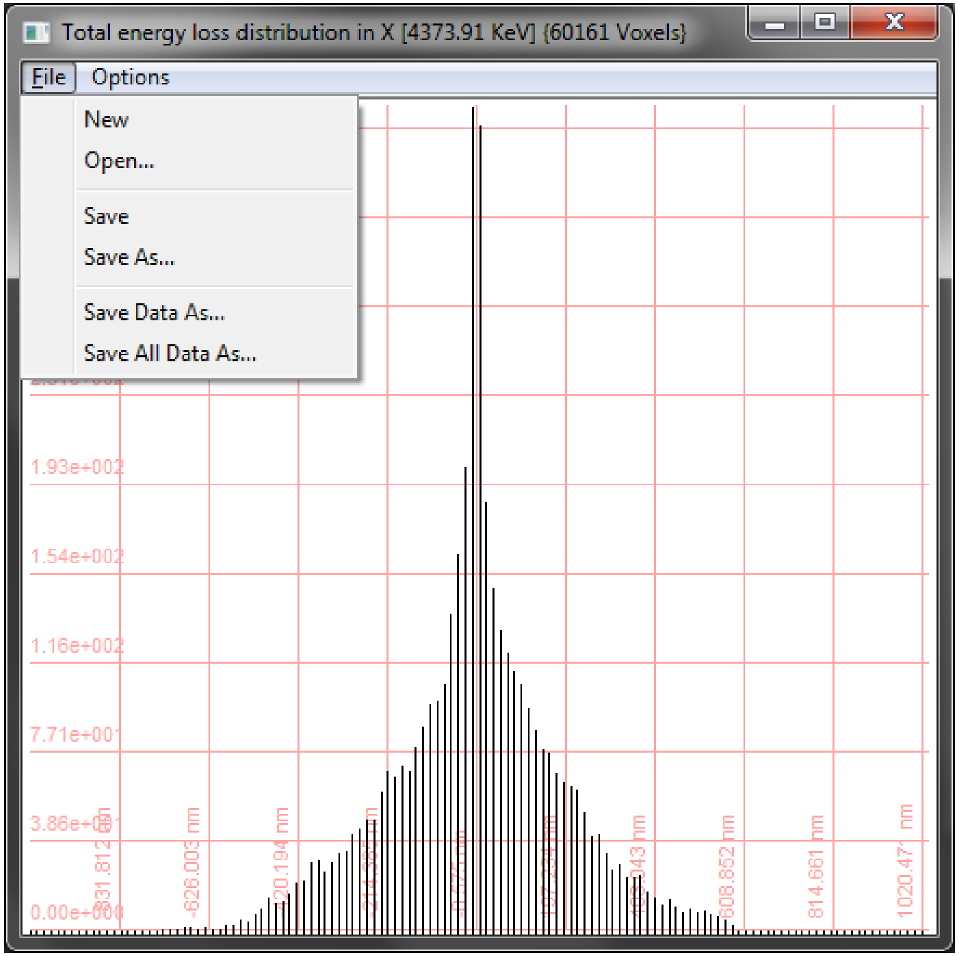


Au NP

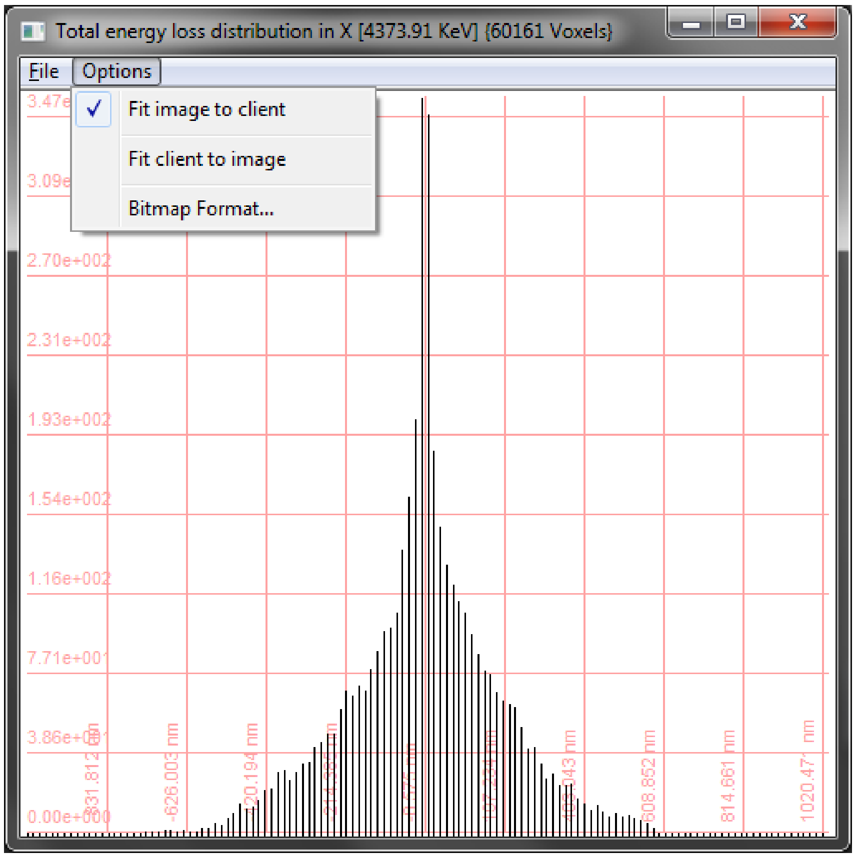
Display Results File Menu

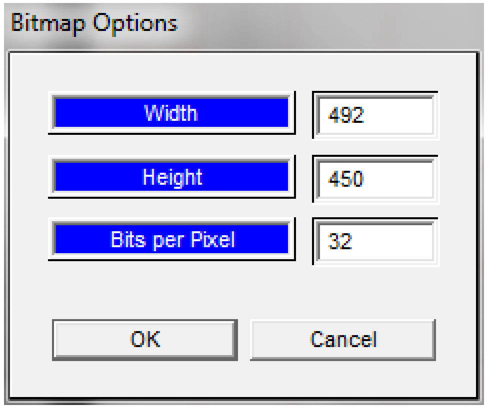
Save the graphic
In a bitmap file

Save the data
in a text file



Display Results Options Menu





Examples

- AlMgBulk5keV.sim
- CuAlGrainBoundary20kV.sim
- CrSiMultilayer10kV.sim
- AuParticleInC20keV.sim
- AuParticleOnC20keV.sim
- AuParticleInCFilm10keV.sim
- AuParticleOnCFilm10keV.sim
- AuParticleBelowCFilm10keV.sim
- CarbonNanotube_10nm_5keV.sim

Example: AlMgBulk5keV.sim

- AlMg Alloy (bulk) at 5keV.
- Al 50% weight fraction, Mg 50%.

Example: CuAlGrainBoundary20kV.sim

- Two regions having a vertical interface
  - Cu region 1: X position maximum = 1000000000 (default value)
  - Al region 2: Y position minimum = 0

Example: CrSiMultilayer10kV.sim

- Two regions having a horizontal interface
  - Cr region 1: Z position maximum = 2000000000 (default value)
  - Si region 2: Z position minimum = 50

Example: AuParticleInC20keV.sim

- Au nanoparticle (NP) in C substrate at 20 keV.
- NP diameter 20 nm just below the surface (position Z = 10.1 nm).
- Line scan
  - X: -50 to 50 nm with 15 step
  - Y = 0 to 0 with 1 step

Example: AuParticleOnC20keV.sim

- Au nanoparticle (NP) on C substrate at 20 keV.
- Region 1 is vacuum.
- NP diameter 20 nm just above the surface (position z = 10.1 nm, region 2).
- C bulk surface start at z = 20.2 nm (region 3).
- Line scan
  - X: -50 to 50 nm with 15 step
  - Y = 0 to 0 with 1 step

Example: AuParticleInCFilm10keV.sim

- Au nanoparticle (NP) in C film at 10 keV.
- C film 100 nm thick (region 1)
- NP diameter 20 nm just below the surface (position Z = 10.1 nm, region 2)
- Line scan
  - X: -50 to 50 nm with 15 step
  - Y = 0 to 0 with 1 step

Example: AuParticleOnCFilm10keV.sim

- Au nanoparticle (NP) on C film at 10 keV.
- Region 1 is vacuum.
- NP diameter 20 nm just above the surface (position z = 10.1 nm, region 2).
- C film surface start at z = 20.2 nm and end at z = 120.2 nm (region 3).
- Line scan
  - X: -50 to 50 nm with 15 step
  - Y = 0 to 0 with 1 step

Example: AuParticleBelowCFilm10keV.sim

- Au nanoparticle (NP) on C film at 10 keV.
- Region 1 is vacuum.
- C film surface start at z = 0 nm and end at z = 100 nm (region 2).
- NP diameter 20 nm just below the bottom surface (position z = 110.1 nm, region 3).
- Line scan
  - X: -50 to 50 nm with 15 step
  - Y = 0 to 0 with 1 step

Example: CarbonNanotube_10nm_5keV.sim

- Carbon nanotube at 5 keV.
- Region 1 is vacuum.
- Outer radius 100 nm carbon region 2
  - Z = 100.1 nm
  - Direction Y = 1
  - Length 1000 nm
  - Radius of 100 nm
- inner radius 50 nm, center vacuum region 3.
  - Z = 100.1 nm
  - Direction Y = 1
  - Length 1000 nm
  - Radius of 50 nm
- Pt NP 10 nm on the right side of the CNT region 4.
  - X 100.1 nm
  - Z 100.1 nm
  - Radius of 10 nm
- Line scan
  - X: -200 to 200 nm with 15 step
  - Y = 0 to 0 with 1 step