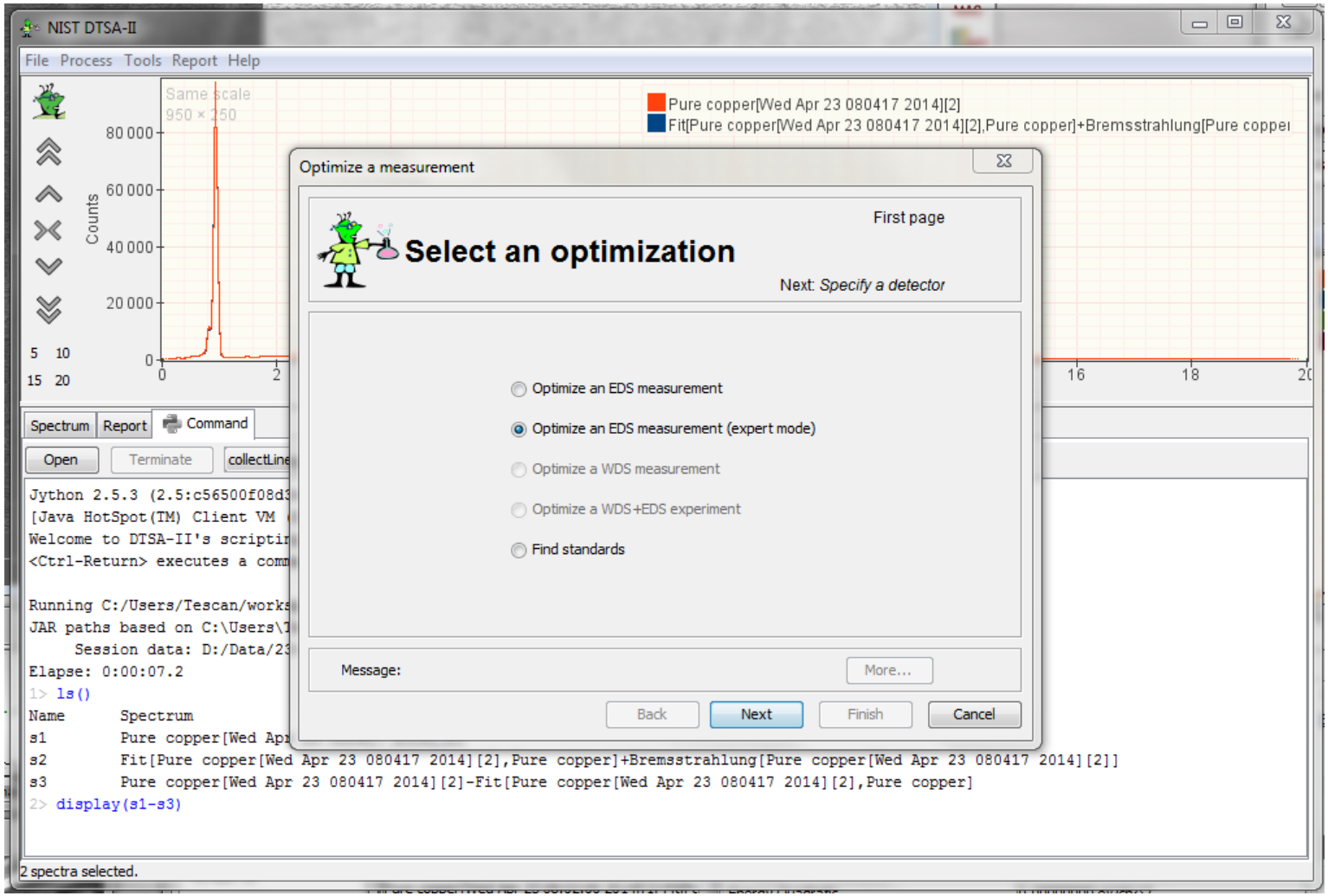
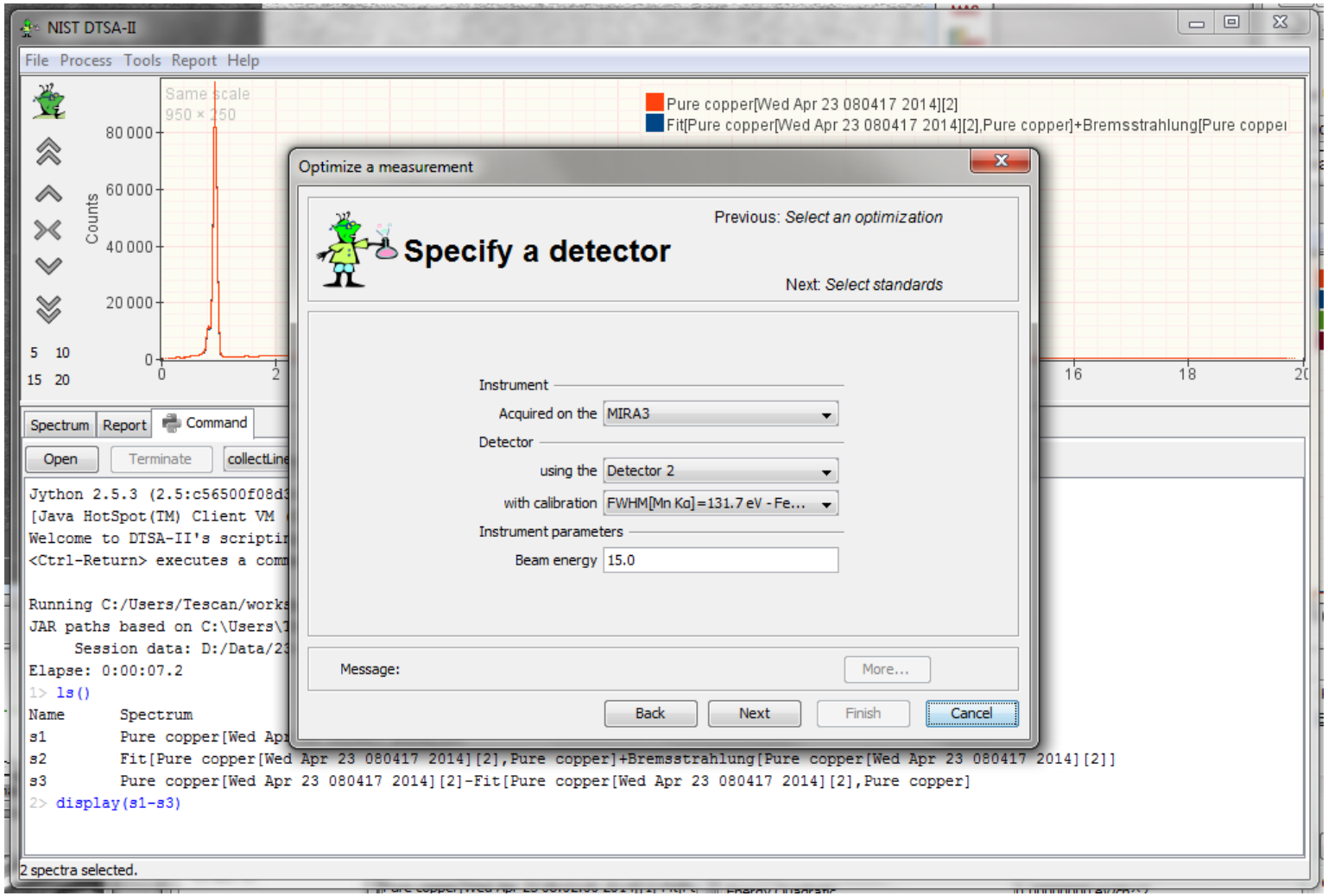
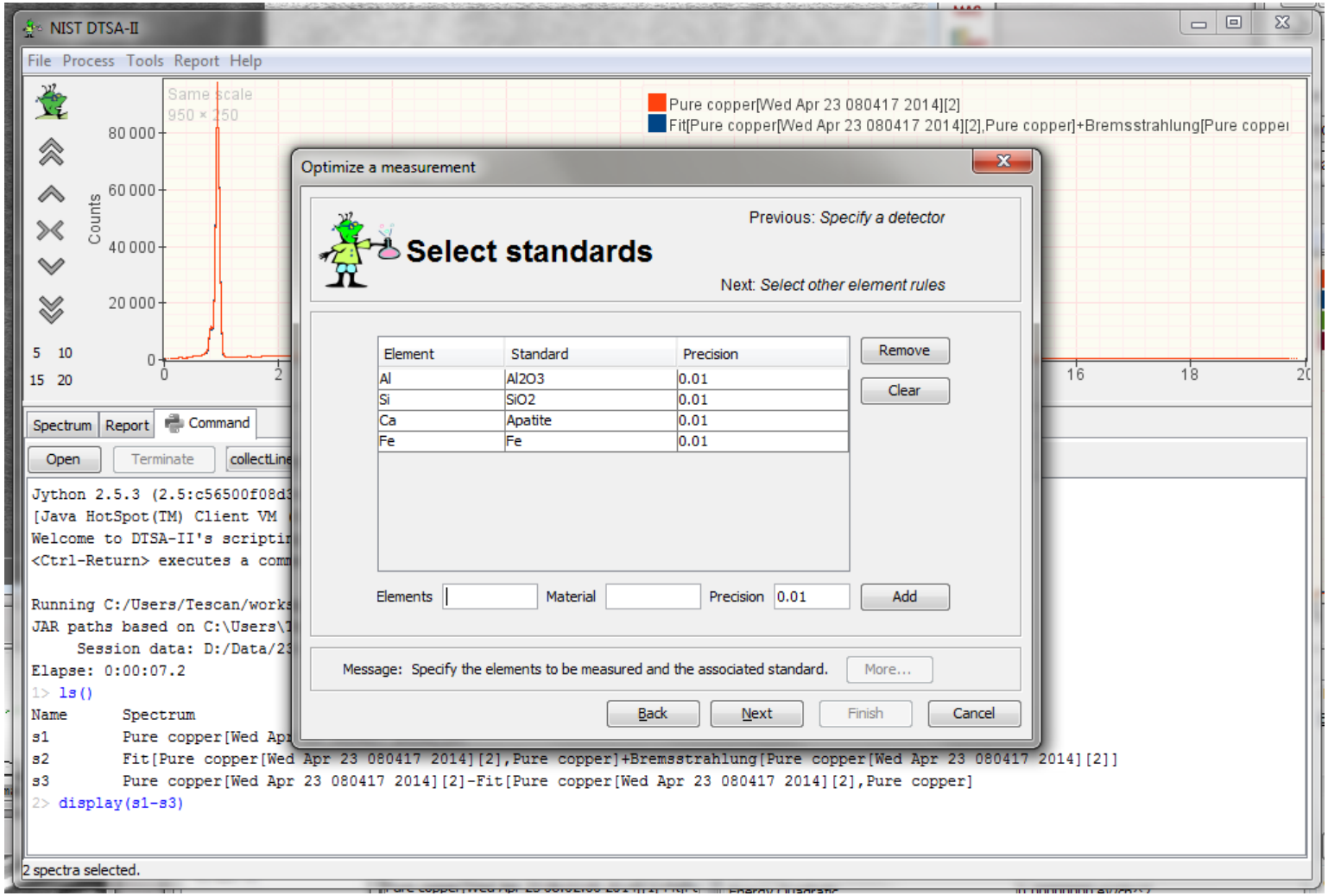
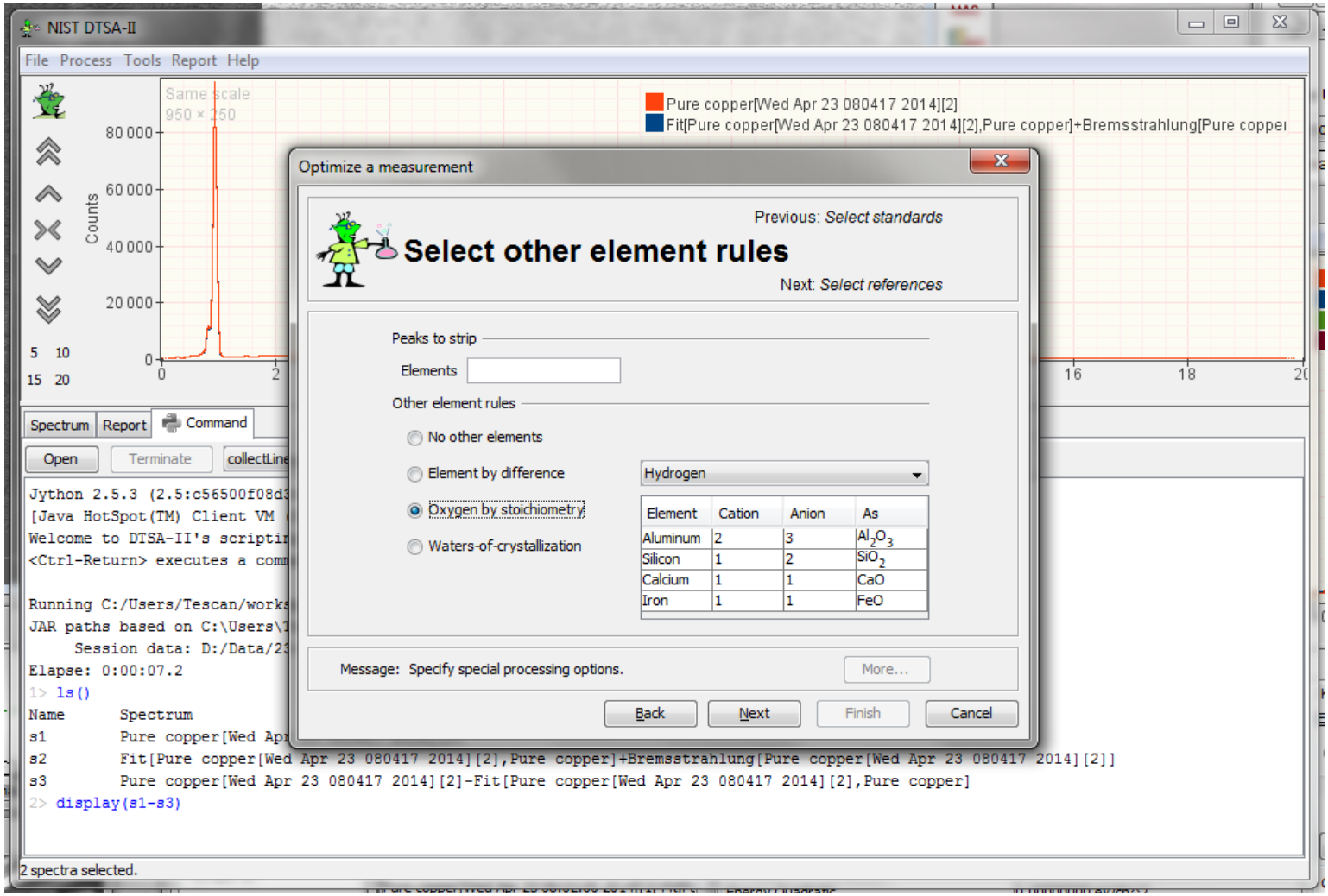
Optimization

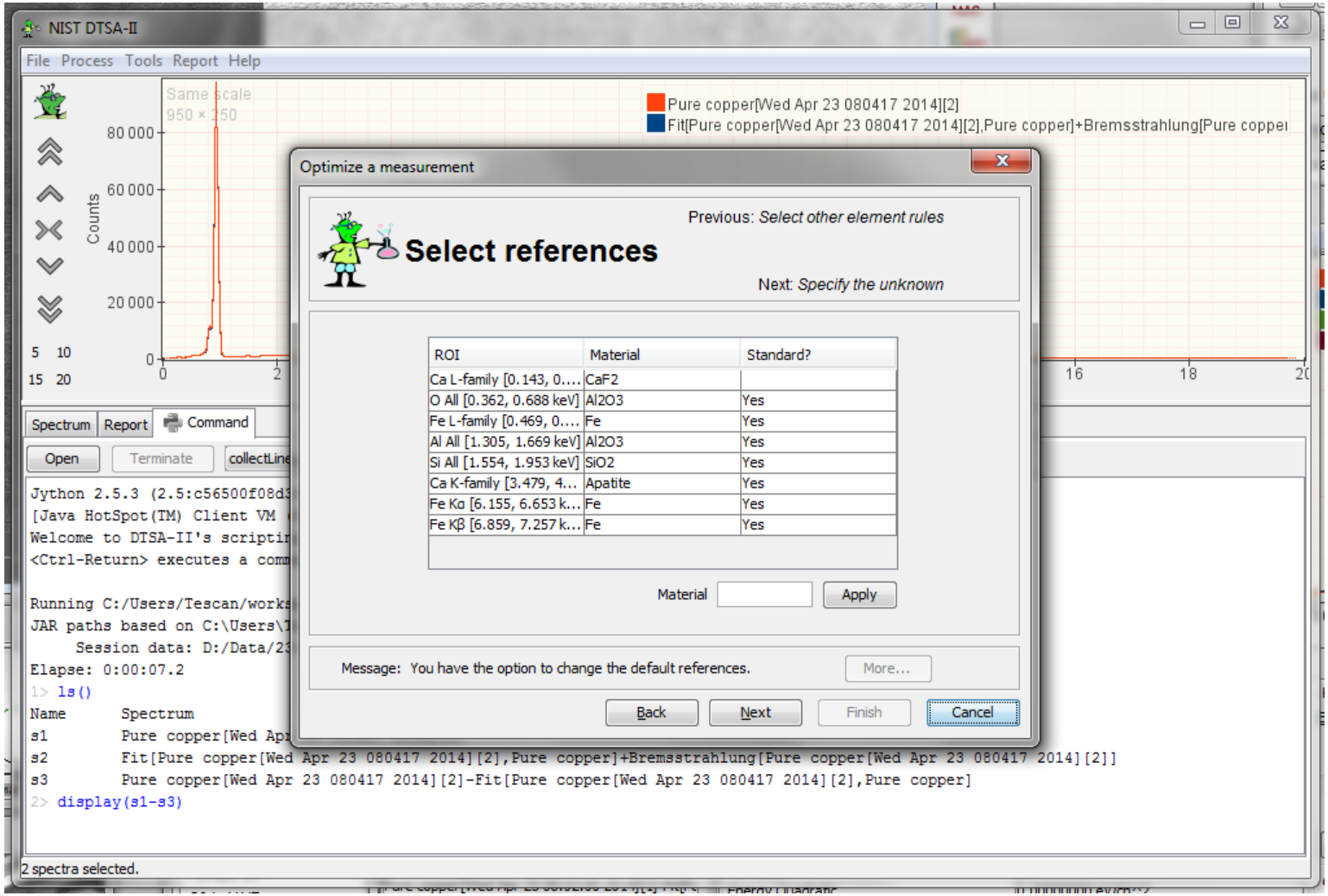
Designing a measurement protocol to optimally address the measurement need

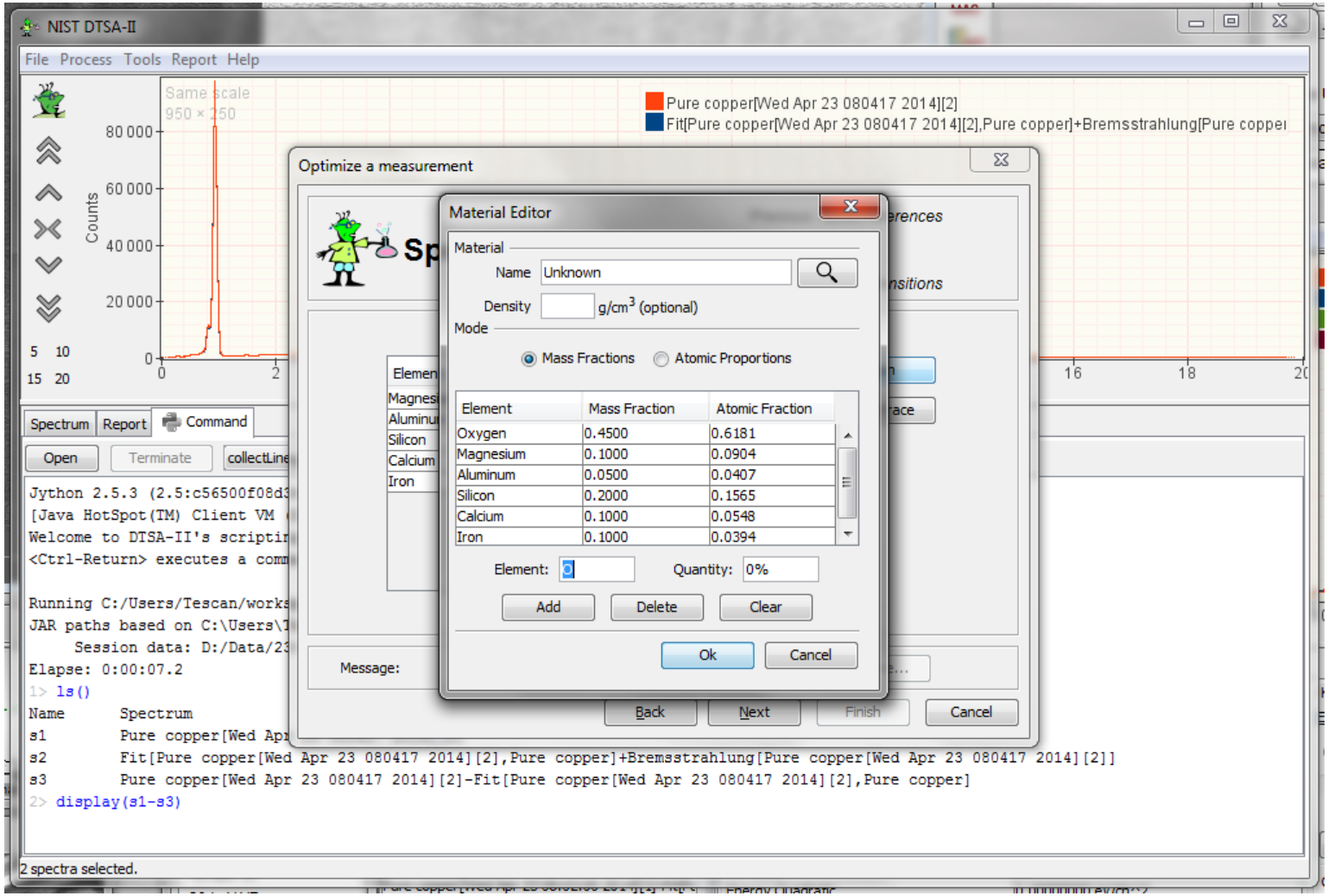

NIST DTSA-II
File Process Tools Report Help
Same scale
950 × 250
Pure copper[Wed Apr 23 080417 2014][2]
Fit[Pure copper[Wed Apr 23 080417 2014][2],Pure copper]+Bremsstrahlung[Pure copper
Counts
80 000
60 000
40 000
20 000
0
Optimize a measurement
First page
Select an optimization
Next: Specify a detector
Optimize an EDS measurement
Optimize an EDS measurement (expert mode)
Optimize a WDS measurement
Optimize a WDS+EDS experiment
Find standards
Message:
More...
Back
Next
Finish
Cancel
Spectrum
Report
Command
Open
Terminate
Jython 2.5.3 (2.5:c56500f08d3
[Java HotSpot(TM) Client VM
Welcome to DTSA-II's scriptin
<Ctrl-Return> executes a comm
Running C:/Users/Tescan/works
JAR paths based on C:\Users\
Session data: D:/Data/23
Elapse: 0:00:07.2
1> ls()
Name Spectrum
s1 Pure copper[Wed Ap
s2 Fit[Pure copper[Wed Apr 23 080417 2014][2],Pure copper]+Bremsstrahlung[Pure copper[Wed Apr 23 080417 2014][2]]
s3 Pure copper[Wed Apr 23 080417 2014][2]-Fit[Pure copper[Wed Apr 23 080417 2014][2],Pure copper]
2> display(s1-s3)
2 spectra selected.

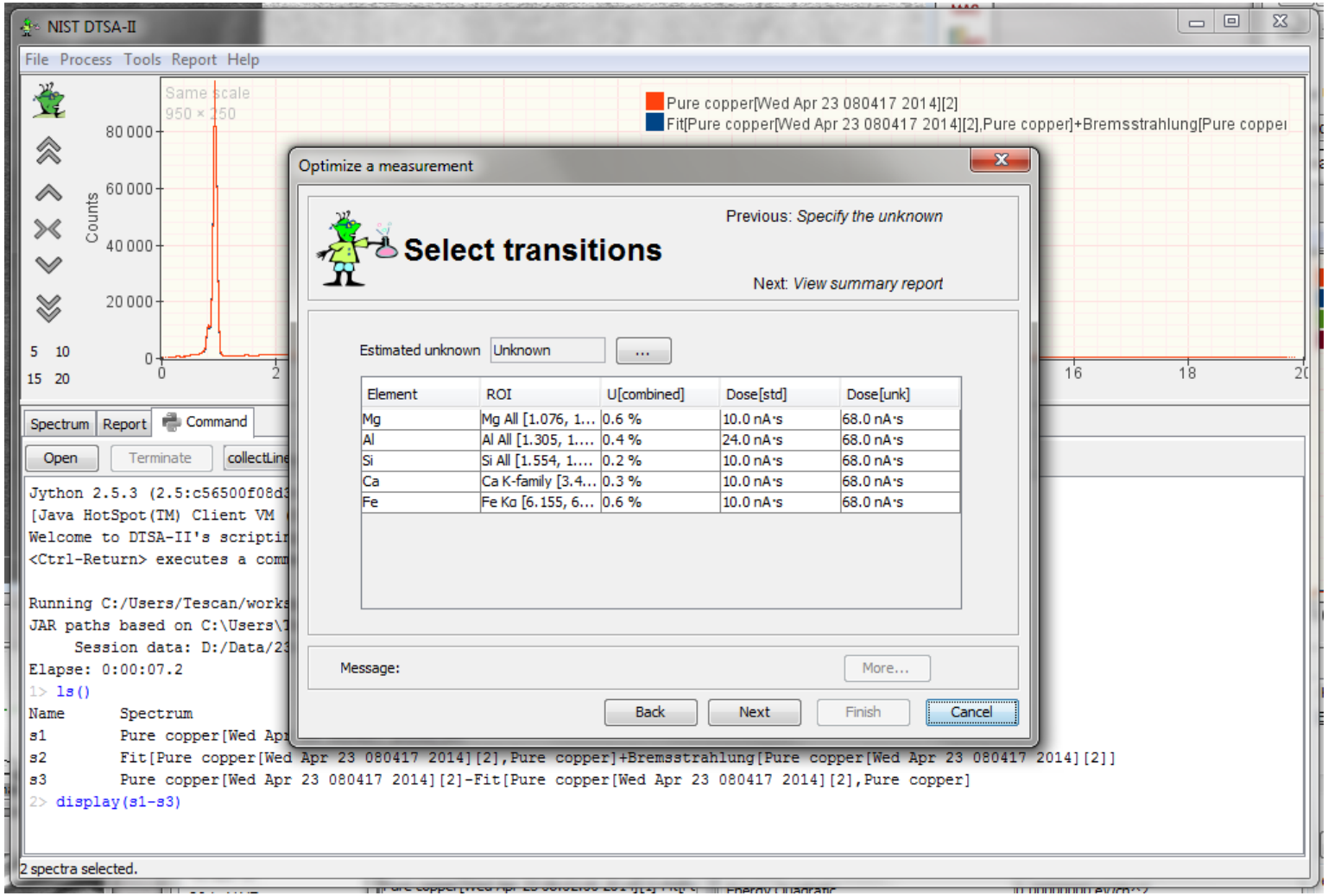

NIST DTSA-II
File Process Tools Report Help
Same scale
950 × 250
Pure copper[Wed Apr 23 080417 2014][2]
Fit[Pure copper[Wed Apr 23 080417 2014][2],Pure copper]+Bremsstrahlung[Pure copper
Counts
80 000
60 000
40 000
20 000
0
Optimize a measurement
Previous: Select an optimization
Specify a detector
Next: Select standards
Instrument
Acquired on the MIRA3
Detector
using the Detector 2
with calibration FWHM[Mn Kα]=131.7 eV - Fe...
Instrument parameters
Beam energy 15.0
Message:
More...
Back
Next
Finish
Cancel
Spectrum
Report
Command
Open
Terminate
Jython 2.5.3 (2.5:c56500f08d
[Java HotSpot(TM) Client VM
Welcome to DTSA-II's scriptin
<Ctrl-Return> executes a comm
Running C:/Users/Tescan/works
JAR paths based on C:\Users\
Session data: D:/Data/2
Elapse: 0:00:07.2
1> ls()
Name Spectrum
s1 Pure copper[Wed Ap
s2 Fit[Pure copper[Wed Apr 23 080417 2014][2],Pure copper]+Bremsstrahlung[Pure copper[Wed Apr 23 080417 2014][2]]
s3 Pure copper[Wed Apr 23 080417 2014][2]-Fit[Pure copper[Wed Apr 23 080417 2014][2],Pure copper]
2> display(s1-s3)
2 spectra selected.

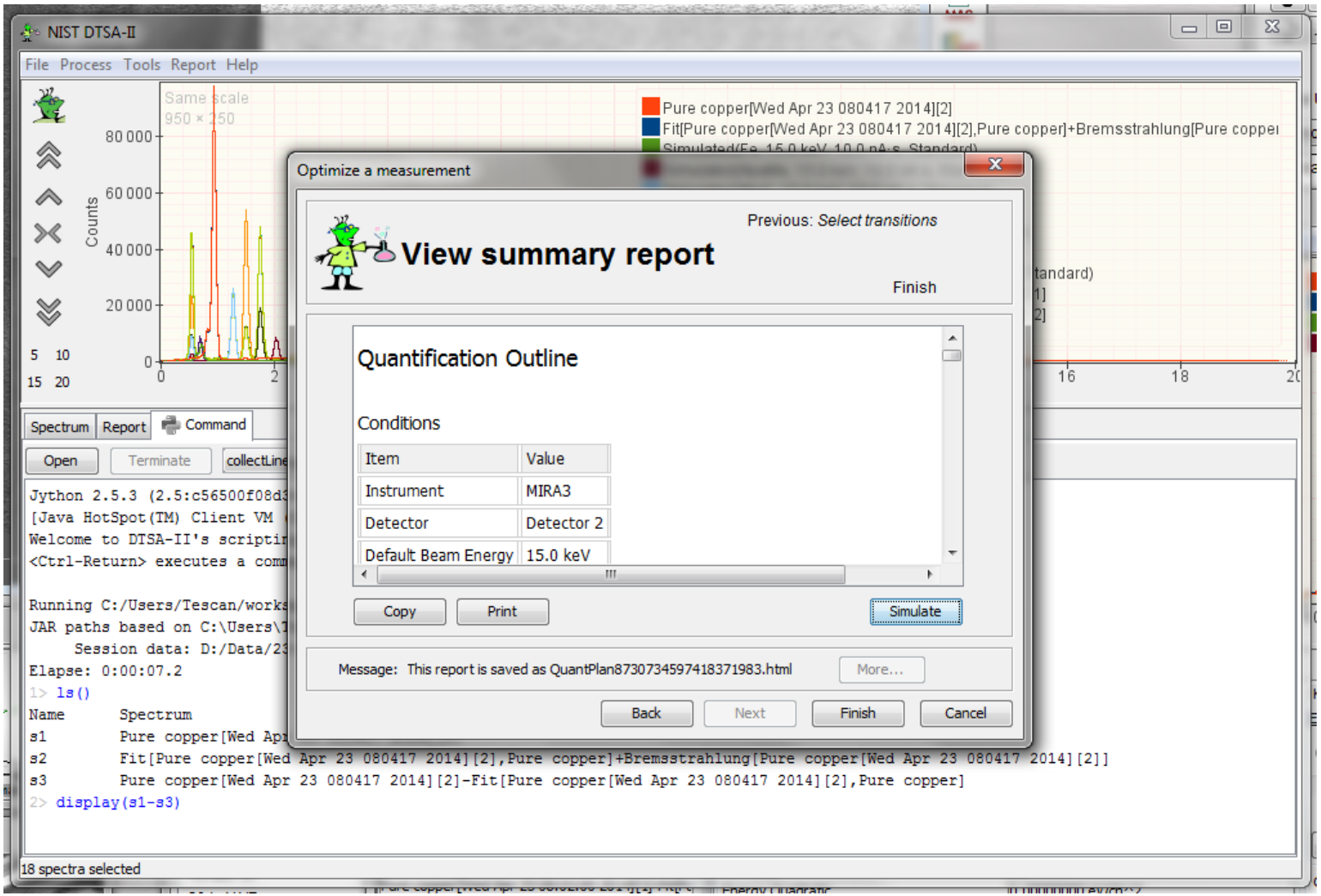

NIST DTSA-II
File Process Tools Report Help
Same scale
950 × 250
Pure copper[Wed Apr 23 080417 2014][2]
Fit[Pure copper[Wed Apr 23 080417 2014][2],Pure copper]+Bremsstrahlung[Pure copper
Counts
80 000
60 000
40 000
20 000
0
Spectrum Report Command
Open Terminate collectLine
Jython 2.5.3 (2.5:c56500f08d3
[Java HotSpot(TM) Client VM
Welcome to DTSA-II's scriptin
<Ctrl-Return> executes a comm
Running C:/Users/Tescan/works
JAR paths based on C:\Users\
Session data: D:/Data/23
Elapse: 0:00:07.2
1> ls()
Name Spectrum
s1 Pure copper[Wed Ap
s2 Fit[Pure copper[Wed Apr 23 080417 2014][2],Pure copper]+Bremsstrahlung[Pure copper[Wed Apr 23 080417 2014][2]]
s3 Pure copper[Wed Apr 23 080417 2014][2]-Fit[Pure copper[Wed Apr 23 080417 2014][2],Pure copper]
2> display(s1-s3)
2 spectra selected.
Optimize a measurement
Previous: Specify a detector
Select standards
Next: Select other element rules
Element Standard Precision
Al Al2O3 0.01
Si SiO2 0.01
Ca Apatite 0.01
Fe Fe 0.01
Remove
Clear
Elements
Material
Precision 0.01
Add
Message: Specify the elements to be measured and the associated standard.
More...
Back Next Finish Cancel


NIST DTSA-II
File Process Tools Report Help
Same scale
950 × 250
Pure copper[Wed Apr 23 080417 2014][2]
Fit[Pure copper[Wed Apr 23 080417 2014][2],Pure copper]+Bremsstrahlung[Pure copper
Counts
80 000
60 000
40 000
20 000
0
Spectrum
Report
Command
Open
Terminate
Jython 2.5.3 (2.5:c56500f08d3
[Java HotSpot(TM) Client VM
Welcome to DTSA-II's scriptin
<Ctrl-Return> executes a comm
Running C:/Users/Tescan/works
JAR paths based on C:\Users\
Session data: D:/Data/23
Elapse: 0:00:07.2
1> ls()
Name Spectrum
s1 Pure copper[Wed Apr
s2 Fit[Pure copper[Wed Apr 23 080417 2014][2],Pure copper]+Bremsstrahlung[Pure copper[Wed Apr 23 080417 2014][2]]
s3 Pure copper[Wed Apr 23 080417 2014][2]-Fit[Pure copper[Wed Apr 23 080417 2014][2],Pure copper]
2> display(s1-s3)
2 spectra selected.
Optimize a measurement
Previous: Select standards
Select other element rules
Next: Select references
Peaks to strip
Elements
Other element rules
No other elements
Element by difference
Hydrogen
Oxygen by stoichiometry
Waters-of-crystallization
Element Cation Anion As
Aluminum 2 3 Al2O3
Silicon 1 2 SiO2
Calcium 1 1 CaO
Iron 1 1 FeO
Message: Specify special processing options.
More...
Back
Next
Finish
Cancel


NIST DTSA-II
File Process Tools Report Help
Same scale
950 × 250
Pure copper[Wed Apr 23 080417 2014][2]
Fit[Pure copper[Wed Apr 23 080417 2014][2],Pure copper]+Bremsstrahlung[Pure copper
Counts
80 000
60 000
40 000
20 000
0
Spectrum
Report
Command
Open
Terminate
Jython 2.5.3 (2.5:c56500f08d3
[Java HotSpot(TM) Client VM
Welcome to DTSA-II's scriptin
<Ctrl-Return> executes a comm
Running C:/Users/Tescan/works
JAR paths based on C:\Users\1
Session data: D:/Data/23
Elapse: 0:00:07.2
1> ls()
Name Spectrum
s1 Pure copper[Wed Apr 23 080417 2014][2]
s2 Fit[Pure copper[Wed Apr 23 080417 2014][2],Pure copper]+Bremsstrahlung[Pure copper[Wed Apr 23 080417 2014][2]]
s3 Pure copper[Wed Apr 23 080417 2014][2]-Fit[Pure copper[Wed Apr 23 080417 2014][2],Pure copper]
2> display(s1-s3)
2 spectra selected.
Optimize a measurement
Previous: Select other element rules
Select references
Next: Specify the unknown
ROI | Material | Standard?
Ca L-family [0.143, 0.... | CaF2 |
O All [0.362, 0.688 keV] | Al2O3 | Yes
Fe L-family [0.469, 0.... | Fe | Yes
Al All [1.305, 1.669 keV] | Al2O3 | Yes
Si All [1.554, 1.953 keV] | SiO2 | Yes
Ca K-family [3.479, 4... | Apatite | Yes
Fe Kα [6.155, 6.653 k... | Fe | Yes
Fe Kβ [6.859, 7.257 k... | Fe | Yes
Material
Apply
Message: You have the option to change the default references.
More...
Back
Next
Finish
Cancel

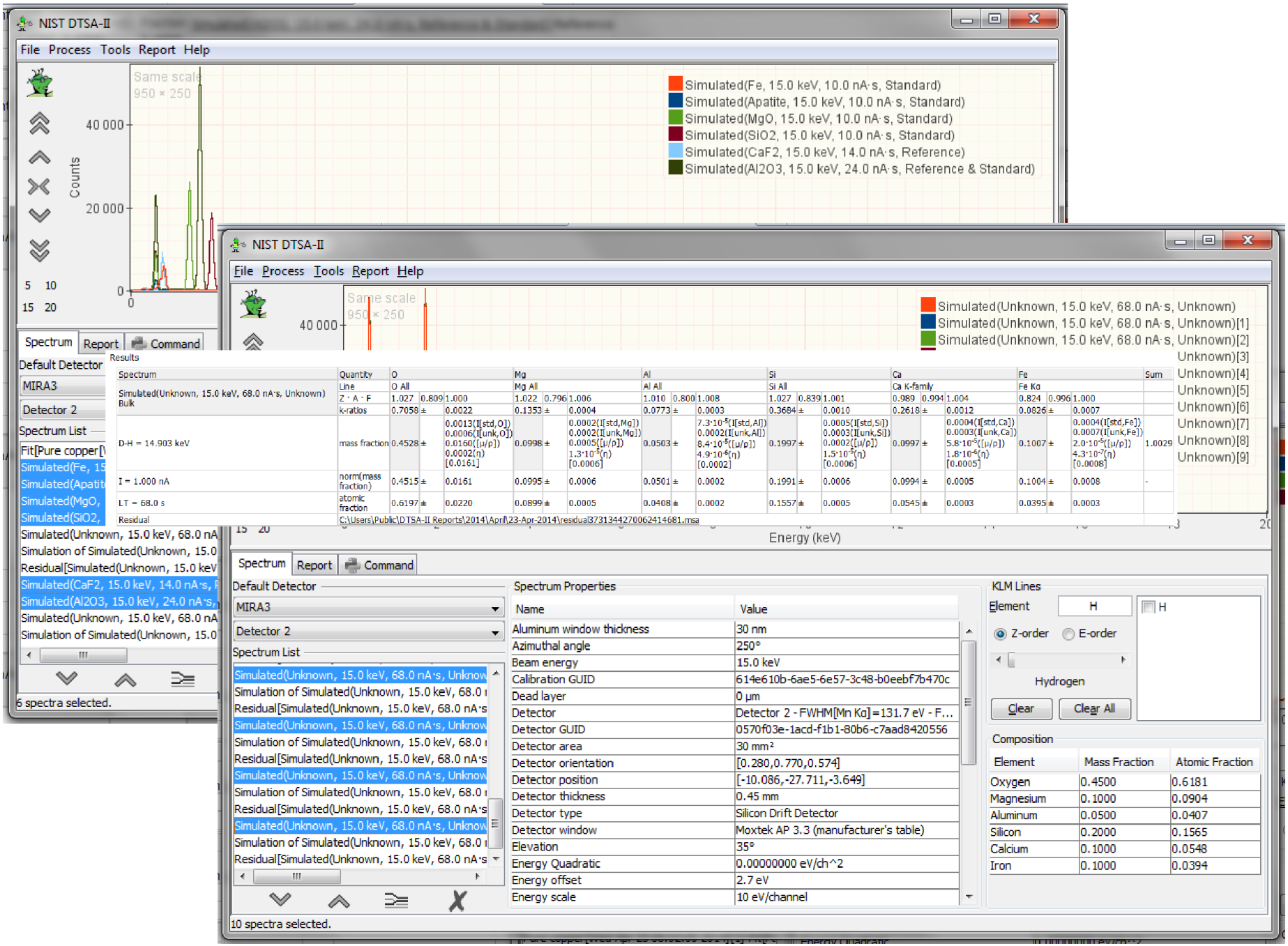

NIST DTSA-II
File Process Tools Report Help
Same scale
950 × 250
Pure copper[Wed Apr 23 080417 2014][2]
Fit[Pure copper[Wed Apr 23 080417 2014][2],Pure copper]+Bremsstrahlung[Pure copper
Counts
80 000
60 000
40 000
20 000
0
Spectrum
Report
Command
Open
Terminate
Optimize a measurement
Material Editor
Material
Name
Unknown
Density
g/cm3 (optional)
Mode
Mass Fractions
Atomic Proportions
Element
Mass Fraction
Atomic Fraction
Oxygen 0.4500 0.6181
Magnesium 0.1000 0.0904
Aluminum 0.0500 0.0407
Silicon 0.2000 0.1565
Calcium 0.1000 0.0548
Iron 0.1000 0.0394
Element:
Quantity: 0%
Add
Delete
Clear
Ok
Cancel
Message:
Back
Next
Finish
Cancel
Jython 2.5.3 (2.5:c56500f08d3
[Java HotSpot(TM) Client VM
Welcome to DTSA-II's scriptin
<Ctrl-Return> executes a comm
Running C:/Users/Tescan/works
JAR paths based on C:\Users\
Session data: D:/Data/23
Elapse: 0:00:07.2
1> ls()
Name Spectrum
s1 Pure copper[Wed Apr
s2 Fit[Pure copper[Wed Apr 23 080417 2014][2],Pure copper]+Bremsstrahlung[Pure copper[Wed Apr 23 080417 2014][2]]
s3 Pure copper[Wed Apr 23 080417 2014][2]-Fit[Pure copper[Wed Apr 23 080417 2014][2],Pure copper]
2> display(s1-s3)
2 spectra selected.


NIST DTSA-II
File Process Tools Report Help
Same scale
950 × 250
Pure copper[Wed Apr 23 080417 2014][2]
Fit[Pure copper[Wed Apr 23 080417 2014][2],Pure copper]+Bremsstrahlung[Pure copper
Counts
80 000
60 000
40 000
20 000
0
Spectrum
Report
Command
Open
Terminate
Jython 2.5.3 (2.5:c56500f08d3
[Java HotSpot(TM) Client VM
Welcome to DTSA-II's scriptir
<Ctrl-Return> executes a comm
Running C:/Users/Tescan/works
JAR paths based on C:\Users\
Session data: D:/Data/23
Elapse: 0:00:07.2
1> ls()
Name Spectrum
s1 Pure copper[Wed Apr
s2 Fit[Pure copper[Wed Apr 23 080417 2014][2],Pure copper]+Bremsstrahlung[Pure copper[Wed Apr 23 080417 2014][2]]
s3 Pure copper[Wed Apr 23 080417 2014][2]-Fit[Pure copper[Wed Apr 23 080417 2014][2],Pure copper]
2> display(s1-s3)
2 spectra selected.
Optimize a measurement
Select transitions
Previous: Specify the unknown
Next: View summary report
Estimated unknown
Unknown
...
Element
ROI
U[combined]
Dose[std]
Dose[unk]
Mg
Mg All [1.076, 1...
0.6 %
10.0 nA·s
68.0 nA·s
Al
Al All [1.305, 1....
0.4 %
24.0 nA·s
68.0 nA·s
Si
Si All [1.554, 1....
0.2 %
10.0 nA·s
68.0 nA·s
Ca
Ca K-family [3.4...
0.3 %
10.0 nA·s
68.0 nA·s
Fe
Fe Kα [6.155, 6...
0.6 %
10.0 nA·s
68.0 nA·s
Message:
More...
Back
Next
Finish
Cancel


NIST DTSA-II
File Process Tools Report Help
Same scale
950 × 250
Counts
80 000
60 000
40 000
20 000
0
Pure copper[Wed Apr 23 080417 2014][2]
Fit[Pure copper[Wed Apr 23 080417 2014][2],Pure copper]+Bremsstrahlung[Pure copper
Spectrum
Report
Command
Open
Terminate
Jython 2.5.3 (2.5:c56500f08d3
[Java HotSpot(TM) Client VM
Welcome to DTSA-II's scriptin
<Ctrl-Return> executes a comm
Running C:/Users/Tescan/works
JAR paths based on C:\Users\
Session data: D:/Data/23
Elapse: 0:00:07.2
1> ls()
Name Spectrum
s1 Pure copper[Wed Ap
s2 Fit[Pure copper[Wed Apr 23 080417 2014][2],Pure copper]+Bremsstrahlung[Pure copper[Wed Apr 23 080417 2014][2]]
s3 Pure copper[Wed Apr 23 080417 2014][2]-Fit[Pure copper[Wed Apr 23 080417 2014][2],Pure copper]
2> display(s1-s3)
18 spectra selected
Optimize a measurement
Previous: Select transitions
View summary report
Finish
Quantification Outline
Conditions
Item
Value
Instrument
MIRA3
Detector
Detector 2
Default Beam Energy
15.0 keV
Copy
Print
Simulate
Message: This report is saved as QuantPlan8730734597418371983.html
More...
Back
Next
Finish
Cancel

Measurement plan

Composition				Beam Energy (keV)	Form	Preparation	Dose (nA·s)	Type
Unknown				15.0	Bulk	Polished to a 50.0 nm finish	68.0	Unknown
Element	Mass Fraction	Mass Fraction (normalized)	Atomic Fraction					
O	0.4500	0.4500	0.6181					
Mg	0.1000	0.1000	0.0904					
Al	0.0500	0.0500	0.0407					
Si	0.2000	0.2000	0.1565					
Ca	0.1000	0.1000	0.0548					
Fe	0.1000	0.1000	0.0394					
CaF2				15.0	Bulk	Polished to a 50.0 nm finish	14.0	Reference
Element	Mass Fraction	Mass Fraction (normalized)	Atomic Fraction					
F	0.4867	0.4867	0.6667					
Ca	0.5133	0.5133	0.3333					
Al2O3				15.0	Bulk	Polished to a 50.0 nm finish	24.0	Reference & Standard
Element	Mass Fraction	Mass Fraction (normalized)	Atomic Fraction					
O	0.4707	0.4707	0.6000					
Al	0.5293	0.5293	0.4000					
MgO				15.0	Bulk	Polished to a 50.0 nm finish	10.0	Standard
Element	Mass Fraction	Mass Fraction (normalized)	Atomic Fraction					
O	0.3970	0.3970	0.5000					
Mg	0.6030	0.6030	0.5000					
SiO2				15.0	Bulk	Polished to a 50.0 nm finish	10.0	Standard
Element	Mass Fraction	Mass Fraction (normalized)	Atomic Fraction					
O	0.5326	0.5326	0.6667					
Si	0.4674	0.4674	0.3333					
Apatite				15.0	Bulk	Polished to a 50.0 nm finish	10.0	Standard
Element	Mass Fraction	Mass Fraction (normalized)	Atomic Fraction					
H	0.0019	0.0019	0.0435					
O	0.3900	0.3900	0.5652					
P	0.2323	0.2323	0.1739					
Ca	0.3758	0.3758	0.2174					
Fe				15.0	Bulk	Polished to a 50.0 nm finish	10.0	Standard
Element	Mass Fraction	Mass Fraction (normalized)	Atomic Fraction					
Fe	1.0000	1.0000	1.0000					


NIST DTSA-II
File Process Tools Report Help
Same scale
950 × 250
Counts
40 000
20 000
0
Simulated(Fe, 15.0 keV, 10.0 nA·s, Standard)
Simulated(Apatite, 15.0 keV, 10.0 nA·s, Standard)
Simulated(MgO, 15.0 keV, 10.0 nA·s, Standard)
Simulated(SiO2, 15.0 keV, 10.0 nA·s, Standard)
Simulated(CaF2, 15.0 keV, 14.0 nA·s, Reference)
Simulated(Al2O3, 15.0 keV, 24.0 nA·s, Reference & Standard)
Spectrum
Report
Command
Default Detector
MIRA3
Detector 2
Spectrum List
Fit[Pure copper[
Simulated(Fe, 15
Simulated(Apatit
Simulated(MgO,
Simulated(SiO2,
Simulated(Unknown, 15.0 keV, 68.0 nA
Simulation of Simulated(Unknown, 15.0
Residual[Simulated(Unknown, 15.0 keV
Simulated(CaF2, 15.0 keV, 14.0 nA·s,
Simulated(Al2O3, 15.0 keV, 24.0 nA·s,
Simulated(Unknown, 15.0 keV, 68.0 nA
Simulation of Simulated(Unknown, 15.0
6 spectra selected.
Simulated(Unknown, 15.0 keV, 68.0 nA·s, Unknown)
Simulated(Unknown, 15.0 keV, 68.0 nA·s, Unknown)[1]
Simulated(Unknown, 15.0 keV, 68.0 nA·s, Unknown)[2]
Unknown)[3]
Unknown)[4]
Unknown)[5]
Unknown)[6]
Unknown)[7]
Unknown)[8]
Unknown)[9]
Results
Spectrum | Quantity | O | Mg | Al | Si | Ca | Fe | Sum
Simulated(Unknown, 15.0 keV, 68.0 nA·s, Unknown) Bulk | Line | O All | Mg All | Al All | Si All | Ca K-family | Fe Kα
Z · A · F | 1.027 0.809 1.000 | 1.022 0.796 1.006 | 1.010 0.800 1.008 | 1.027 0.839 1.001 | 0.989 0.994 1.004 | 0.824 0.996 1.000
k-ratios | 0.7058 ± 0.0022 | 0.1353 ± 0.0004 | 0.0773 ± 0.0003 | 0.3684 ± 0.0010 | 0.2618 ± 0.0012 | 0.0826 ± 0.0007
D-H = 14.903 keV | mass fraction | 0.4528 ± 0.0013(I[std,O]) 0.0006(I[unk,O]) 0.0160([μ/ρ]) 0.0002(η) [0.0161] | 0.0998 ± 0.0002(I[std,Mg]) 0.0002(I[unk,Mg]) 0.0005([μ/ρ]) 1.3·10⁻⁵(η) [0.0006] | 0.0503 ± 7.3·10⁻⁵(I[std,Al]) 0.0002(I[unk,Al]) 8.4·10⁻⁵([μ/ρ]) 4.9·10⁻⁶(η) [0.0002] | 0.1997 ± 0.0005(I[std,Si]) 0.0003(I[unk,Si]) 0.0002([μ/ρ]) 1.5·10⁻⁵(η) [0.0006] | 0.0997 ± 0.0004(I[std,Ca]) 0.0003(I[unk,Ca]) 5.8·10⁻⁵([μ/ρ]) 1.8·10⁻⁶(η) [0.0005] | 0.1007 ± 0.0004(I[std,Fe]) 0.0007(I[unk,Fe]) 2.0·10⁻⁵([μ/ρ]) 4.3·10⁻⁷(η) [0.0008] | 1.0029
I = 1.000 nA | norm(mass fraction) | 0.4515 ± 0.0161 | 0.0995 ± 0.0006 | 0.0501 ± 0.0002 | 0.1991 ± 0.0006 | 0.0994 ± 0.0005 | 0.1004 ± 0.0008 | -
LT = 68.0 s | atomic fraction | 0.6197 ± 0.0220 | 0.0899 ± 0.0005 | 0.0408 ± 0.0002 | 0.1557 ± 0.0005 | 0.0545 ± 0.0003 | 0.0395 ± 0.0003
Residual | C:\Users\Public\DTSA-II Reports\2014\April\23-Apr-2014\residual3731344270062414681.msa
Energy (keV)
Spectrum
Report
Command
Default Detector
MIRA3
Detector 2
Spectrum List
Simulated(Unknown, 15.0 keV, 68.0 nA·s, Unknow
Simulation of Simulated(Unknown, 15.0 keV, 68.0
Residual[Simulated(Unknown, 15.0 keV, 68.0 nA·s
Simulated(Unknown, 15.0 keV, 68.0 nA·s, Unknow
Simulation of Simulated(Unknown, 15.0 keV, 68.0
Residual[Simulated(Unknown, 15.0 keV, 68.0 nA·s
Simulated(Unknown, 15.0 keV, 68.0 nA·s, Unknow
Simulation of Simulated(Unknown, 15.0 keV, 68.0
Residual[Simulated(Unknown, 15.0 keV, 68.0 nA·s
Simulated(Unknown, 15.0 keV, 68.0 nA·s, Unknow
Simulation of Simulated(Unknown, 15.0 keV, 68.0
Residual[Simulated(Unknown, 15.0 keV, 68.0 nA·s
10 spectra selected.
Spectrum Properties
Name | Value
Aluminum window thickness | 30 nm
Azimuthal angle | 250°
Beam energy | 15.0 keV
Calibration GUID | 614e610b-6ae5-6e57-3c48-b0eebf7b470c
Dead layer | 0 μm
Detector | Detector 2 - FWHM[Mn Kα] = 131.7 eV - F...
Detector GUID | 0570f03e-1acd-f1b1-80b6-c7aad8420556
Detector area | 30 mm²
Detector orientation | [0.280,0.770,0.574]
Detector position | [-10.086,-27.711,-3.649]
Detector thickness | 0.45 mm
Detector type | Silicon Drift Detector
Detector window | Moxtek AP 3.3 (manufacturer's table)
Elevation | 35°
Energy Quadratic | 0.00000000 eV/ch^2
Energy offset | 2.7 eV
Energy scale | 10 eV/channel
KLM Lines
Element
H
Z-order
E-order
Hydrogen
Clear
Clear All
Composition
Element | Mass Fraction | Atomic Fraction
Oxygen | 0.4500 | 0.6181
Magnesium | 0.1000 | 0.0904
Aluminum | 0.0500 | 0.0407
Silicon | 0.2000 | 0.1565
Calcium | 0.1000 | 0.0548
Iron | 0.1000 | 0.0394

Name	O	Mg	Al	Si	Ca	Fe
Simulated(Unknown, 15.0 keV, 68.0 nA·s, Unknown)	45.28	9.98	5.03	19.97	9.97	10.07
Simulated(Unknown, 15.0 keV, 68.0 nA·s, Unknown)[1]	45.41	10.01	5.02	19.97	10.08	10.01
Simulated(Unknown, 15.0 keV, 68.0 nA·s, Unknown)[2]	45.00	9.94	4.99	19.93	10.03	9.90
Simulated(Unknown, 15.0 keV, 68.0 nA·s, Unknown)[3]	45.16	9.95	4.98	19.93	9.97	9.95
Simulated(Unknown, 15.0 keV, 68.0 nA·s, Unknown)[4]	45.06	9.96	5.02	19.92	9.96	9.92
Simulated(Unknown, 15.0 keV, 68.0 nA·s, Unknown)[5]	45.38	9.92	5.02	19.96	10.00	9.95
Simulated(Unknown, 15.0 keV, 68.0 nA·s, Unknown)[6]	45.10	9.96	5.00	19.92	10.00	9.82
Simulated(Unknown, 15.0 keV, 68.0 nA·s, Unknown)[7]	45.23	10.01	5.01	19.97	9.99	9.98
Simulated(Unknown, 15.0 keV, 68.0 nA·s, Unknown)[8]	45.27	9.98	5.02	19.95	10.02	10.06
Simulated(Unknown, 15.0 keV, 68.0 nA·s, Unknown)[9]	45.51	10.00	5.05	20.02	10.09	9.91
Average	45.24	9.97	5.01	19.95	10.01	9.96
Std. Dev.	0.1535	0.0274	0.0179	0.0297	0.0427	0.0702
Fractional	0.34%	0.27%	0.36%	0.15%	0.43%	0.71%