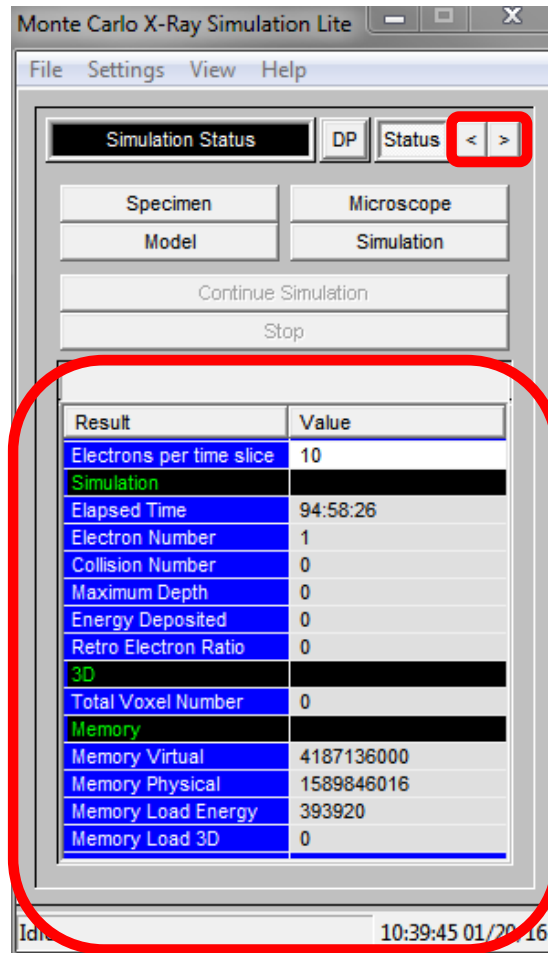


MC X-Ray Lite User Manual

Version 1.6

January 2016

MC X-Ray Lite



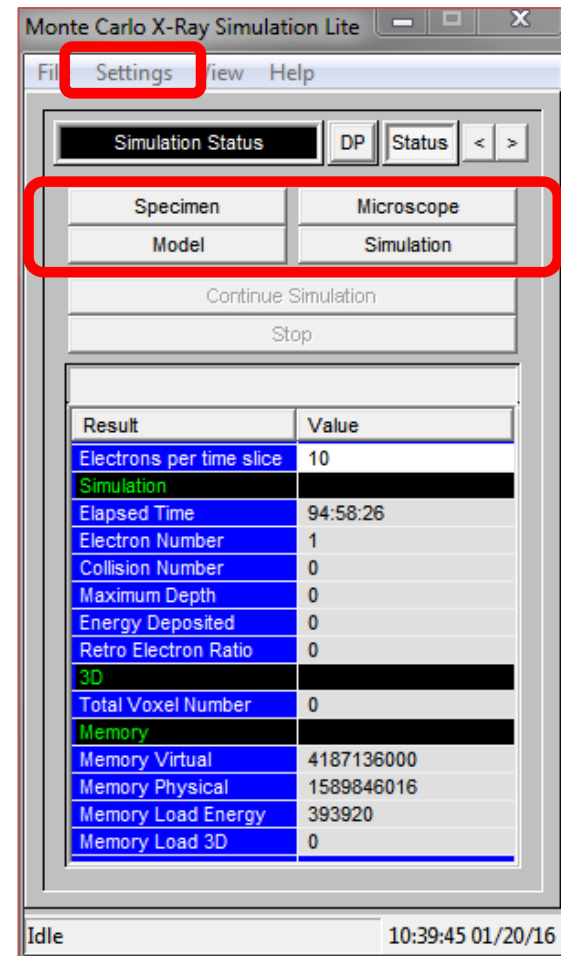
Navigate between main and spectrum simulation dialogs

Information about the simulation progress

Settings

- Specimen
- Microscope
- Models
- Simulation Parameters

Can be access either by the buttons or the menu



Specimen Settings

Specimen Settings

Select region

| Parameter | Value |
|-------------------|------------------------|
| Number of Regions | 1 |
| Regions Topology | No Predefined Topology |
| X extent min (nm) | -1000000000 |
| X extent max (nm) | 1000000000 |
| Y extent min (nm) | -1000000000 |
| Y extent max (nm) | 1000000000 |
| Z extent min (nm) | 0 |
| Z extent max (nm) | 2000000000 |

Add Region

| Parameter | Value |
|----------------------------|-------------|
| Number of Elements | 1 |
| Mean Atomic Number | 6 |
| Mean Atomic Weight (g/mol) | 12.01 |
| Mass Density (g/cm3) | 2.26 |
| Atomic Density (1/A3) | 0.11333871 |
| Geometry | Box |
| X position min (nm) | -1000000000 |
| X position max (nm) | 1000000000 |

Remove Region User Density

Select region shape
Set dimensions

| Z | Element | S | Weight (g/... | Density (g/... |
|----|-----------|------|---------------|----------------|
| 1 | Hydrogen | H | 1.008 | 7.1e-002 |
| 2 | Helium | H... | 4.003 | 0.126 |
| 3 | Lithium | Li | 6.94 | 0.53 |
| 4 | Beryllium | Be | 9.01 | 1.85 |
| 5 | Boron | B | 10.81 | 2.35 |
| 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 | N... | 20.18 | 1.2 |
| 11 | Sodium | N... | 22.99 | 0.97 |
| 12 | Magnesium | M... | 24.31 | 1.74 |

Add element

| Element | Mass Fraction |
|---------|---------------|
| Carbon | 1. |

Set composition

Clear Compute Selection
Clear Selected Fractions Invert Selection

OK Cancel

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

Region Box

Specimen Settings

| Specimen | | Region 1 | |
|-------------------|------------------------|-----------------------|-------------------|
| Parameter | Value | Parameter | Value |
| Number of Regions | 1 | Atomic Density (1/A3) | 0.113338717735221 |
| Regions Topology | No Predefined Topology | Geometry | Box |
| X extent min (nm) | -1000000000 | X position min (nm) | -1000000000 |
| X extent max (nm) | 1000000000 | X position max (nm) | 1000000000 |
| Y extent min (nm) | -1000000000 | Y position min (nm) | -1000000000 |
| Y extent max (nm) | 1000000000 | Y position max (nm) | 1000000000 |
| Z extent min (nm) | 0 | Z position min (nm) | 0 |
| Z extent max (nm) | 2000000000 | Z position max (nm) | 2000000000 |

Add Region Remove Region U

| Available Elements | | | | | Region Element | |
|--------------------|-----------|------|---------------|----------------|----------------|---------------|
| Z | Element | S | Weight (g/... | Density (g/... | Element | Mass Fraction |
| 1 | Hydrogen | H | 1.008 | 7.1e-002 | Carbon | 1. |
| 2 | Helium | H... | 4.003 | 0.126 | | |
| 3 | Lithium | Li | 6.94 | 0.53 | | |
| 4 | Beryllium | B... | 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 | N... | 20.18 | 1.2 | | |
| 11 | Sodium | N... | 22.99 | 0.97 | | |
| 12 | Magnesium | M... | 24.31 | 1.74 | | |

OK Cancel

Clear Compute Selection
Clear Selected Fractions Invert Selection

Box X, Y, Z dimensions
in nm

Electron travel
toward Z positive

- specimen surface at 0
- bottom at 2 m (2×10^9 nm)

Region Sphere

Specimen Settings

| Specimen | | Region 2 | |
|-------------------|------------------------|----------------------------|--------------------|
| Parameter | Value | Parameter | Value |
| Number of Regions | 2 | Mean Atomic Weight (g/mol) | 196.97 |
| Regions Topology | No Predefined Topology | Mass Density (g/cm3) | 19.3 |
| X extent min (nm) | -100 | Atomic Density (1/A3) | 0.0590160430522415 |
| X extent max (nm) | 100 | Geometry | Sphere |
| Y extent min (nm) | -100 | X position (nm) | 0 |
| Y extent max (nm) | 100 | Y position (nm) | 0 |
| Z extent min (nm) | 1 | Z position (nm) | 101 |
| Z extent max (nm) | 201 | Radius (nm) | 100 |

Add Region Remove Region

| Available Elements | | | | | Region Element | |
|--------------------|-----------|------|---------------|----------------|----------------|---------------|
| Z | Element | S | Weight (g/... | Density (g/... | Element | Mass Fraction |
| 1 | Hydrogen | H | 1.008 | 7.1e-002 | Gold | 1. |
| 2 | Helium | H... | 4.003 | 0.126 | | |
| 3 | Lithium | Li | 6.94 | 0.53 | | |
| 4 | Beryllium | B... | 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 | N... | 20.18 | 1.2 | | |
| 11 | Sodium | N... | 22.99 | 0.97 | | |
| 12 | Magnesium | M... | 24.31 | 1.74 | | |

OK Cancel

Clear Compute Selection
Clear Selected Fractions Invert Selection

Sphere:

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

All in nm

Region Cylinder

Specimen Settings

| Specimen | |
|-------------------|------------------------|
| Parameter | Value |
| Number of Regions | 2 |
| Regions Topology | No Predefined Topology |
| X extent min (nm) | -100 |
| X extent max (nm) | 100 |
| Y extent min (nm) | -100 |
| Y extent max (nm) | 100 |
| Z extent min (nm) | 1 |
| Z extent max (nm) | 201 |

Add Region

| Available Elements | | | | |
|--------------------|-----------|------|---------------|----------------|
| Z | Element | S | Weight (g/... | Density (g/... |
| 1 | Hydrogen | H | 1.008 | 7.1e-002 |
| 2 | Helium | H... | 4.003 | 0.126 |
| 3 | Lithium | Li | 6.94 | 0.53 |
| 4 | Beryllium | B... | 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 | N... | 20.18 | 1.2 |
| 11 | Sodium | N... | 22.99 | 0.97 |
| 12 | Magnesium | M... | 24.31 | 1.74 |

OK

| Region 2 | |
|-----------------|-------|
| Parameter | Value |
| X position (nm) | 0 |
| Y position (nm) | 0 |
| Z position (nm) | 0 |
| X direction | 1 |
| Y direction | 1 |
| Z direction | 1 |
| Length (nm) | 1000 |
| Radius (nm) | 100 |

Remove Region

| Region Elements | |
|-----------------|---------------|
| Element | Mass Fraction |
| Carbon | 1. |
| | |
| | |
| | |
| | |
| | |
| | |
| | |
| | |
| | |

Clear Compute Selection
Clear Selected Fractions Invert Selection

Cancel

Cylinder:

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

All in nm

Region User Density

Specimen Settings

| Specimen | |
|-------------------|------------------------|
| Parameter | Value |
| Number of Regions | 1 |
| Regions Topology | No Predefined Topology |
| X extent min (nm) | -1000000000 |
| X extent max (nm) | 1000000000 |
| Y extent min (nm) | -1000000000 |
| Y extent max (nm) | 1000000000 |
| Z extent min (nm) | 0 |
| Z extent max (nm) | 2000000000 |

Add Region

| Region 1 | |
|------------------------------------|--------------------|
| Parameter | Value |
| Number of Elements | 2 |
| Mean Atomic Number | 12.4739715344122 |
| Mean Atomic Weight (g/mol) | 25.5755039968805 |
| Mass Density (g/cm ³) | 1.23 |
| Atomic Density (1/A ³) | 0.0144831749960892 |
| Geometry | Box |
| X position min (nm) | -1000000000 |
| X position max (nm) | 1000000000 |

Remove Region User Density

| Available Elements | | | | |
|--------------------|-----------|------|----------------|-----------------|
| Z | Element | S | Weight (g/...) | Density (g/...) |
| 1 | Hydrogen | H | 1.008 | 7.1e-002 |
| 2 | Helium | H... | 4.003 | 0.126 |
| 3 | Lithium | Li | 6.94 | 0.53 |
| 4 | Beryllium | B... | 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 | N... | 20.18 | 1.2 |
| 11 | Sodium | N... | 22.99 | 0.97 |
| 12 | Magnesium | M... | 24.31 | 1.74 |

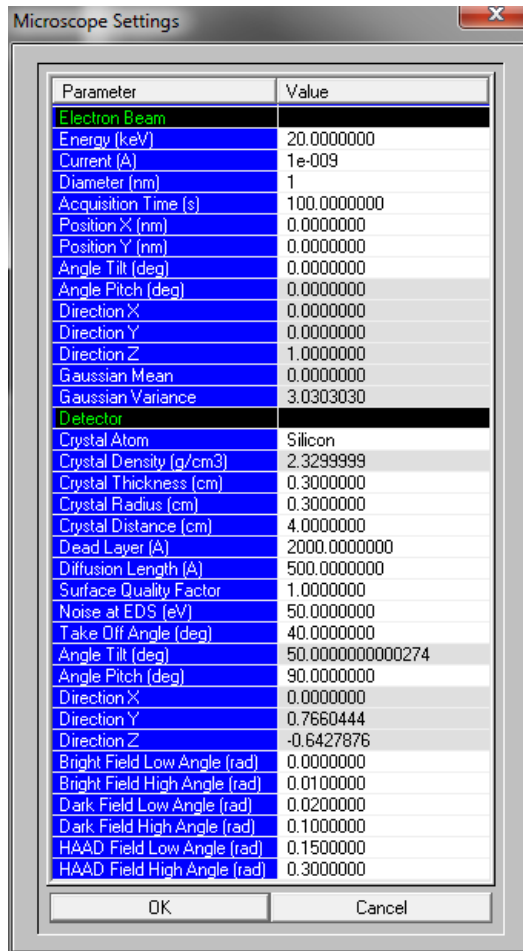
| Region Elements | |
|-----------------|---------------|
| Element | Mass Fraction |
| Magnesium | 0.5 |
| Aluminium | 0.5 |
| | |
| | |
| | |
| | |
| | |
| | |
| | |
| | |

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



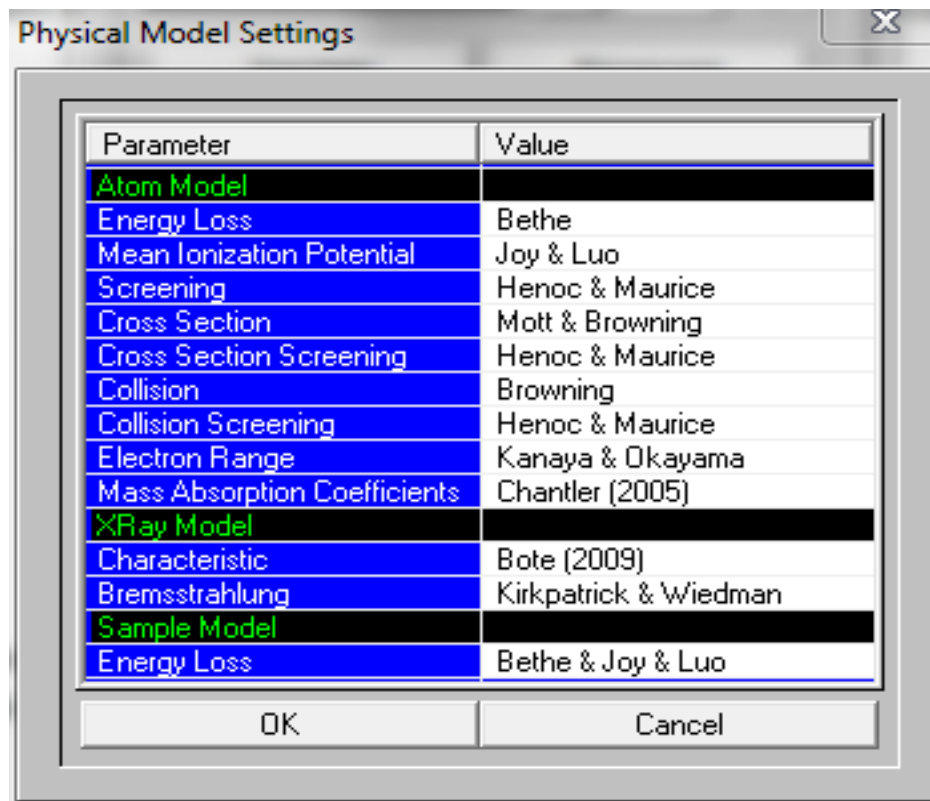
The image shows a 'Microscope Settings' dialog box with a table of parameters and their values. The parameters are grouped into 'Electron Beam' and 'Detector' sections. The 'Electron Beam' section includes parameters like Energy (keV), Current (A), Diameter (nm), Acquisition Time (s), Position X (nm), Position Y (nm), Angle Tilt (deg), Angle Pitch (deg), Direction X, Direction Y, Direction Z, Gaussian Mean, and Gaussian Variance. The 'Detector' section includes parameters like Crystal Atom, Crystal Density (g/cm3), Crystal Thickness (cm), Crystal Radius (cm), Crystal Distance (cm), Dead Layer (A), Diffusion Length (A), Surface Quality Factor, Noise at EDS (eV), Take Off Angle (deg), Angle Tilt (deg), Angle Pitch (deg), Direction X, Direction Y, Direction Z, Bright Field Low Angle (rad), Bright Field High Angle (rad), Dark Field Low Angle (rad), Dark Field High Angle (rad), HAAD Field Low Angle (rad), and HAAD Field High Angle (rad). The 'Take Off Angle (deg)' parameter is highlighted in the original image.

| 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) | 50.00000000000274 |
| 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

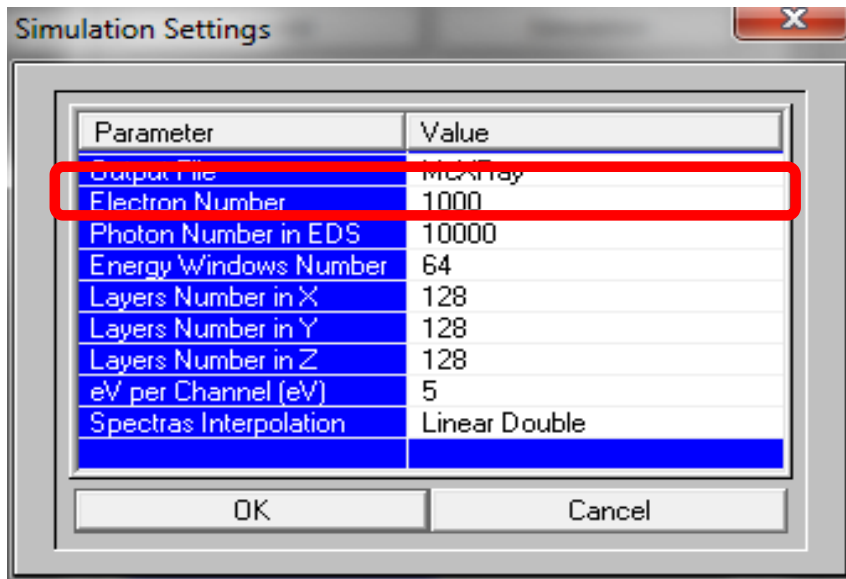
- Electron Beam
 - Incident energy in keV
 - Beam diameter in nm
 - Beam X, Y positions in nm
 - Beam tilt in degree
- X-ray Detector
 - Take off angle in degree
- Transmitted Electron Detectors
 - All angle in radian

Models Settings



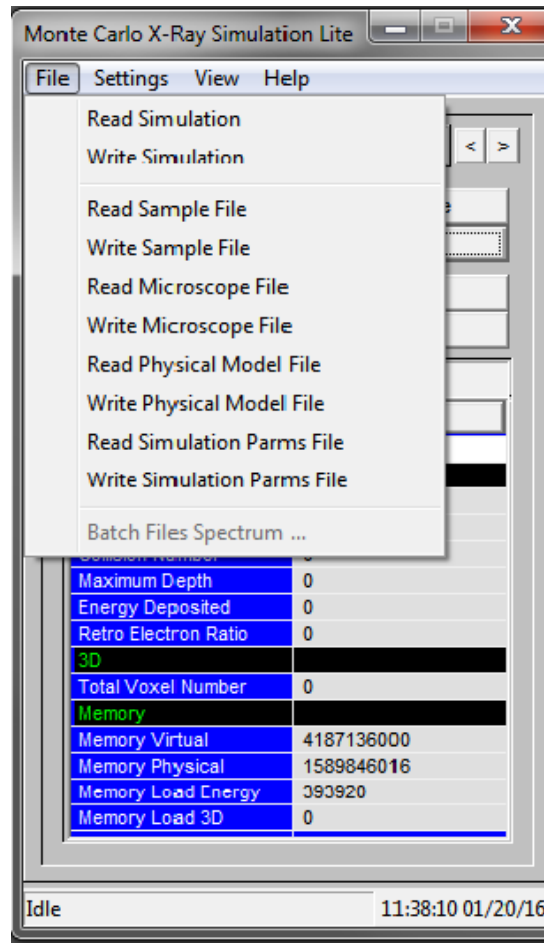
The default models are the best one to use in most simulation

Simulation Parameters



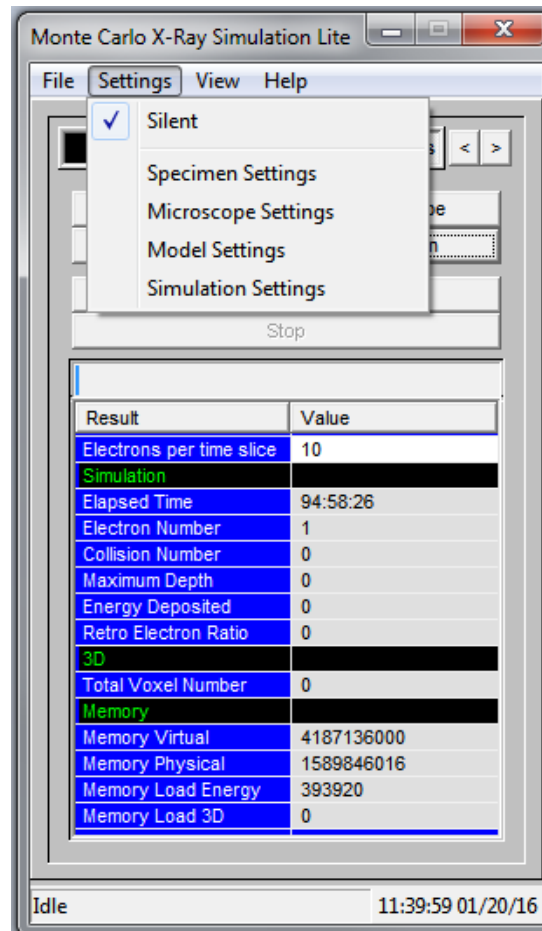
- Set the number of simulated electrons
- Other options are advanced feature, where the default values are good for most simulations

File Menu



Read and write all settings
in separate files

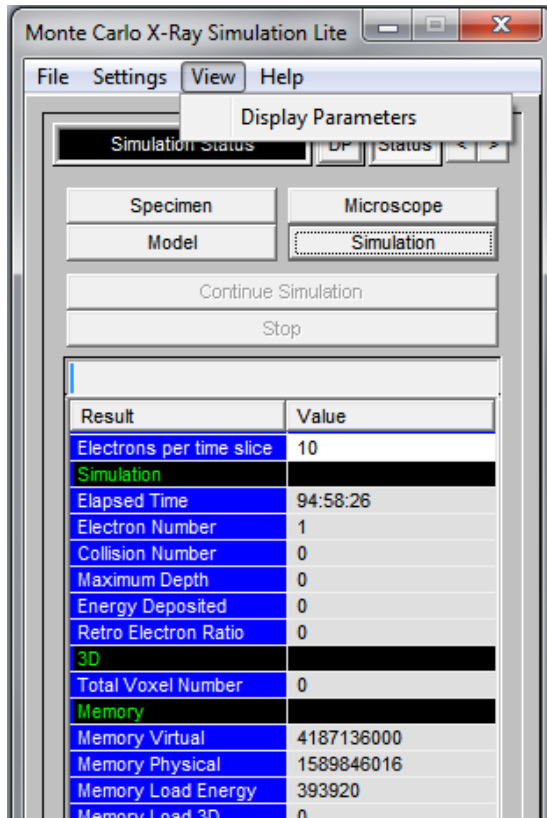
Settings Menu



Can access all settings from the menu

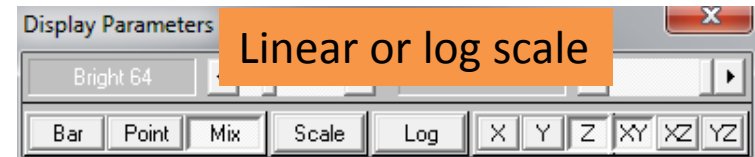
Uncheck Silent to hear a beep when the simulation is finished

View Menu



Open the Display Parameters dialog to adjust the displayed results

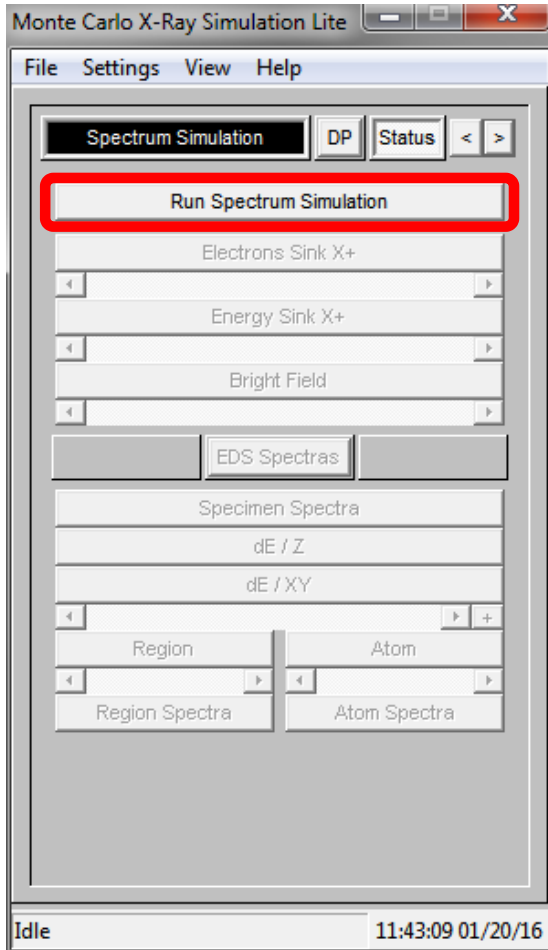
Display Parameters



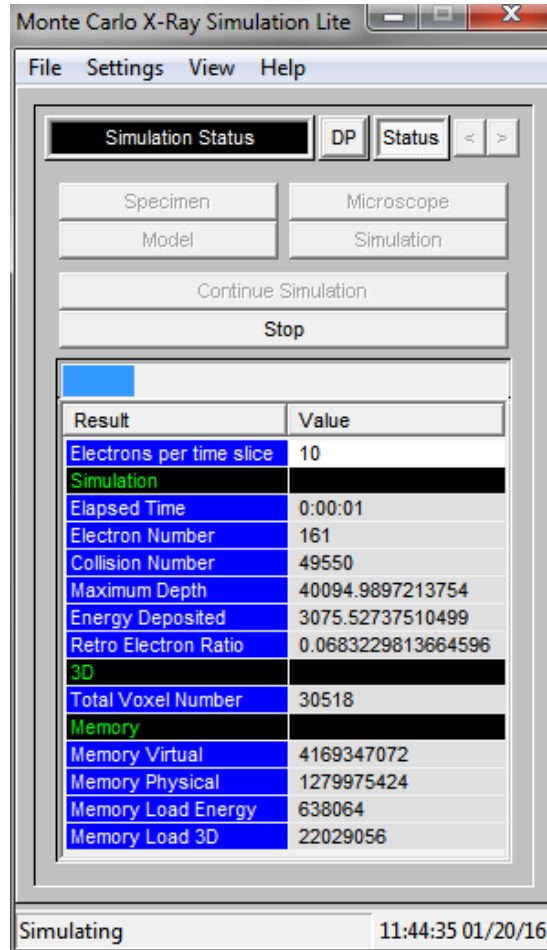
Line type in the graphic

Select the distribution dimension to display

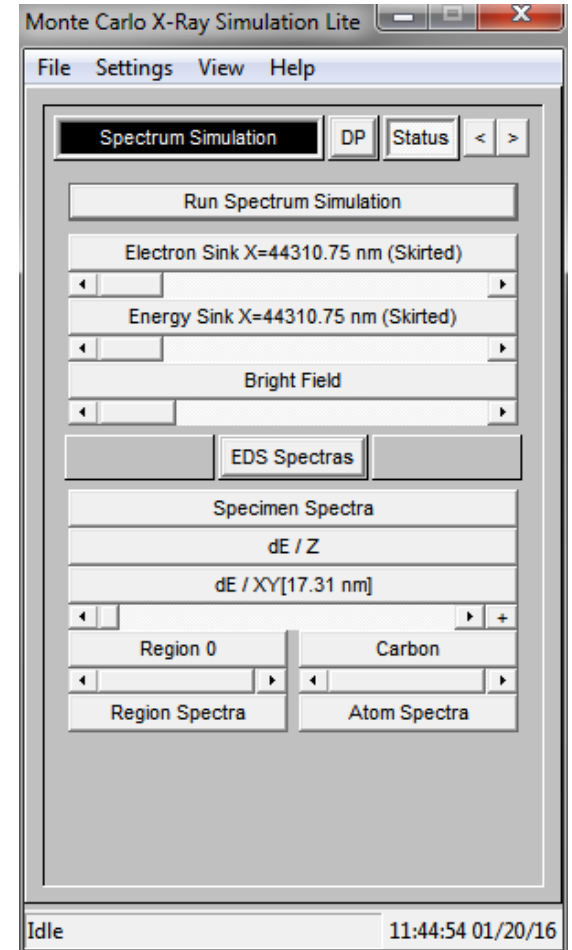
Spectrum Simulation



Start



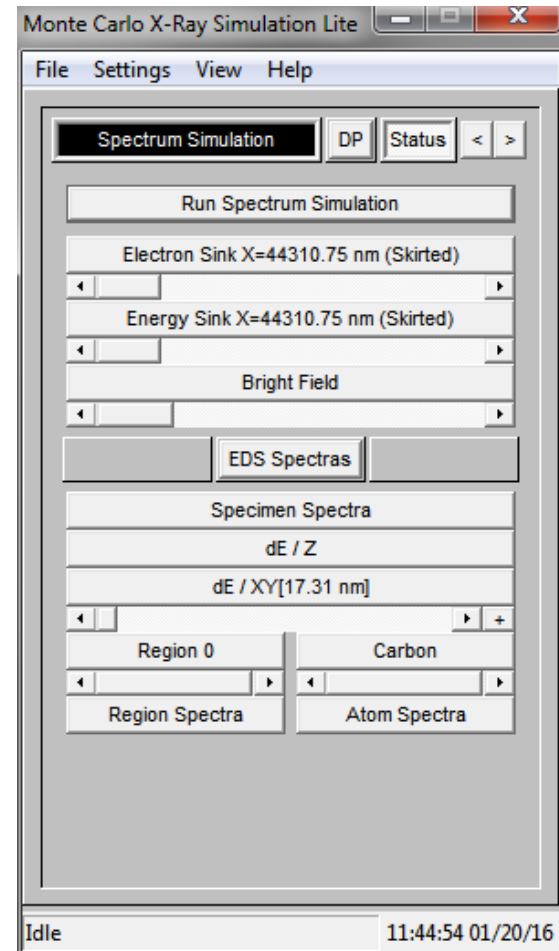
Simulating



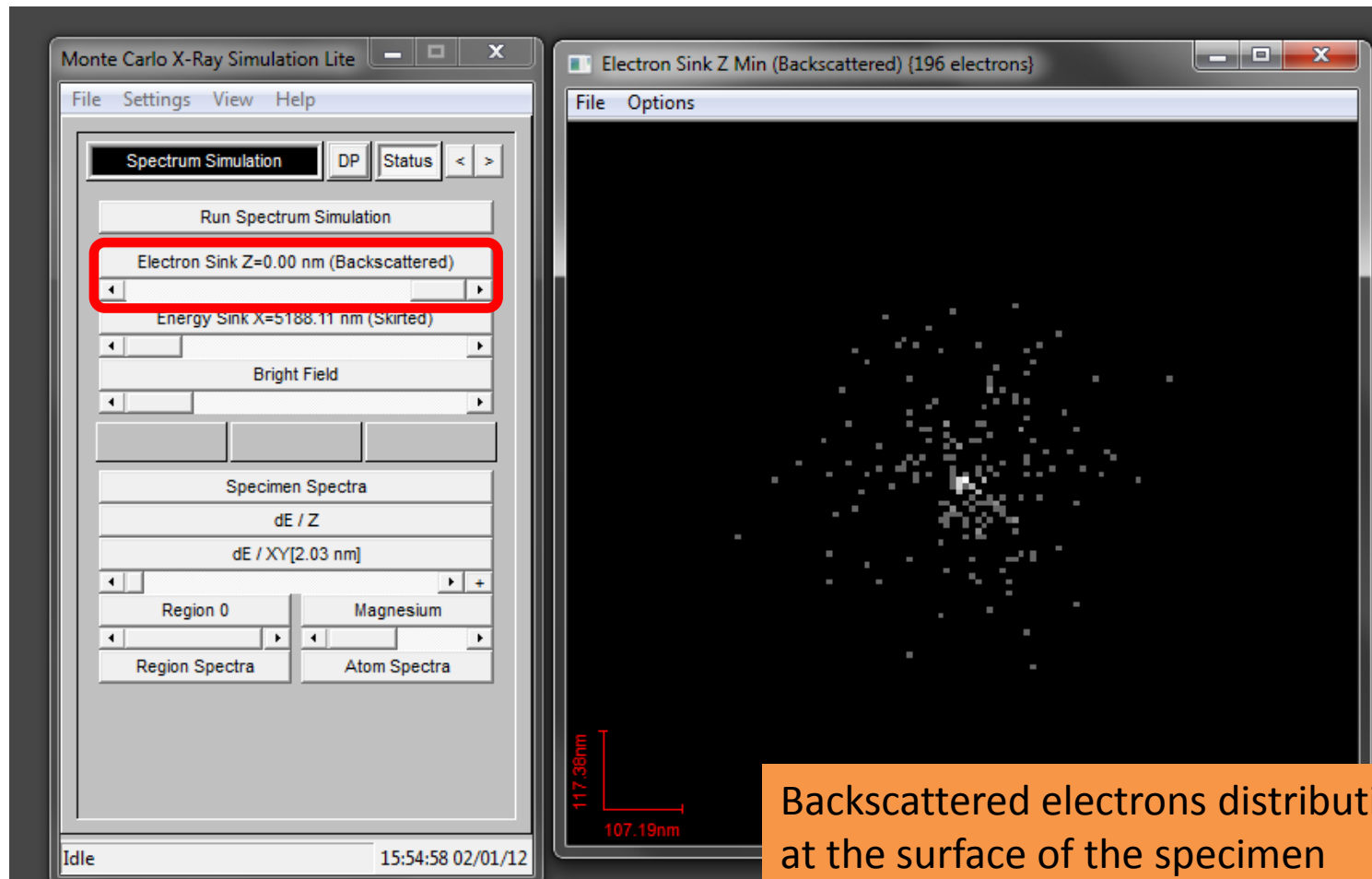
Done

Results

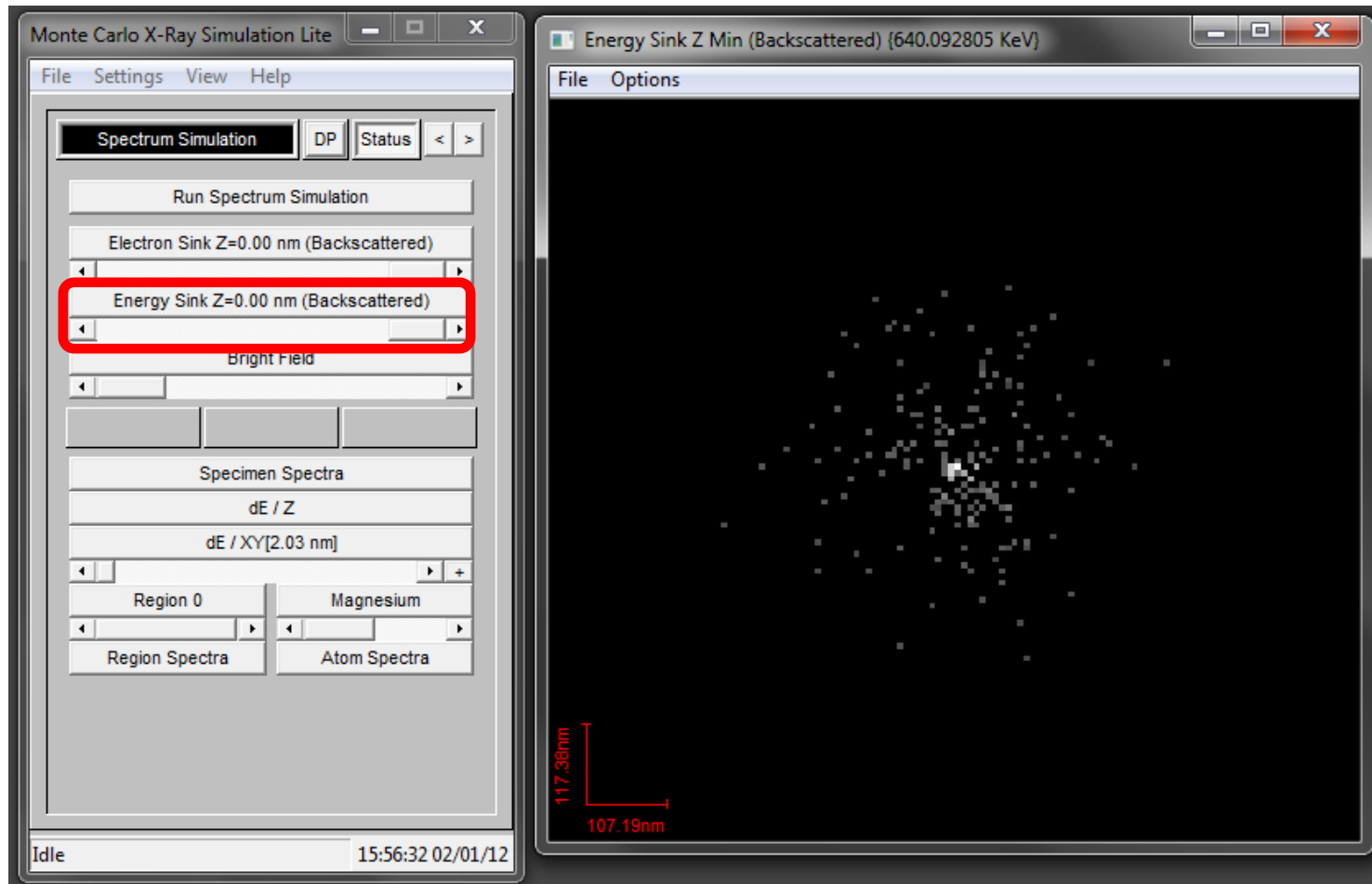
- Click on each label to display the results
- Electron and energy distribution at the specimen surfaces (6)
- Transmitted electrons distribution
- Energy loss distribution
- X-ray spectrum



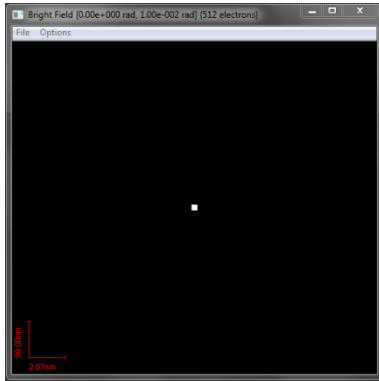
Electrons Sink



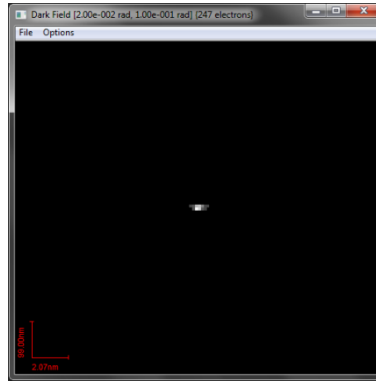
Energy Sink



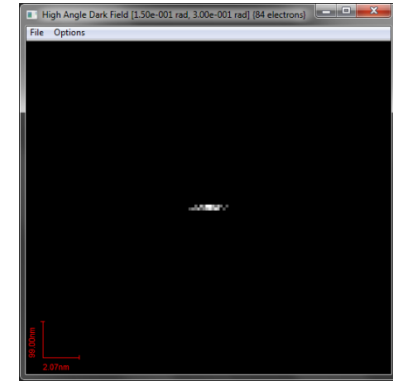
Transmitted Electrons



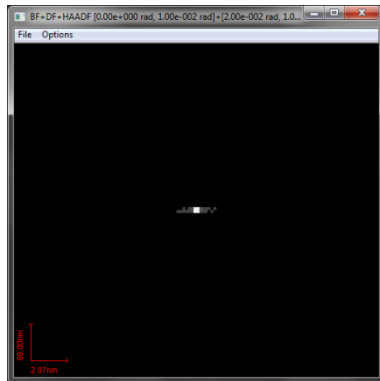
Bright Field



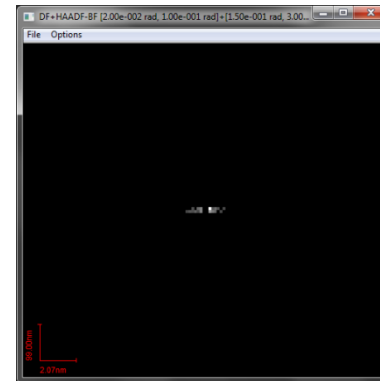
Dark Field



HAADF

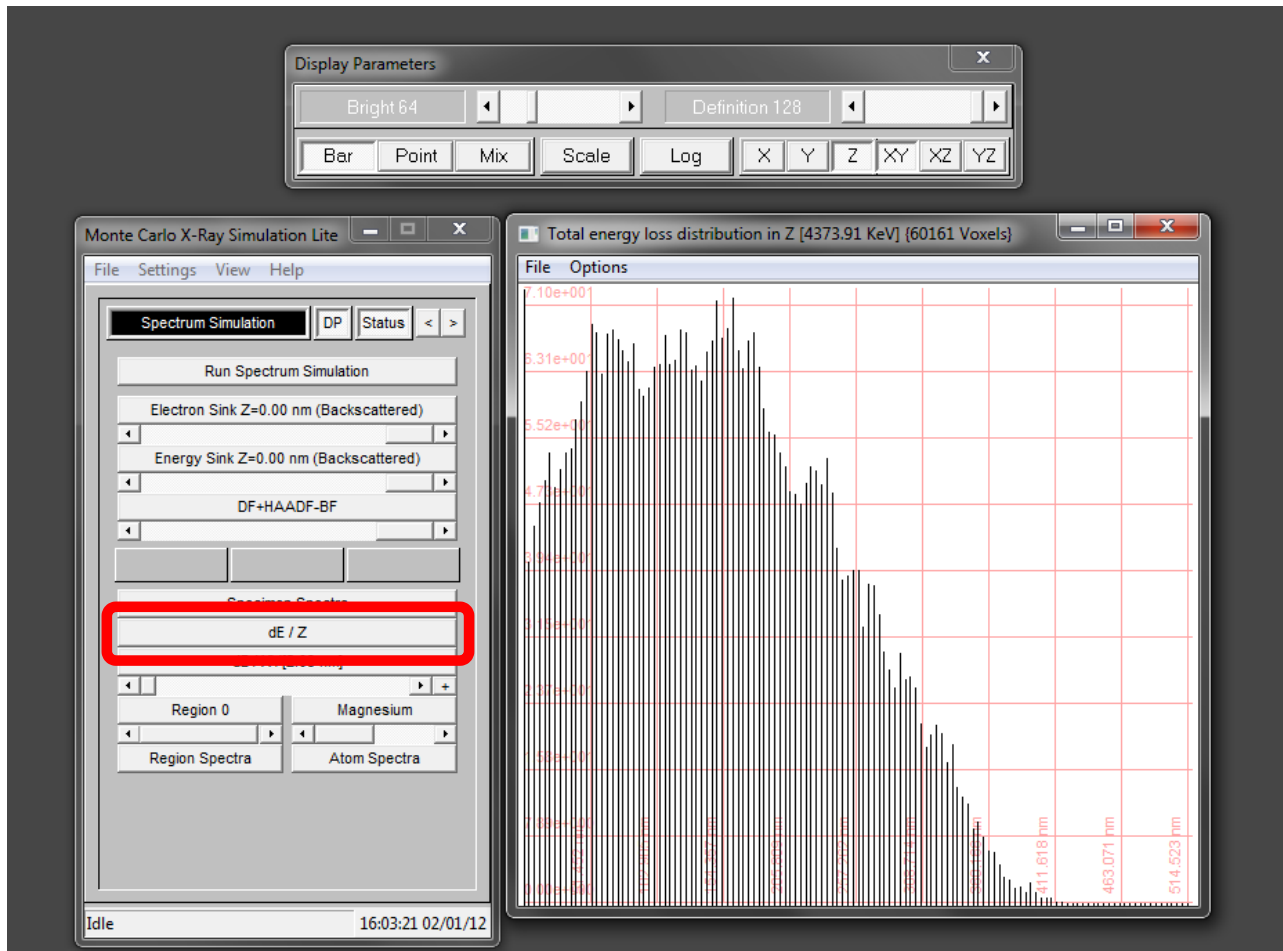


All detectors



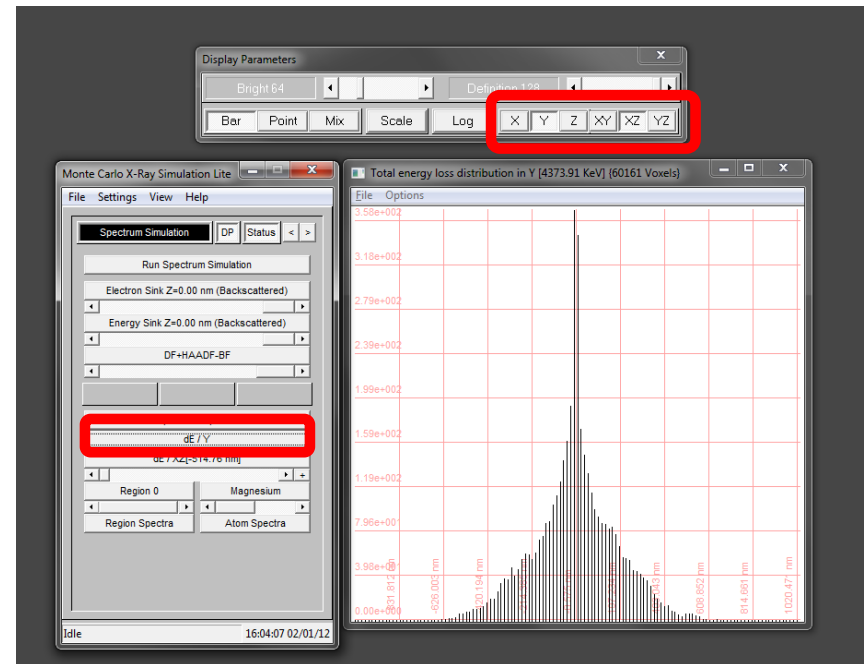
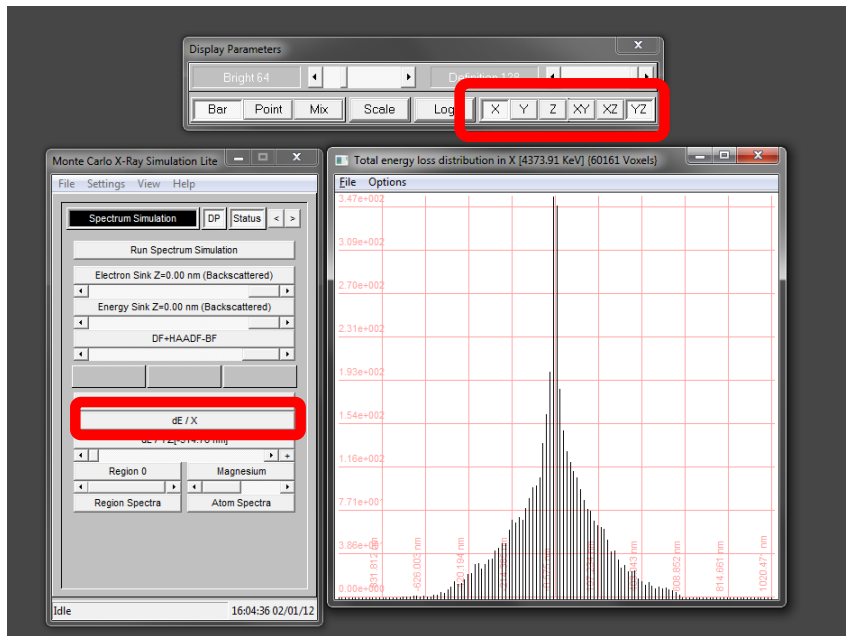
DF + HAADF - BF

Energy Loss Distribution 1D



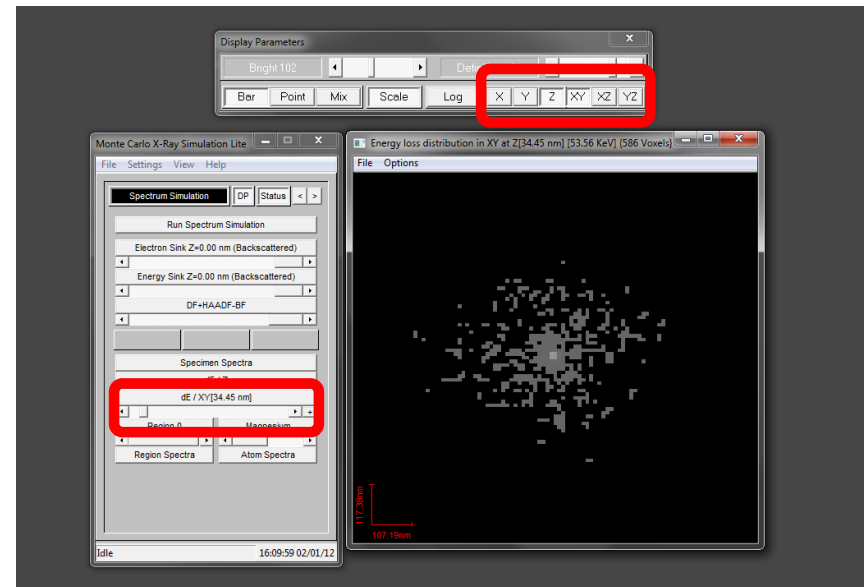
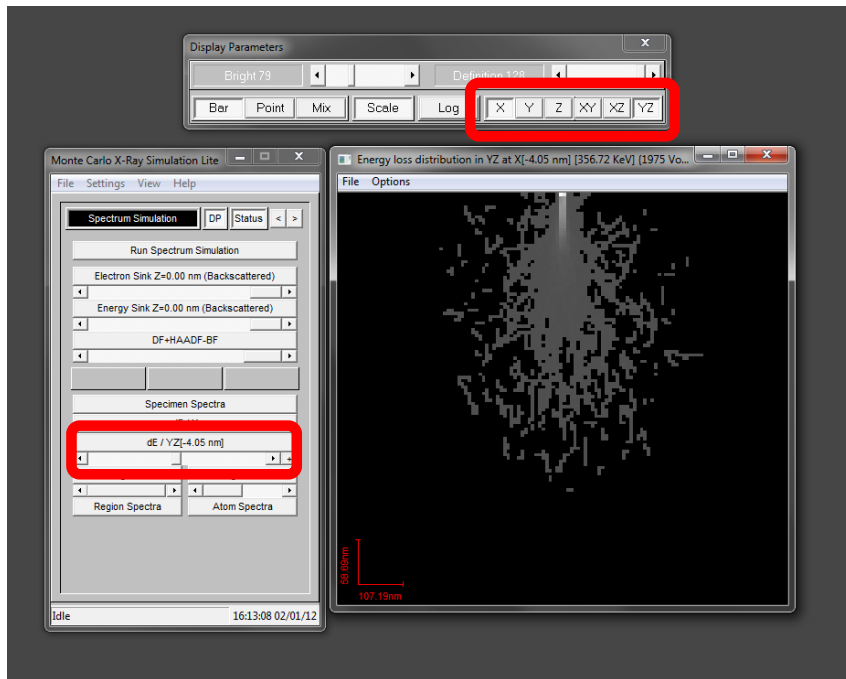
Energy loss depth distribution

Energy Loss Distribution 1D



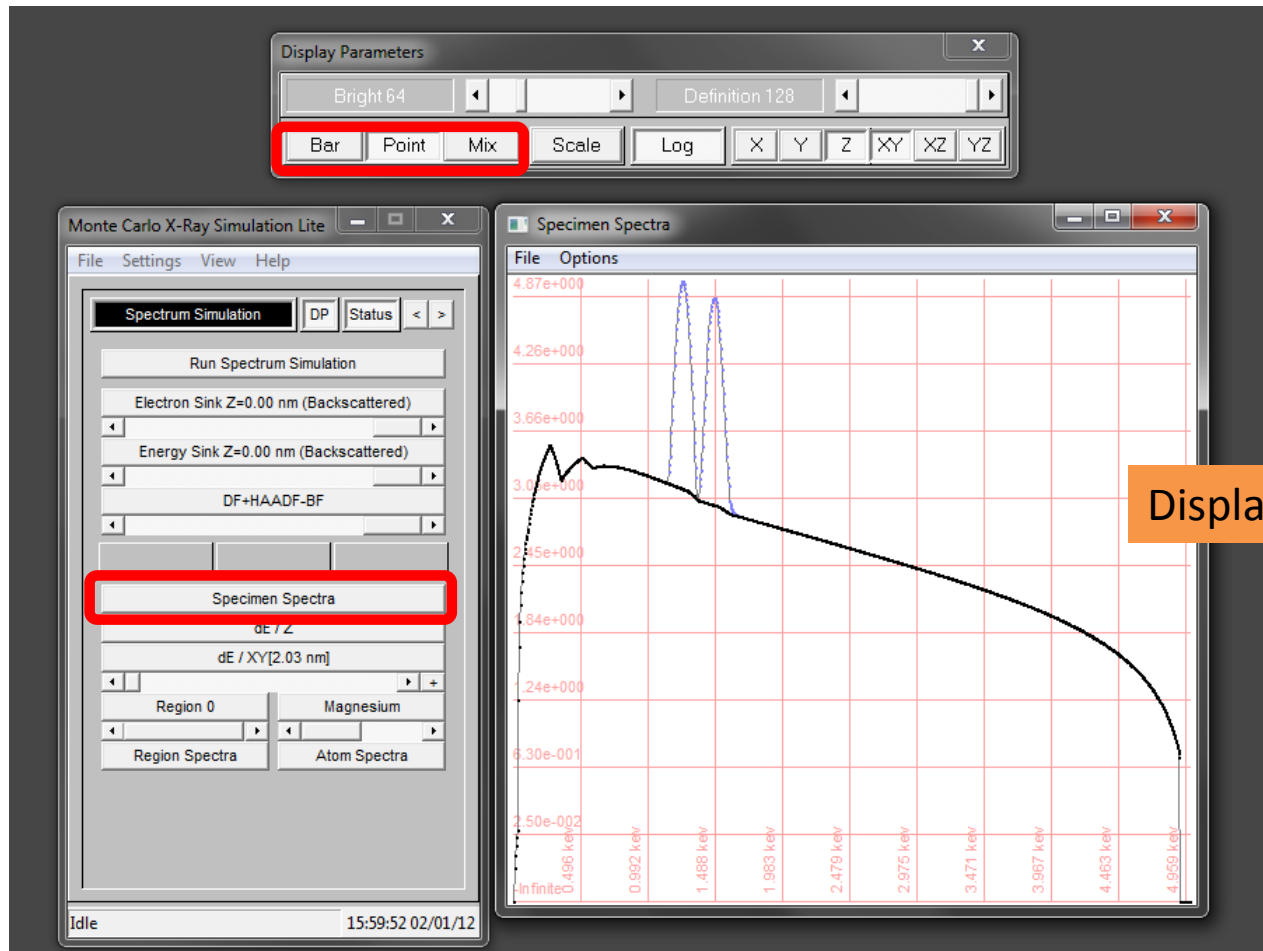
Energy loss lateral distribution

Energy Loss Distribution 2D



Energy loss 2D distribution

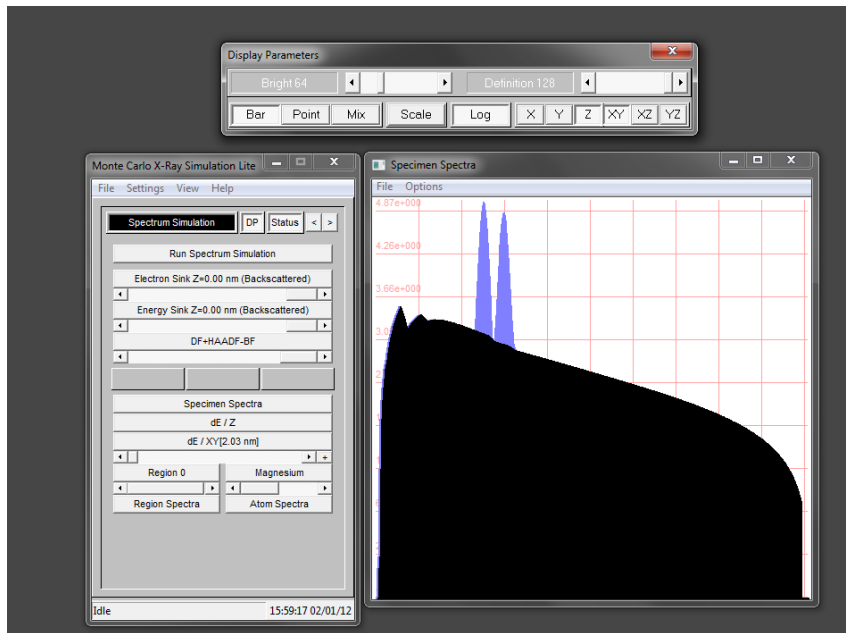
Specimen Spectrum



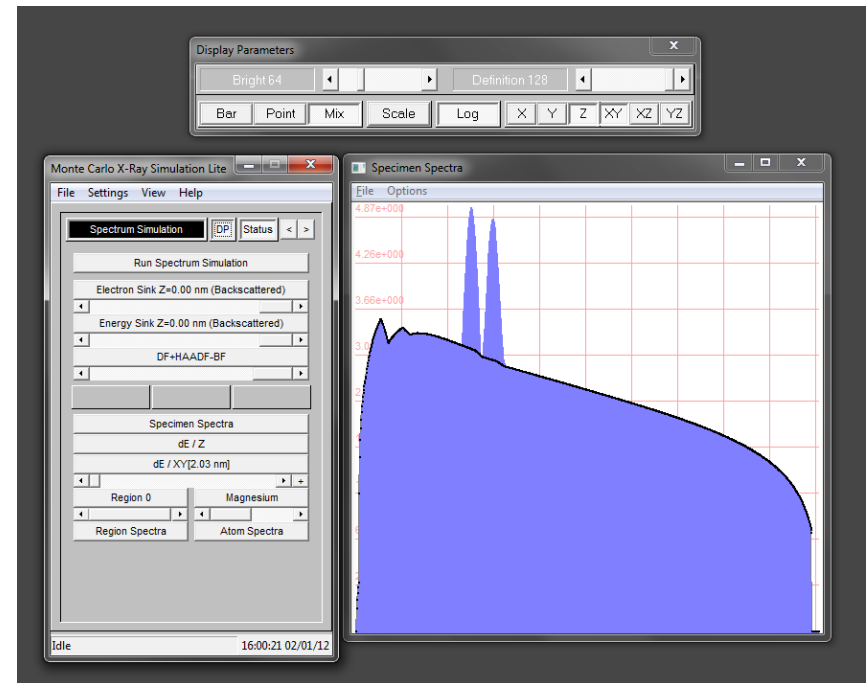
Displayed with points

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

Specimen Spectrum

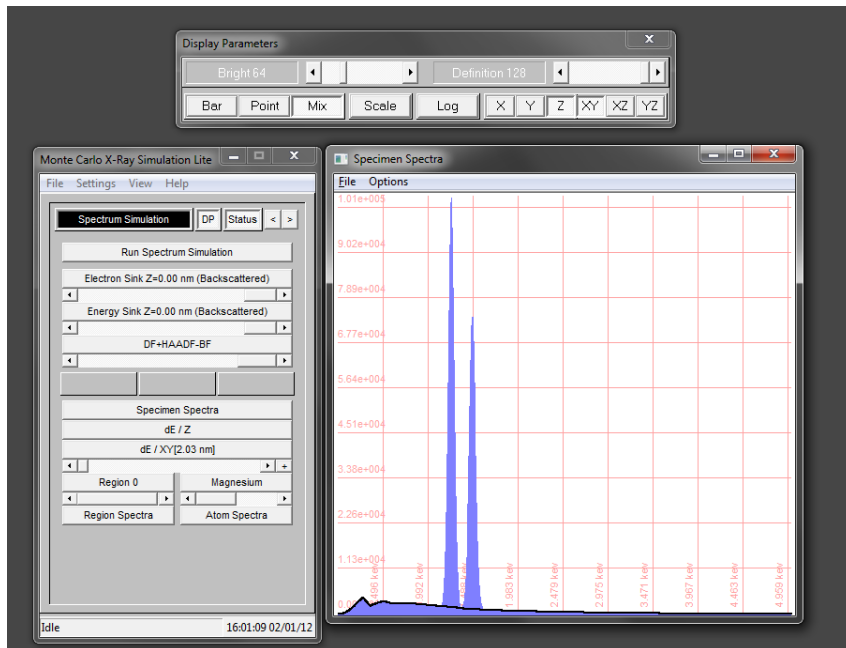


Displayed with bars

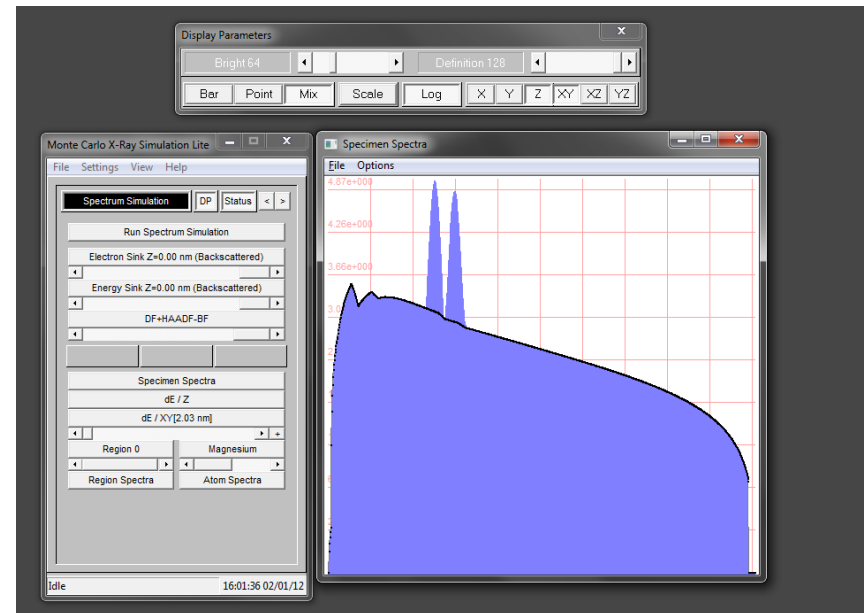


Displayed with points and bars

Specimen Spectrum

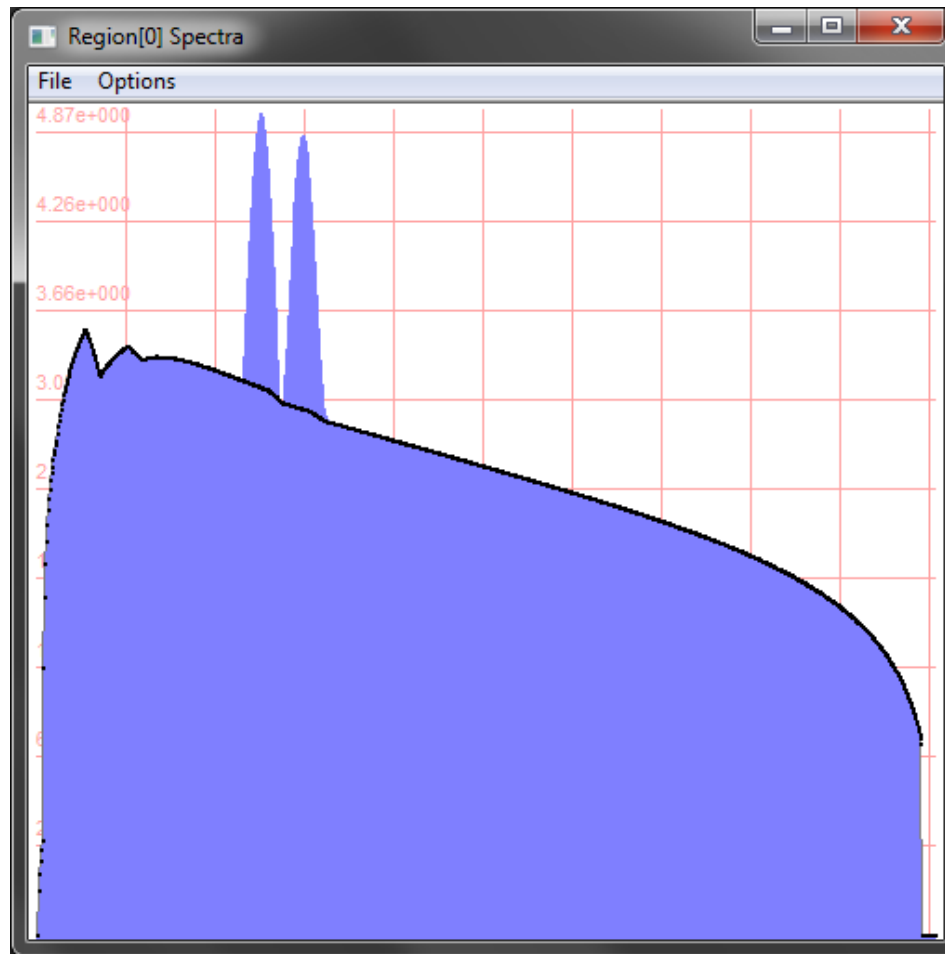


Linear scale



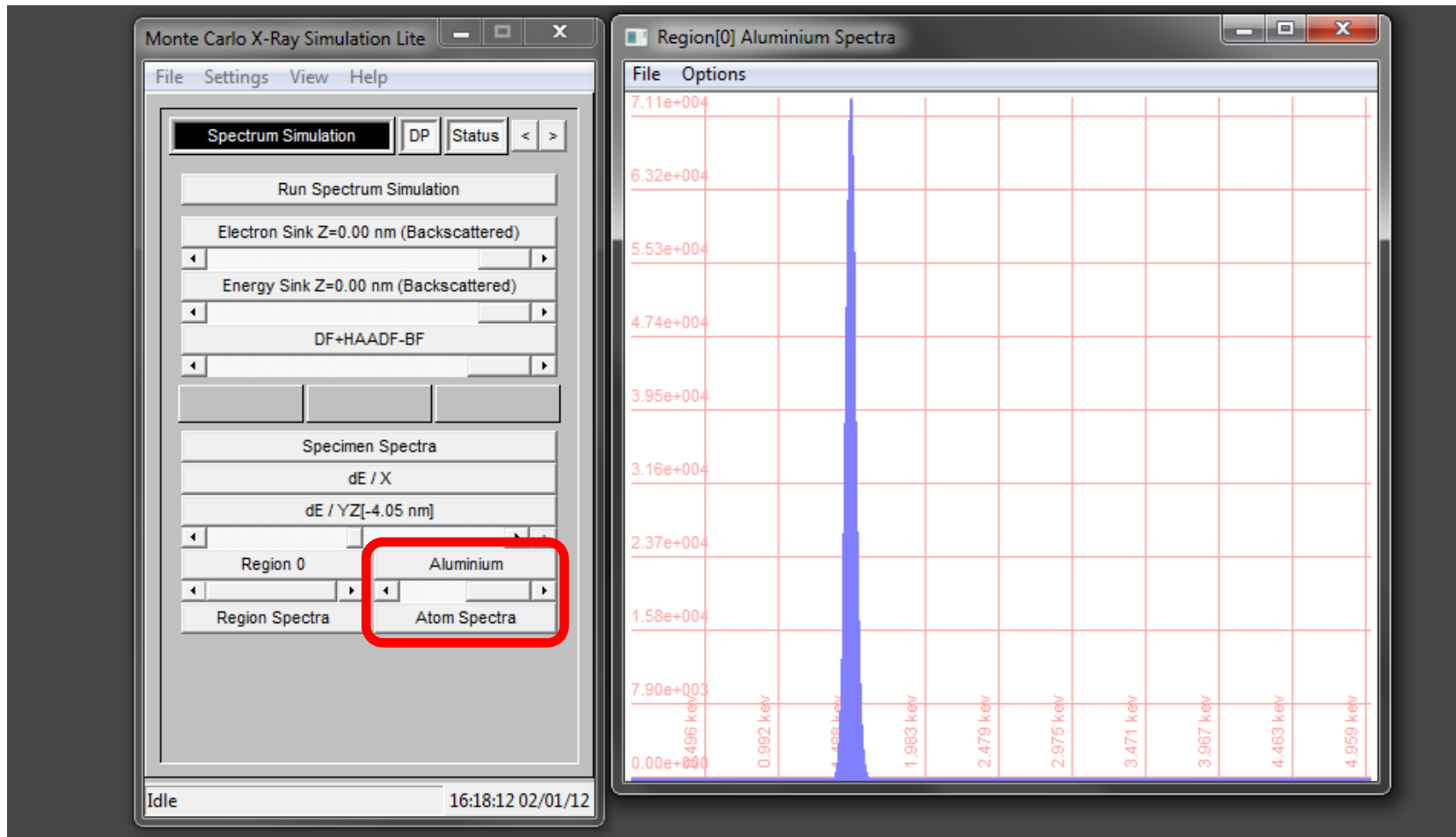
Logarithmic scale

Region Spectrum



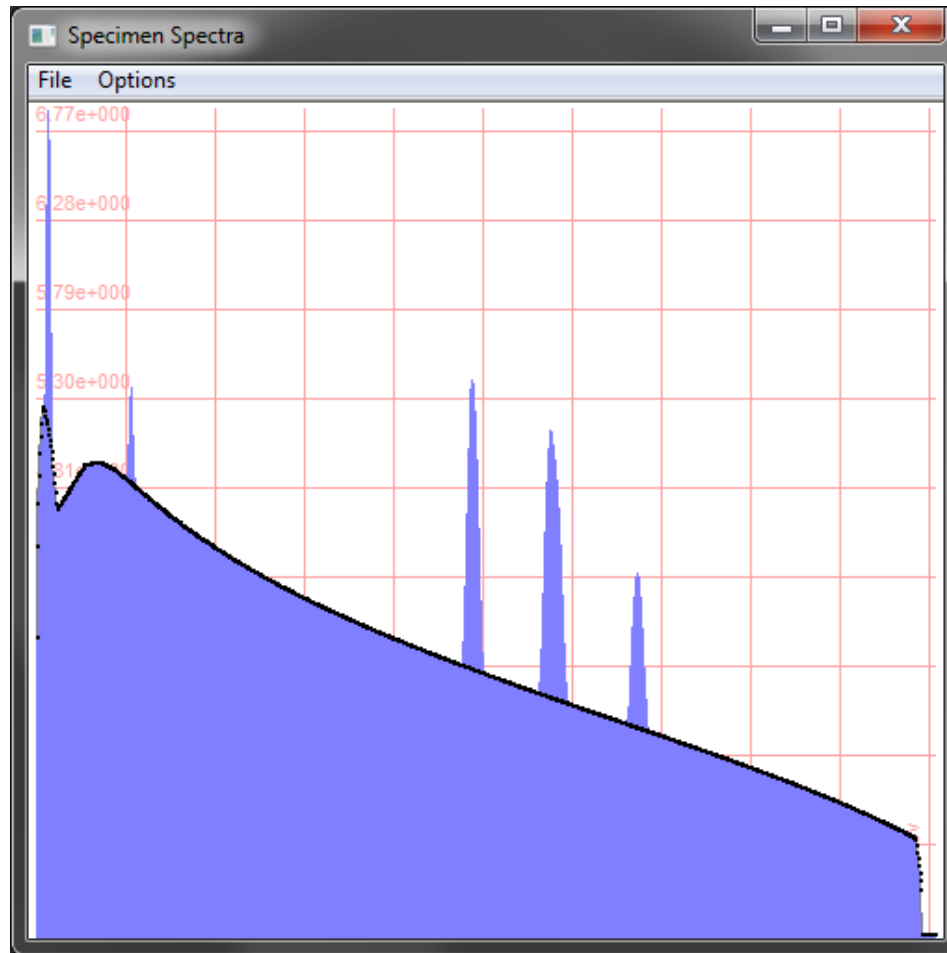
Display spectrum for each region

Atom Spectrum

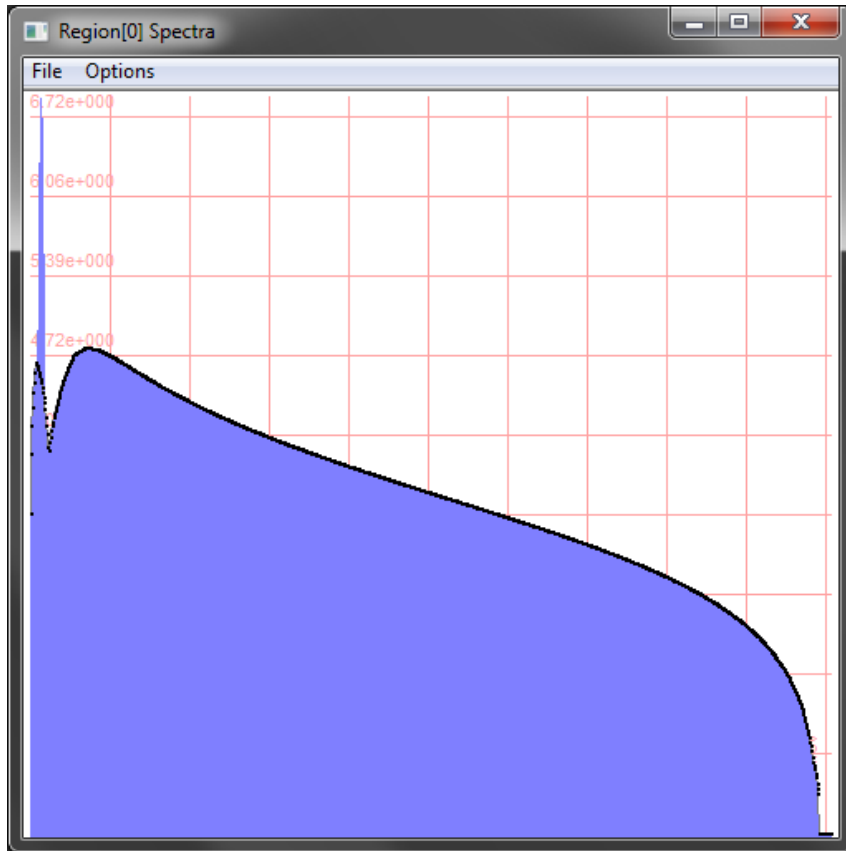


Display spectrum for each atom in a region

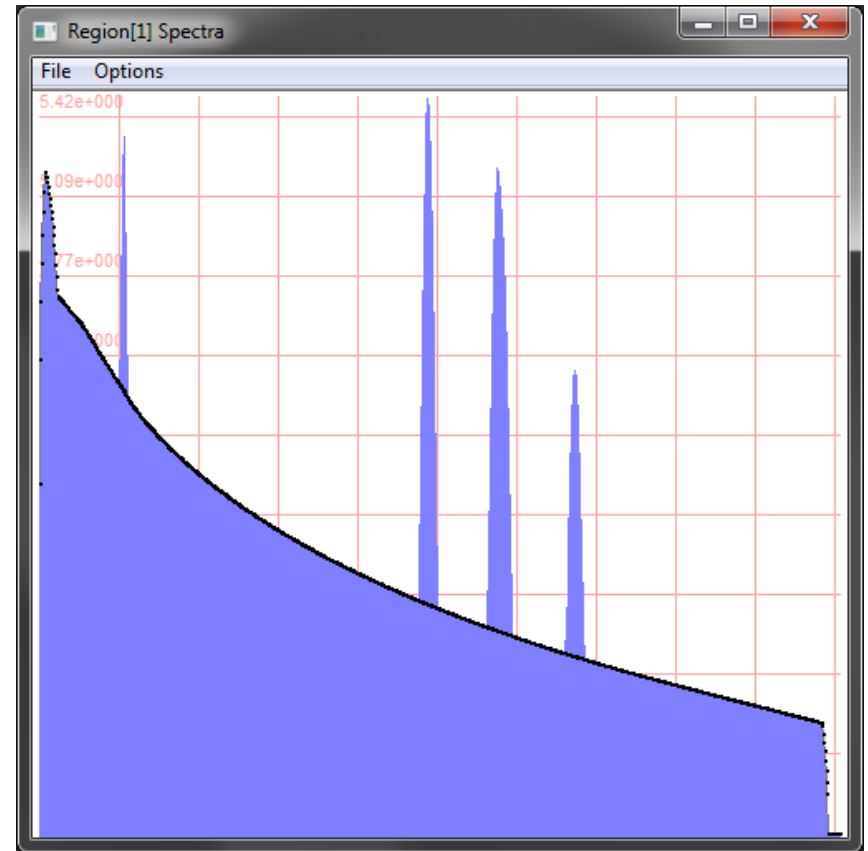
Au NP in C Specimen Spectrum



Au NP in C Region Spectrum

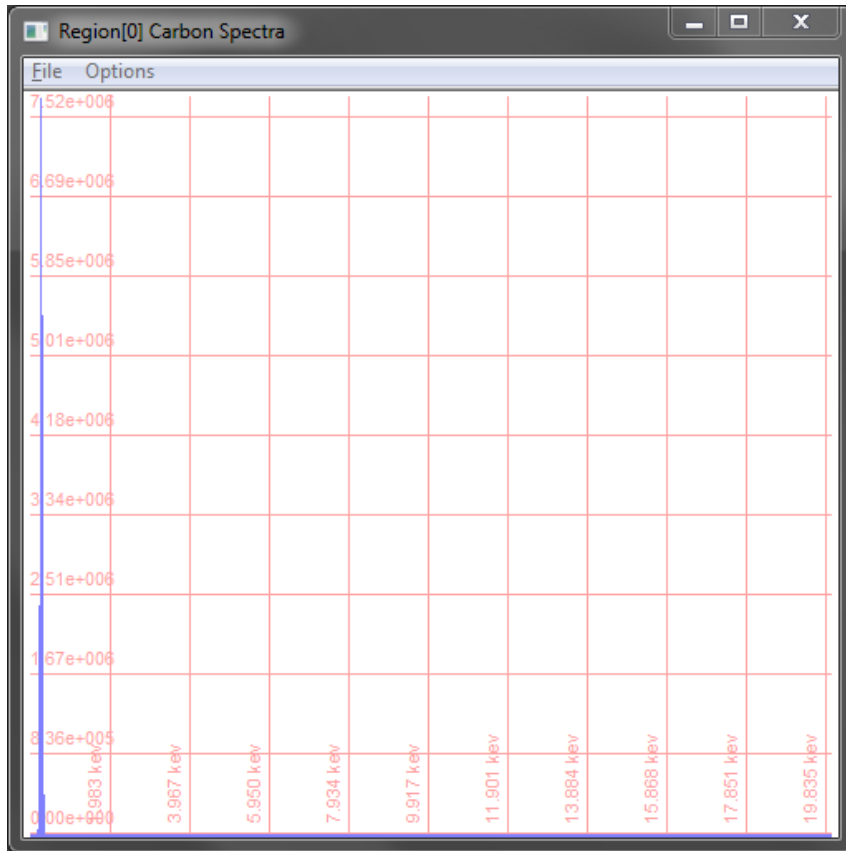


C Substrate

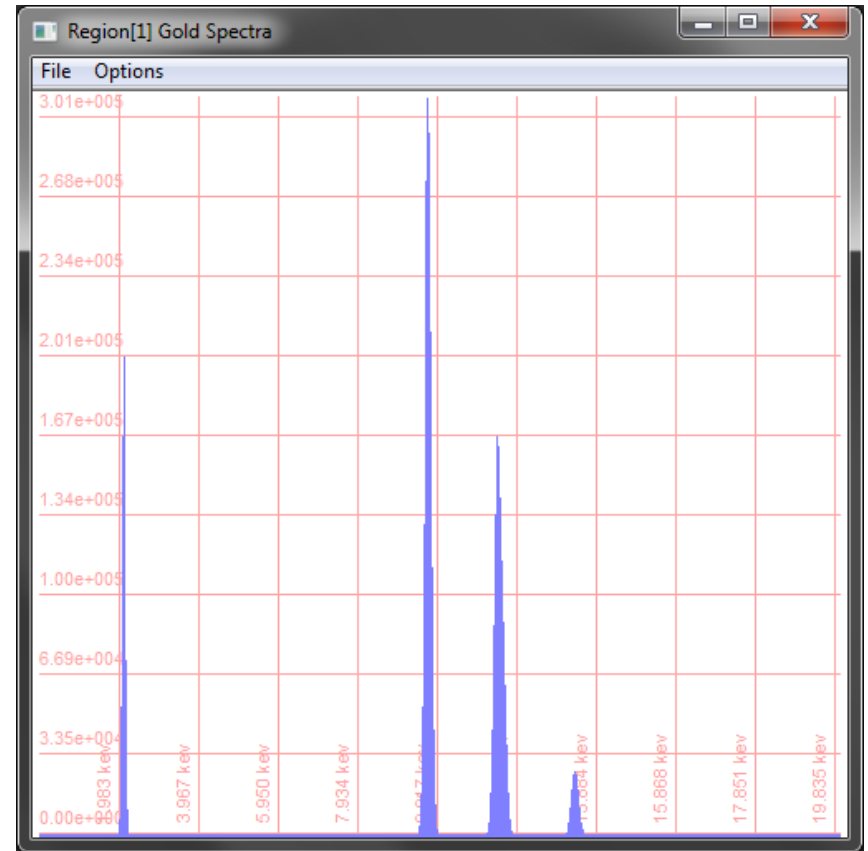


Au NP

Au NP in C Atom Spectrum



C Substrate

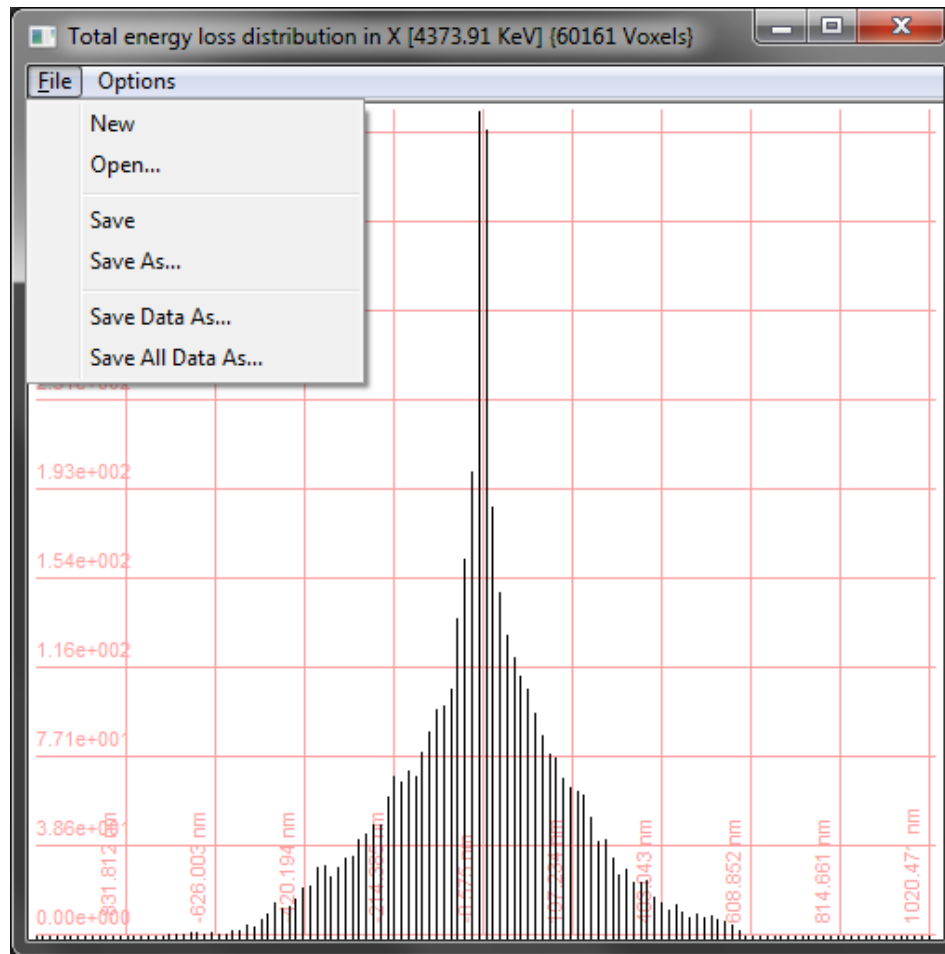


Au NP

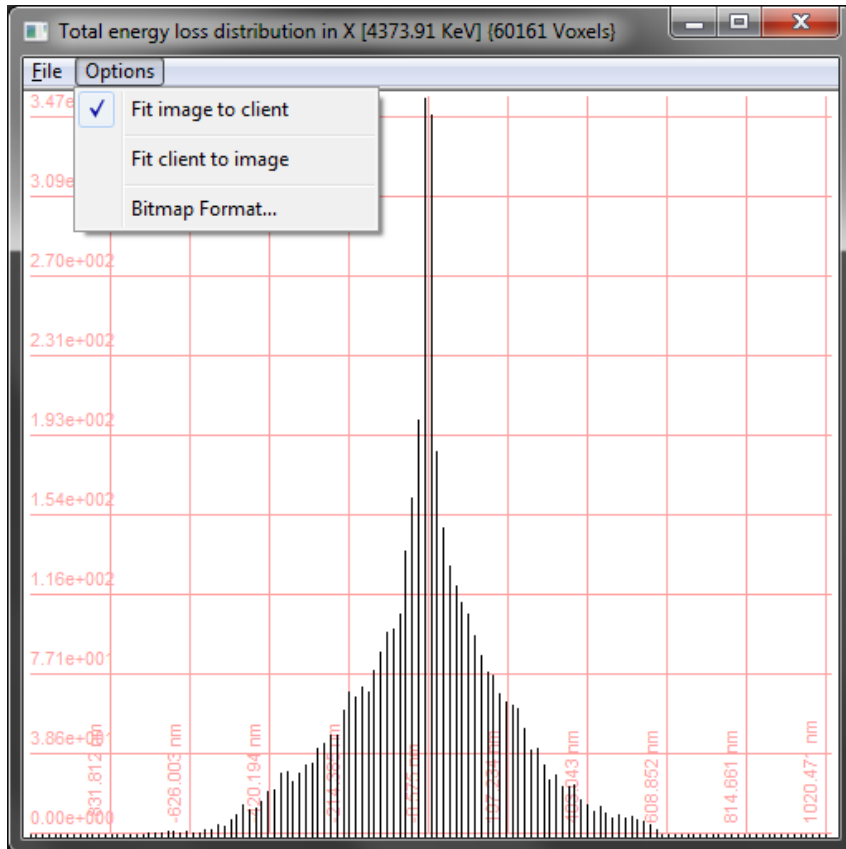
Display Results File Menu

Save the graphic
In a bitmap file

Save the data
in a text file



Display Results Options Menu



Bitmap Options

| | |
|----------------|-----|
| Width | 492 |
| Height | 450 |
| Bits per Pixel | 32 |

OK Cancel

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 = 10000000000 (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.
 - Direction Y = 1
 - Length 1000 nm
 - Radius of 50 nm
- 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
- 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