The Abdus Salam
International Centre for Theoretical Physics

United Nations
Educational, Scientific and
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IAEA
International Atomic Energy Agency

2332

School on Synchrotron and FEL Based Methods and their Multi-Disciplinary Applications

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Additional information lecture 2

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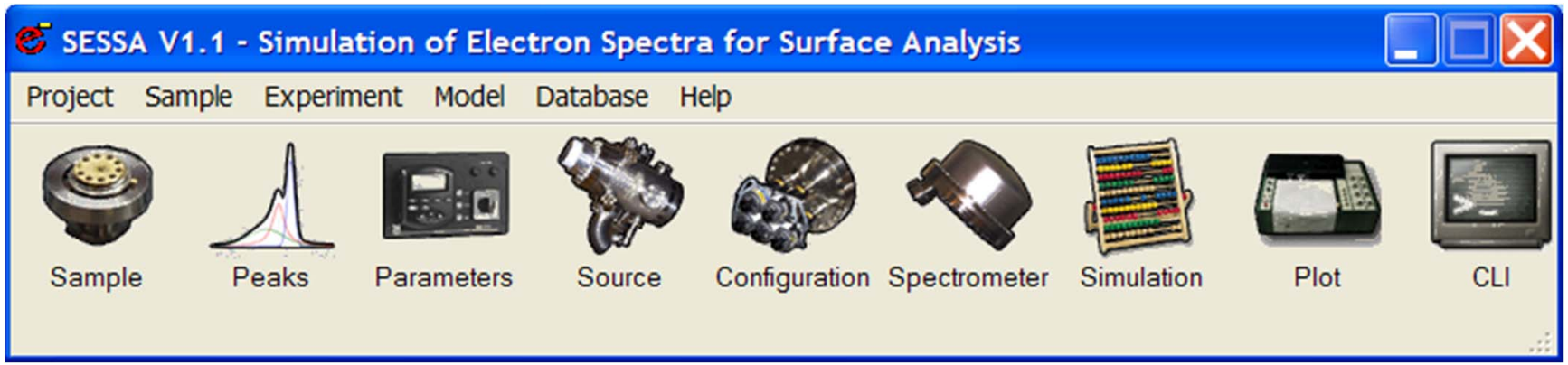
Download prior version of program-1.1:
http://femto.iap.tuwien.ac.at/downloads/SESSAV1_1/

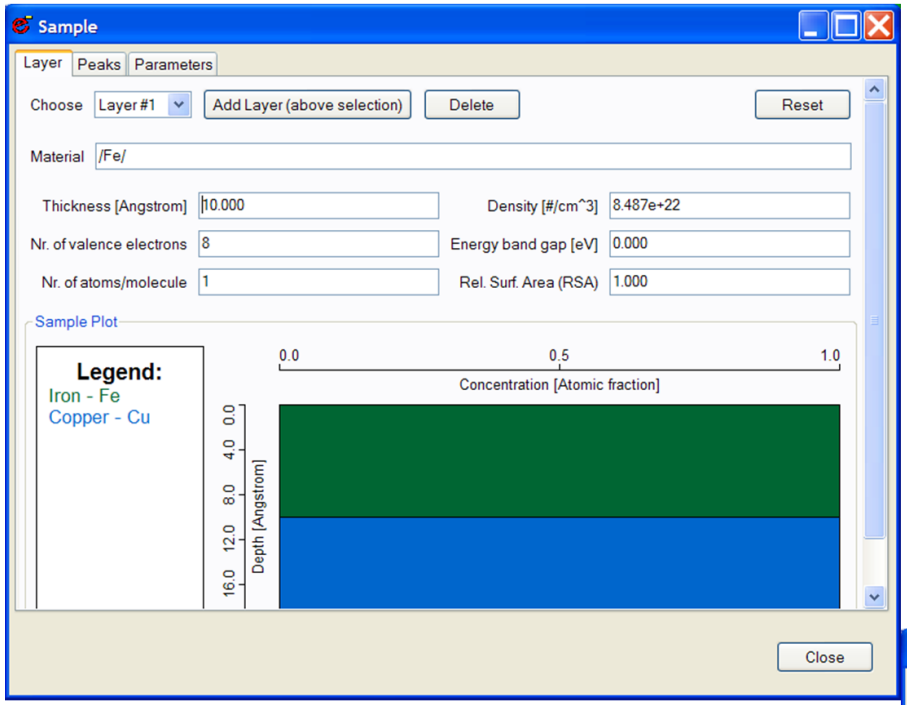
Brief SESSA manual, by CSF:
http://www.physics.ucdavis.edu/Classes/Physics243A/SESSA.BriefManual.pdf
Or use the extensive manual downloadable with pgm.

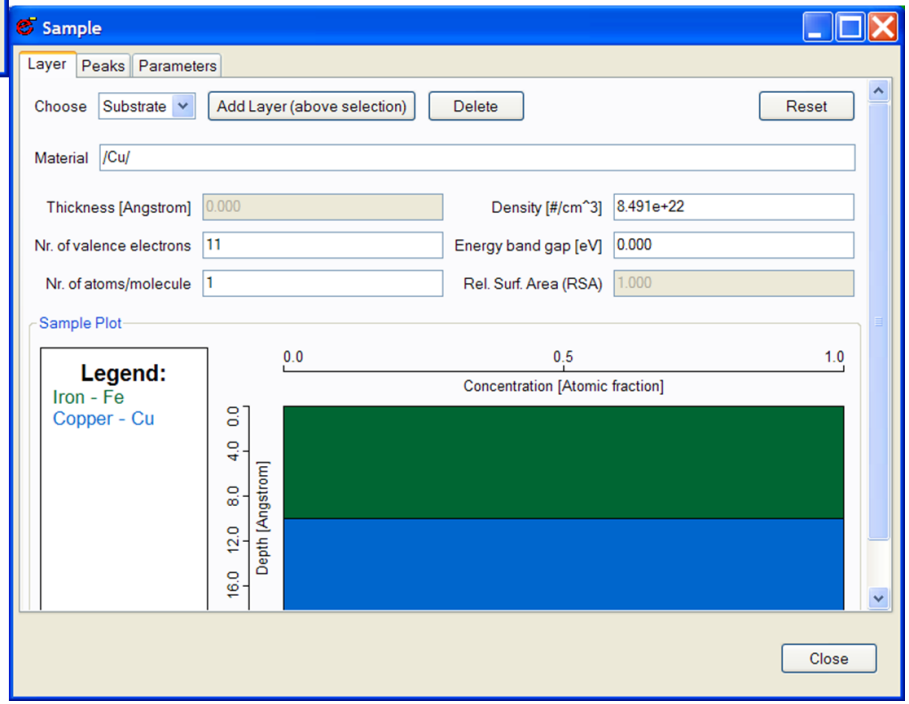
Buy latest version of program-1.2, with variable polarization:
http://nist.gov/data/nist100.htm

Questions of the authors:
http://eaps4.iap.tuwien.ac.at/~werner/sessa.html.

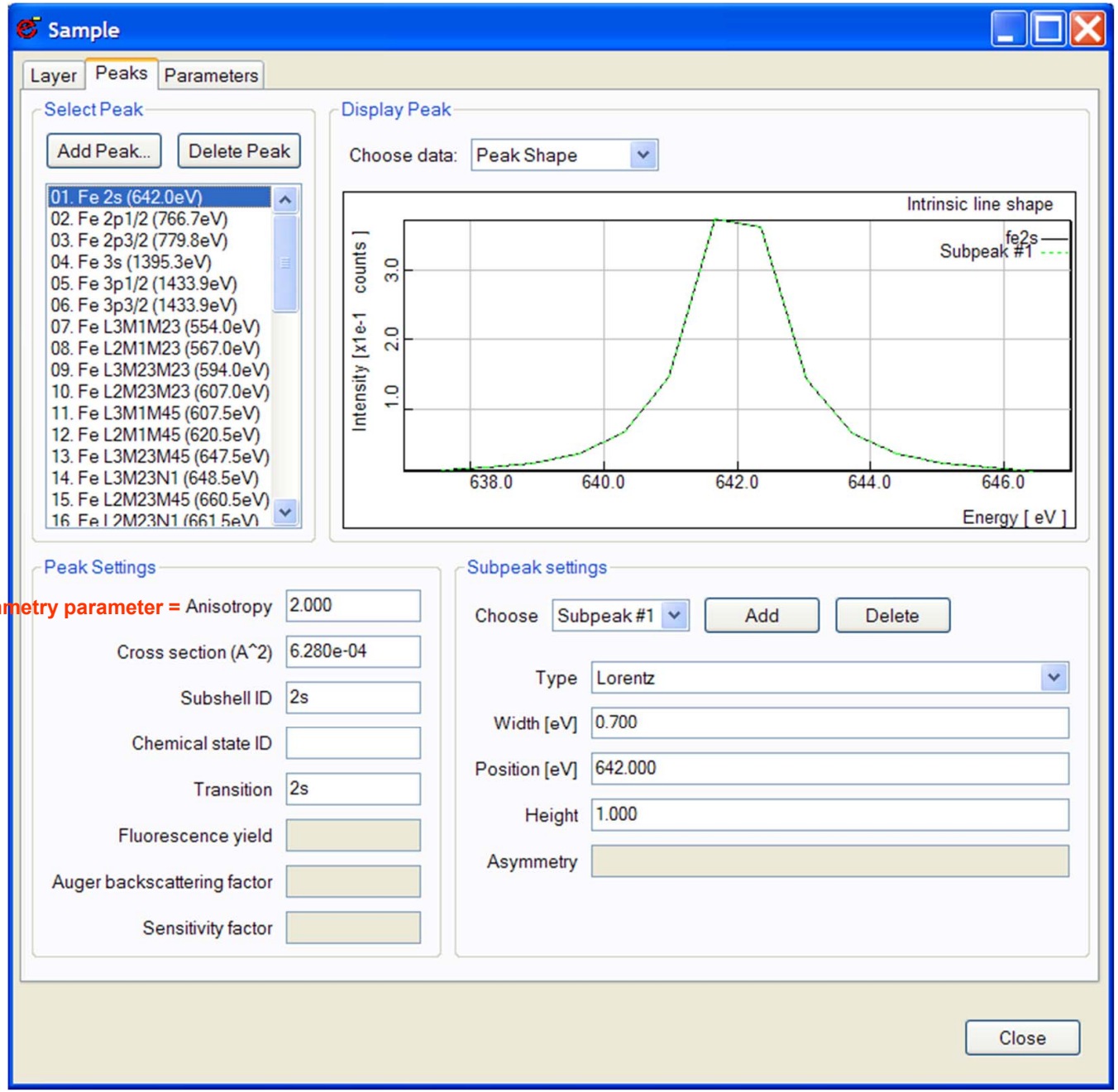


SESSA—Model calculation for 10 Å pure Fe on Cu





SESSA—Model calculation for 10 Å pure Fe on Cu


Sample
Layer
Peaks
Parameters
Select Peak
Add Peak...
Delete Peak
01. Fe 2s (642.0eV)
02. Fe 2p1/2 (766.7eV)
03. Fe 2p3/2 (779.8eV)
04. Fe 3s (1395.3eV)
05. Fe 3p1/2 (1433.9eV)
06. Fe 3p3/2 (1433.9eV)
07. Fe L3M1M23 (554.0eV)
08. Fe L2M1M23 (567.0eV)
09. Fe L3M23M23 (594.0eV)
10. Fe L2M23M23 (607.0eV)
11. Fe L3M1M45 (607.5eV)
12. Fe L2M1M45 (620.5eV)
13. Fe L3M23M45 (647.5eV)
14. Fe L3M23N1 (648.5eV)
15. Fe L2M23M45 (660.5eV)
16. Fe L2M23N1 (661.5eV)
Display Peak
Choose data:
Peak Shape
Intrinsic line shape
fe2s
Subpeak #1
Intensity [x1e-1 counts]
1.0
2.0
3.0
638.0
640.0
642.0
644.0
646.0
Energy [eV]
Peak Settings
Beta = asymmetry parameter =
Anisotropy
2.000
Cross section (A^2)
6.280e-04
Subshell ID
2s
Chemical state ID
Transition
2s
Fluorescence yield
Auger backscattering factor
Sensitivity factor
Subpeak settings
Choose
Subpeak #1
Add
Delete
Type
Lorentz
Width [eV]
0.700
Position [eV]
642.000
Height
1.000
Asymmetry
Close

Sample

Layer | Peaks | Parameters

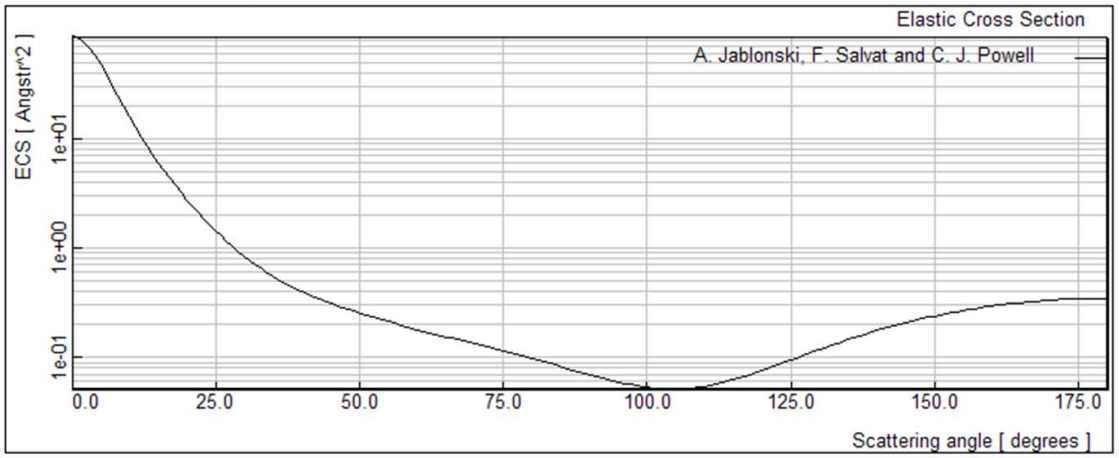
Choose Peak: 01. Fe 2s (642.0eV)

Mean Free Paths

	IMFP (A)	EMFP (A)	TRMFP (A)
Layer #1	11.665	5.292	22.424
Substrate	11.915	6.848	20.979

Choose Layer: Layer #1

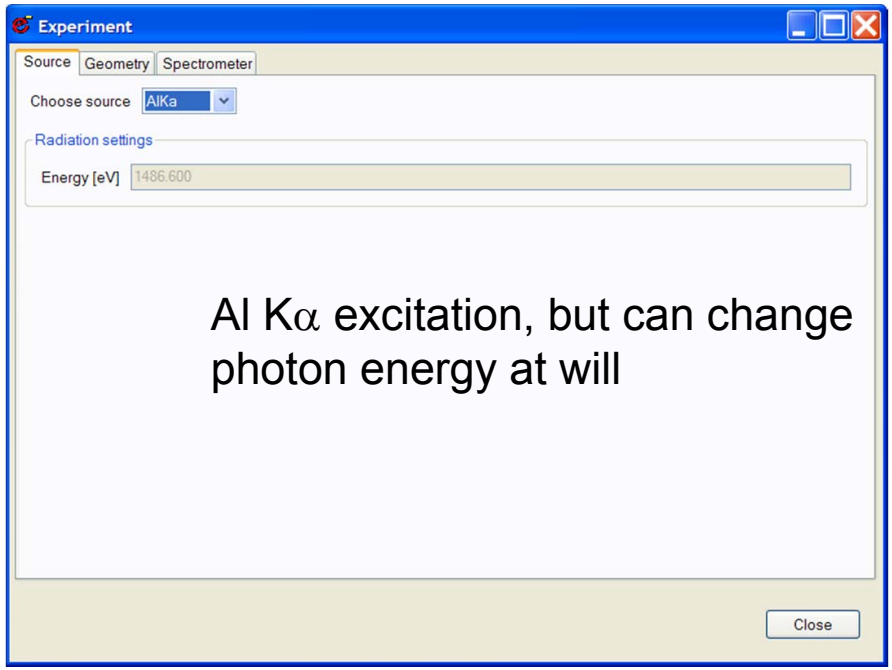
Elastic Cross Section Settings



Differential Inverse Inelastic Mean Free Path

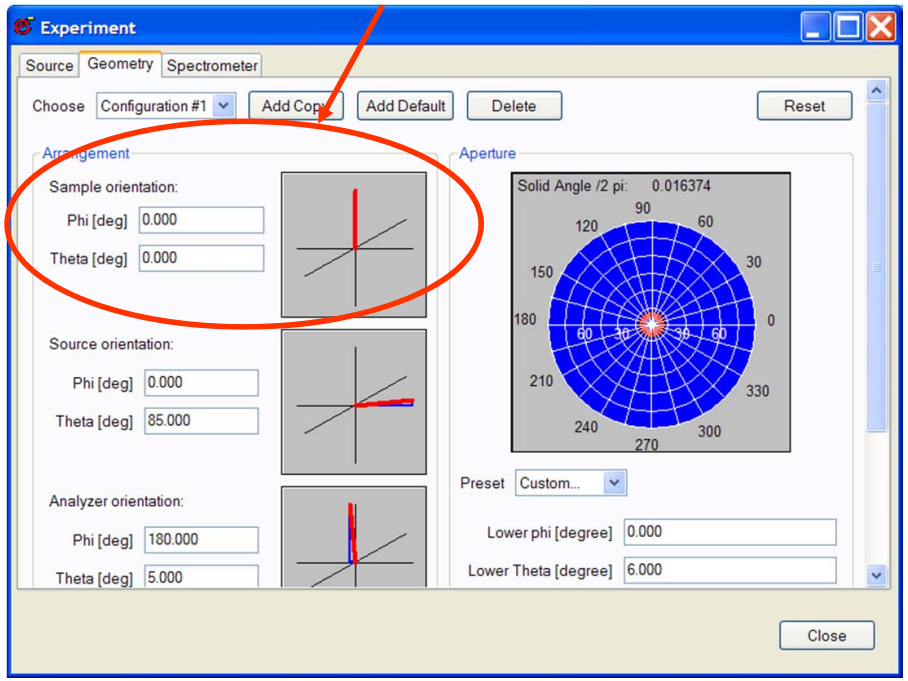
Set Material: /FE/: Iron

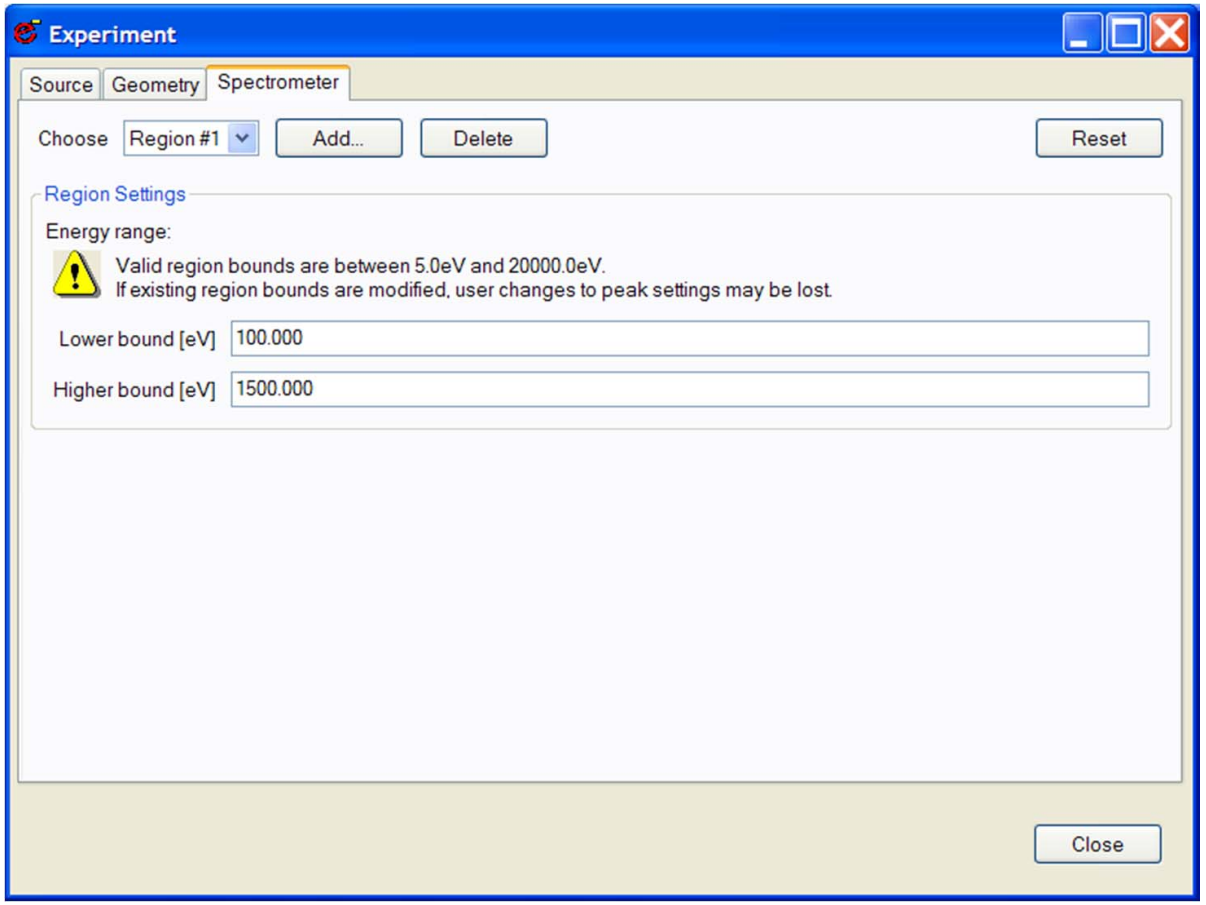
Close

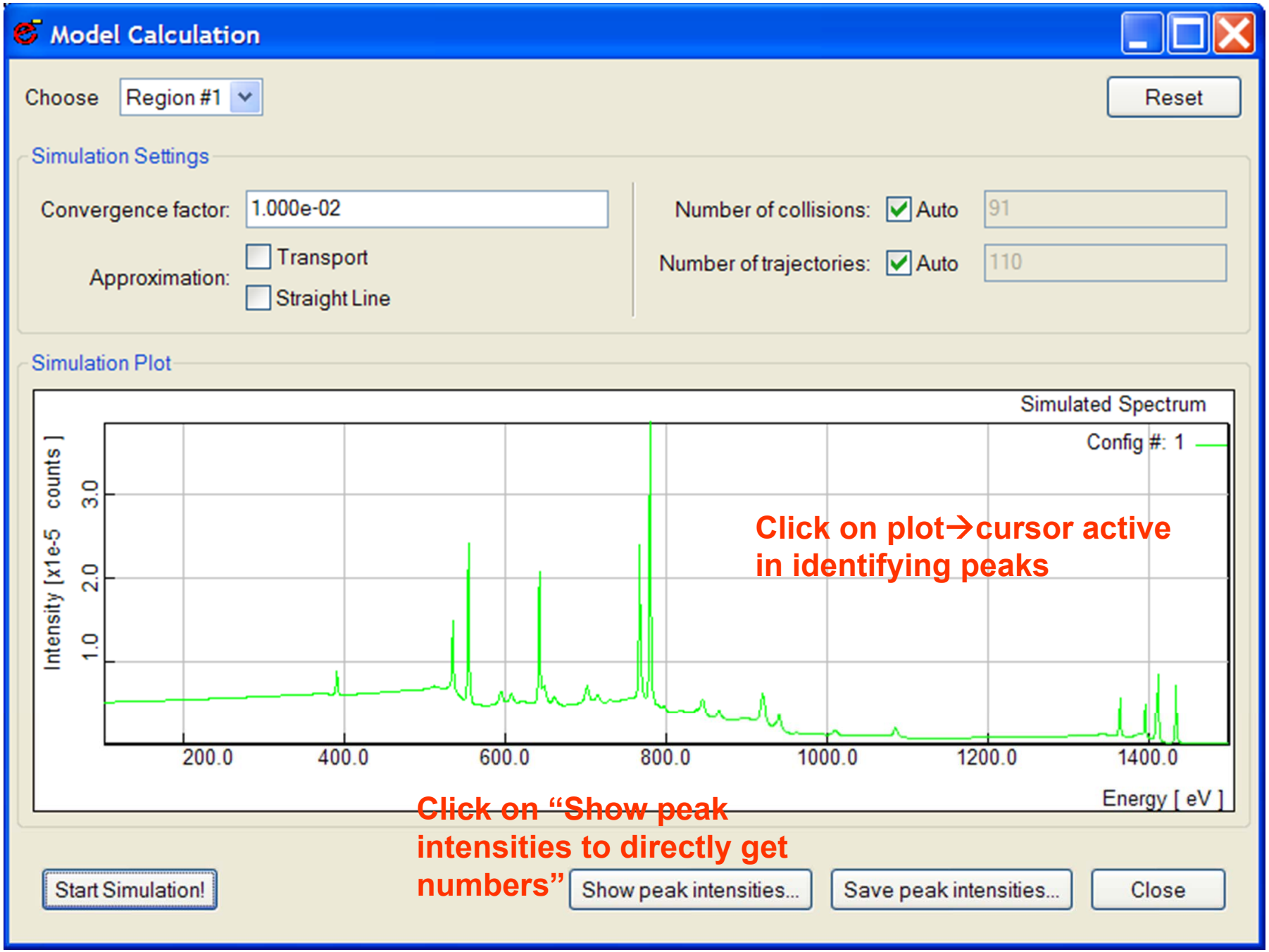


Al Kα excitation, but can change photon energy at will

Leave this alone




Experiment
Source
Geometry
Spectrometer
Choose
Region #1
Add...
Delete
Reset
Region Settings
Energy range:
Valid region bounds are between 5.0eV and 20000.0eV.
If existing region bounds are modified, user changes to peak settings may be lost.
Lower bound [eV]
100.000
Higher bound [eV]
1500.000
Close


Model Calculation
Choose
Region #1
Reset
Simulation Settings
Convergence factor:
1.000e-02
Approximation:
Transport
Straight Line
Number of collisions:
Auto
91
Number of trajectories:
Auto
110
Simulation Plot
Simulated Spectrum
Config #: 1
Intensity [x1e-5 counts]
1.0
2.0
3.0
200.0
400.0
600.0
800.0
1000.0
1200.0
1400.0
Energy [eV]
Click on plot→cursor active in identifying peaks
Click on "Show peak intensities to directly get numbers"
Start Simulation!
Show peak intensities...
Save peak intensities...
Close