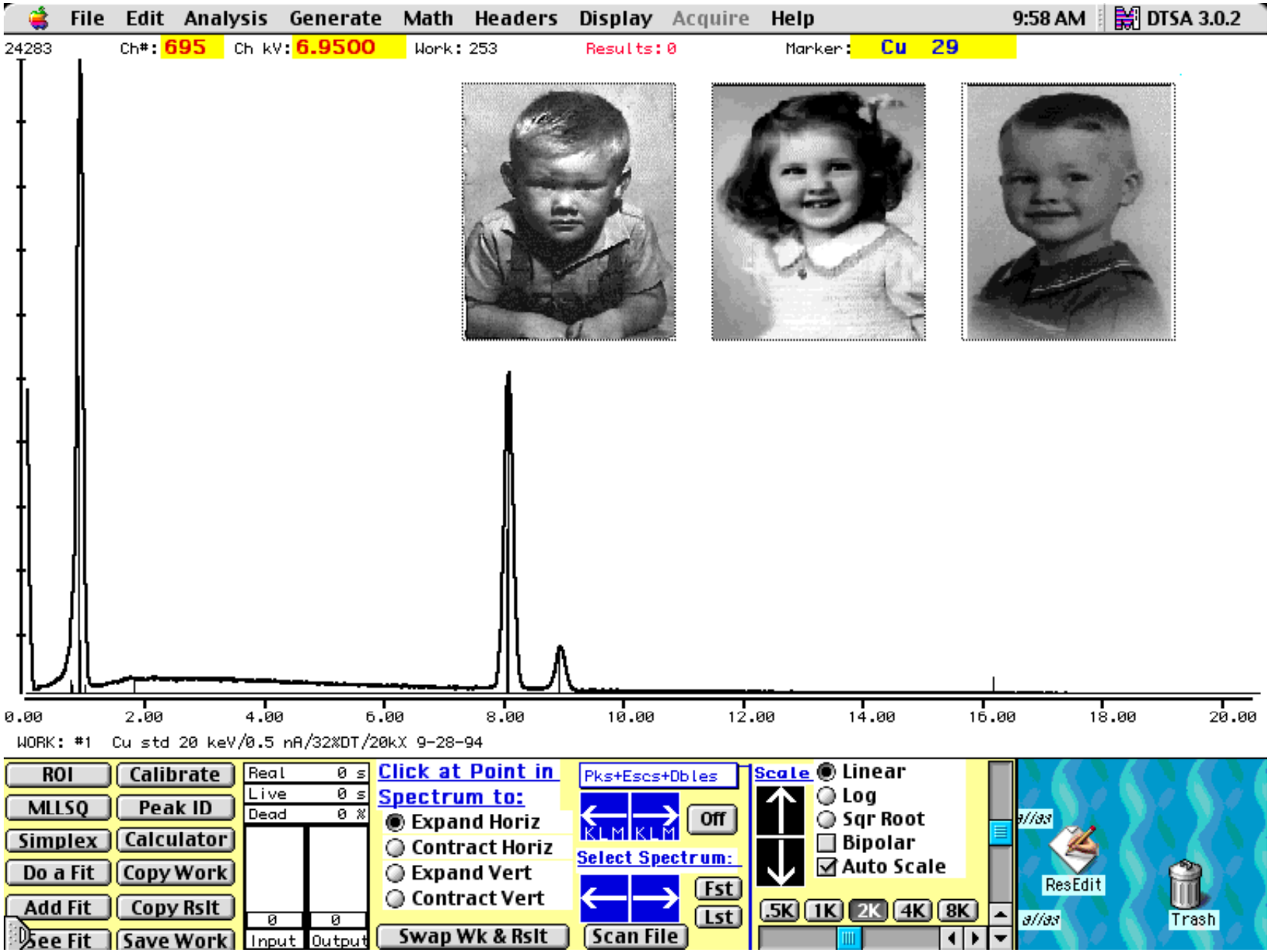
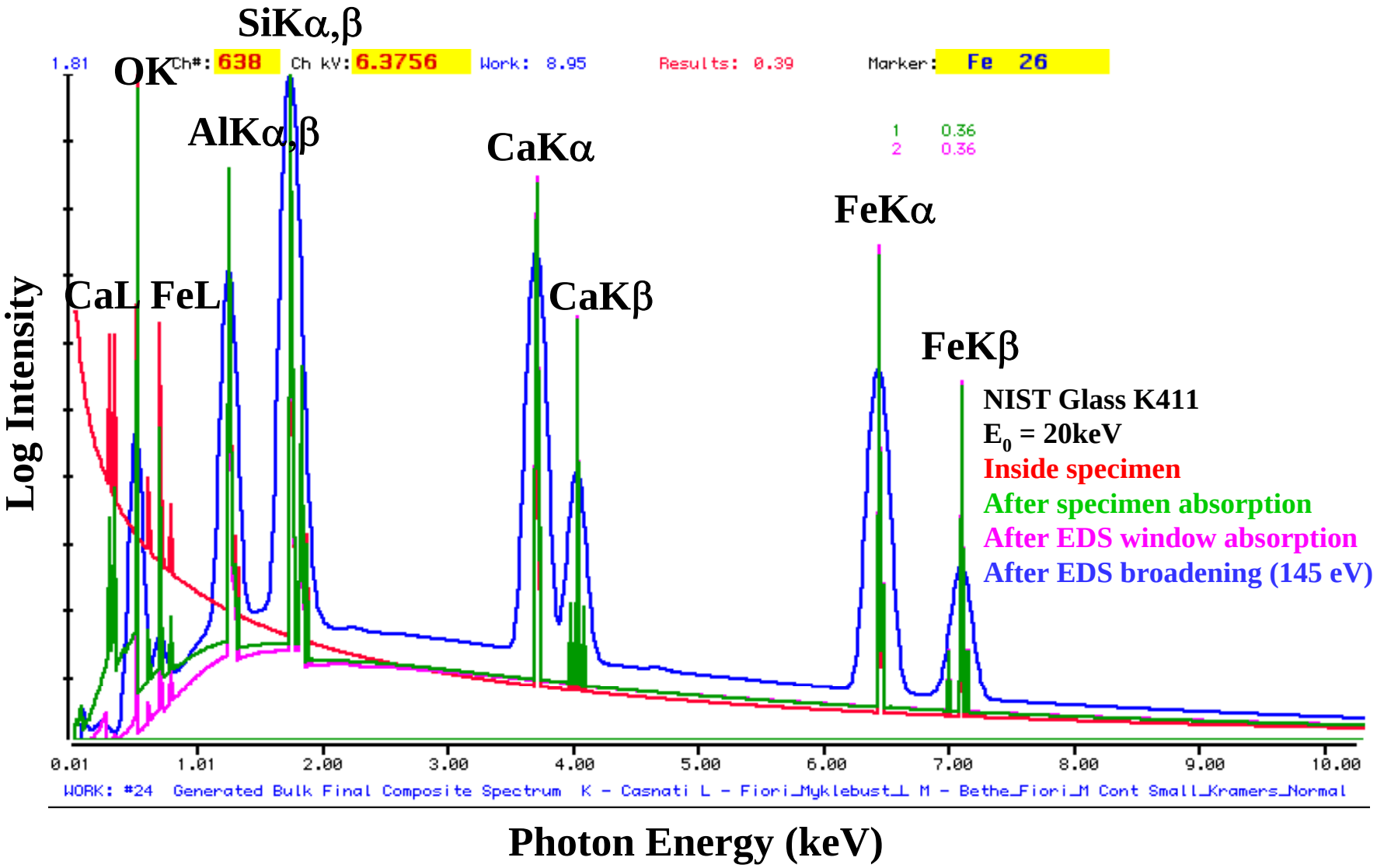
# NIST DTSA-II ("Son of DTSA"): Step-by-Step

Dale E. Newbury (grateful user)
National Institute of Standards and Technology
Gaithersburg, MD 20899-8370

# NIST-NIH Desktop Spectrum Analyzer (DTSA)



# Spectral Simulation with DTSA




**For 16 years, I have heard: "When will you have DTSA for the pc?"**

# NIST DTSA-II

- Created by Nicholas Ritchie of NIST (nicholas.ritchie@nist.gov), inspired by NIST-NIH Desktop Spectrum Analyzer (DTSA) invented 1990-92 by Chuck Fiori (NIH and NIST) and Carol Swyt-Thomas (NIH), and then further developed by Carol and Bob Myklebust (NIST).

# NIST DTSA-II

- Created by Nicholas Ritchie of NIST (nicholas.ritchie@nist.gov), inspired by NIST-NIH Desktop Spectrum Analyzer (DTSA) invented 1990-92 by Chuck Fiori (NIH and NIST) and Carol Swyt-Thomas (NIH), and then further developed by Carol and Bob Myklebust (NIST).
- DTSA ran only on Macintosh, and then only up to system 10. (New Macs won't run DTSA) A painful question heard many, many times: **When will you have DTSA for the pc? DTSA-II is the long awaited answer!!**

# NIST DTSA-II

- Created by Nicholas Ritchie of NIST (nicholas.ritchie@nist.gov), inspired by NIST-NIH Desktop Spectrum Analyzer (DTSA) invented 1990-92 by Chuck Fiori (NIH and NIST) and Carol Swyt-Thomas (NIH), and then further developed by Carol and Bob Myklebust (NIST).
- DTSA ran only on Macintosh, and then only up to system 9. (New Macs won't run DTSA) A painful question heard many, many times: **When will you have DTSA for the pc?** DTSA-II is the long awaited answer!!
- DTSA-II is written in Java and operates on Mac, pc, UNIX, Linux.

# NIST DTSA-II

- Created by Nicholas Ritchie of NIST (nicholas.ritchie@nist.gov), inspired by NIST-NIH Desktop Spectrum Analyzer (DTSA) invented 1990-92 by Chuck Fiori (NIH and NIST) and Carol Swyt-Thomas (NIH), and then further developed by Carol and Bob Myklebust (NIST).
- DTSA ran only on Macintosh, and then only up to system 10. (New Macs won't run DTSA) A painful question heard many, many times: **When will you have DTSA for the pc?** DTSA-II is the long awaited answer!!
- DTSA-II is written in Java and operates on Mac, pc, UNIX, Linux.
- DTSA-II is **NOT** DTSA! Nicholas started from scratch and used DTSA as a guide to develop DTSA-II.

# NIST DTSA-II

- Created by Nicholas Ritchie of NIST (nicholas.ritchie@nist.gov), inspired by NIST-NIH Desktop Spectrum Analyzer (DTSA) invented 1990-92 by Chuck Fiori (NIH and NIST) and Carol Swyt-Thomas (NIH), and then further developed by Carol and Bob Myklebust (NIST).
- DTSA ran only on Macintosh, and then only up to system 10. (New Macs won't run DTSA) A painful question heard many, many times: **When will you have DTSA for the pc?** DTSA-II is the long awaited answer!!
- DTSA-II is written in Java and operates on Mac, pc, UNIX, Linux.
- DTSA-II is **NOT** DTSA! Nicholas started from scratch and used DTSA as a guide to develop DTSA-II.
- DTSA-II is being continually improved and the latest version can be downloaded for free at **http://www.cstl.nist.gov/div837/837.02/epq/dtsa2/index.html**

NIST DTSA-II - Windows Internet Explorer

http://www.cstl.nist.gov/div837/837.02/epq/dtsa2/index.html

File Edit View Favorites Tools Help

Chemical Science and Technology Laboratory

Surface and Microanalysis Science Division

NIST National Institute of Standards and Technology

# DTSA-II

Son of DeskTop Spectrum Analyzer

Geeky scientist in lab coat

## INTRODUCTION

DTSA-II is a multiplatform software package for quantitative x-ray microanalysis. DTSA-II was inspired by the popular Desktop Spectrum Analyzer (DTSA) package developed by Chuck Fiori, Carol Swyt-Thomas, and Bob Myklebust at NIST and NIH in the '80's and early '90's.

DTSA-II has being designed with the goal of making standards-based microanalysis more accessible for the novice microanalyst. *We want to encourage standards-based analysis by making it as easy as possible to get reliable results.* Many operations which had previously required user intervention under DTSA now are performed entirely by the software. Furthermore, the software attempts to guide the user step-by-step through common processes while performing quality control sanity checks. While this might not provide the flexibility that some sophisticated users may desire, we feel that this philosophy is more consistent with the way laboratories are moving towards technicians responsible for multiple techniques and away from experts in single techiques. We encourage users who desire the additional power and flexibility available in the EPQ library to learn to script using Jython or to create their own alternative user interface. EPQ is much more capable than the fraction exposed via DTSA-II.

DTSA-II is based on an entirely new code base written by Nicholas W. M. Ritchie. The codebase has been carefully divided into a shared algorithm library which forms the basis for a handful of software products and a user interface shell. DTSA-II is the user interface shell and the EPQ library is the algorithm library.







Done Local intranet 100%

Start 9:04 AM

# NIST DTSA-II

- Created by Nicholas Ritchie of NIST (nicholas.ritchie@nist.gov), inspired by NIST-NIH Desktop Spectrum Analyzer (DTSA) invented 1990-92 by Chuck Fiori (NIH and NIST) and Carol Swyt-Thomas (NIH), and then further developed by Carol and Bob Myklebust (NIST).
- DTSA ran only on Macintosh, and then only up to system 10. (New Macs won't run DTSA) A painful question heard many, many times: **When will you have DTSA for the pc?** DTSA-II is the long awaited answer.
- DTSA-II is written in Java and operates on Mac, pc, UNIX, Linux.
- DTSA-II is **NOT** DTSA! Nicholas started from scratch and used DTSA as a guide to develop DTSA-II.
- DTSA-II is being continually improved and the latest version can be downloaded for free at **http://www.cstl.nist.gov/div837/837.02/epq/dtsa2/index.html**
- Tools currently embedded in DTSA-II:

# MAJOR FEATURES:

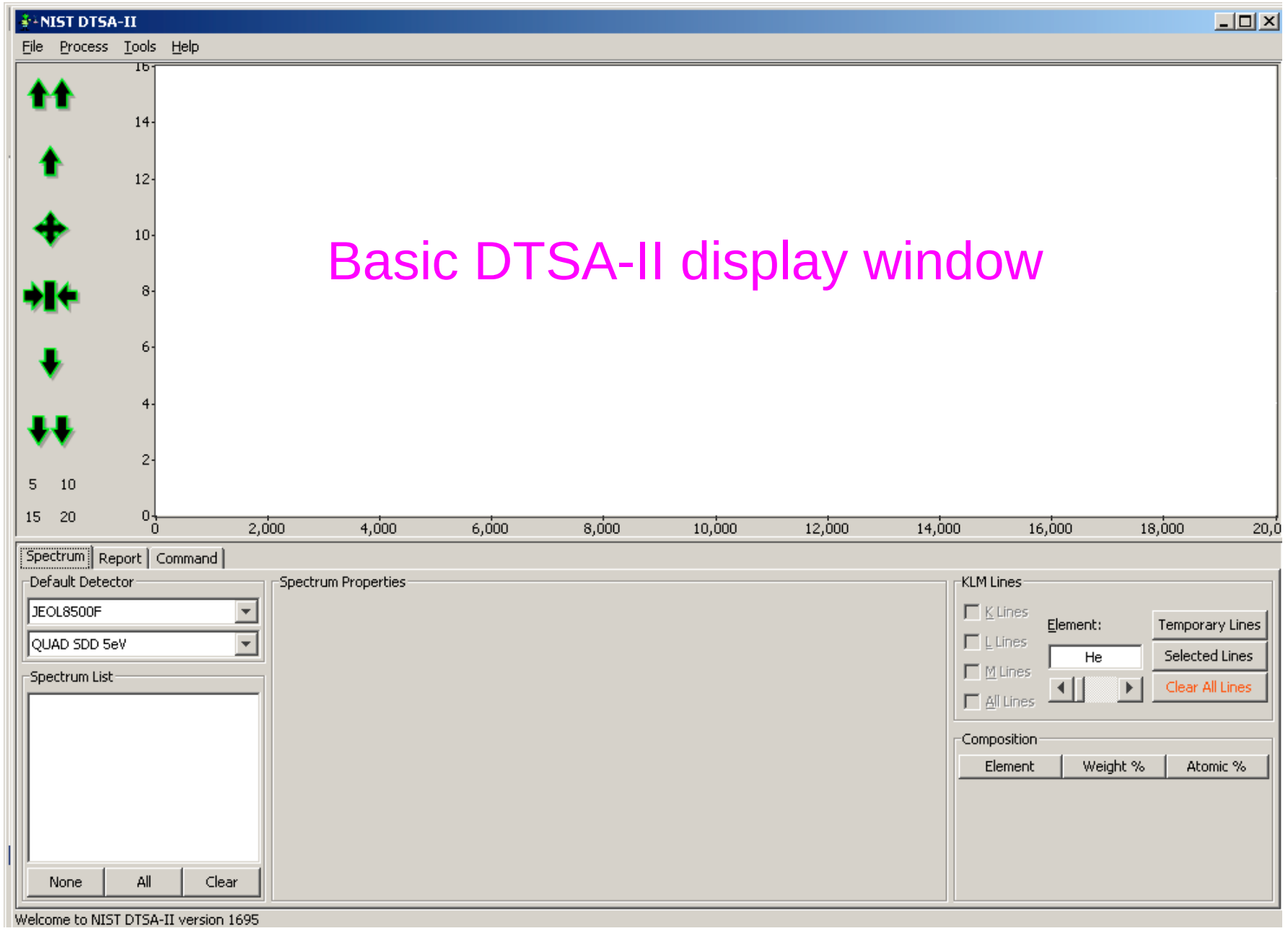
## Basic IO and Display

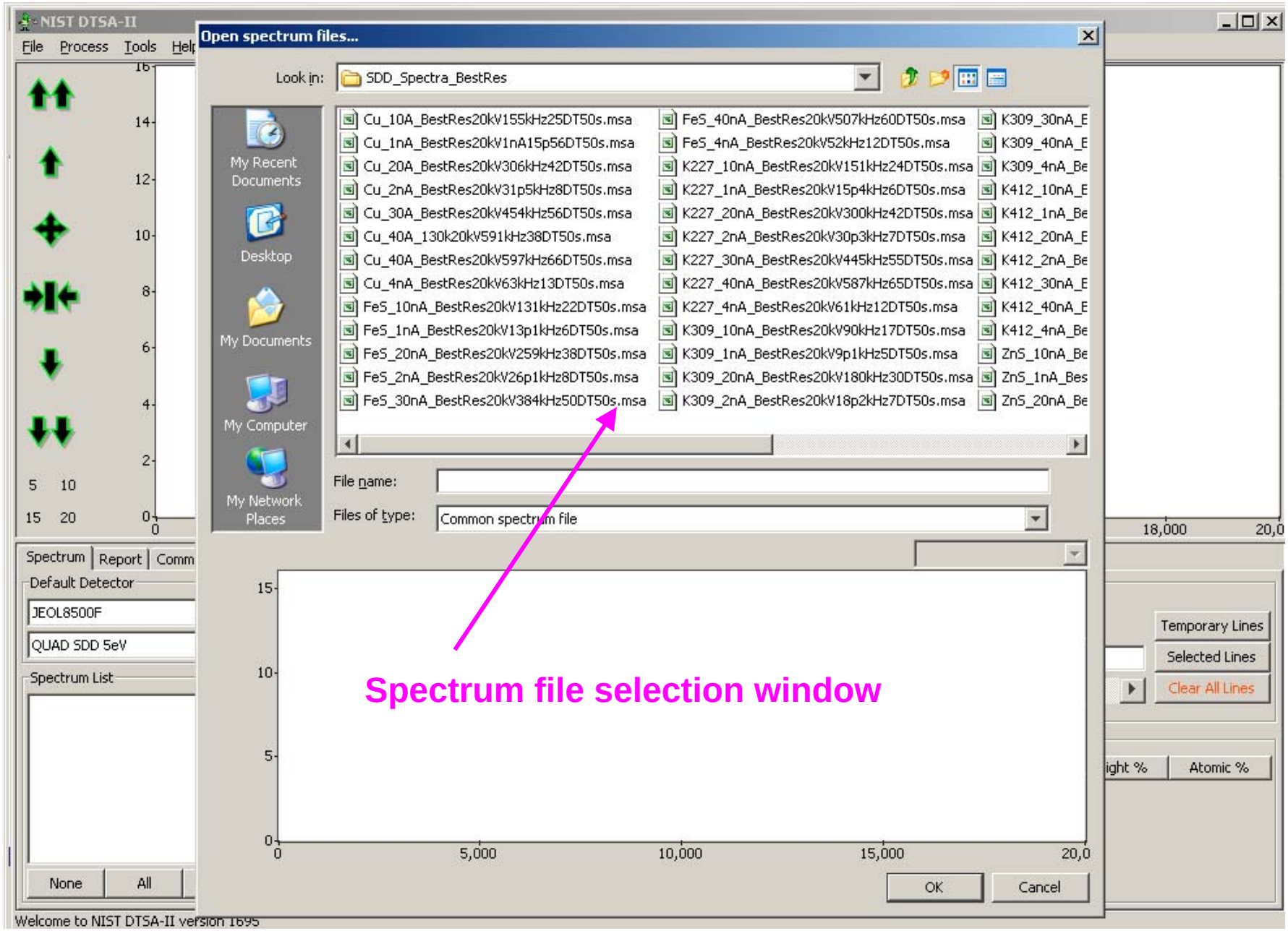
- Read energy dispersive x-ray spectra in a variety of different commercial and non-commercial formats including the industry standard EMSA format
- Display and overlay spectra with various scaling options on linear/log/sqrt axes
- Copy/save/print the spectrum display as a bitmap/PNG file
- Output the spectra as a GNUPlot file for publication quality output
- Overlay labeled x-ray emission lines and x-ray absorption edges
- Define and integrate regions-of-interest
- View spectrum contextual information
- Archive spectra to a searchable database
- Sub-sampling of spectral data to simulate shorter acquisition times

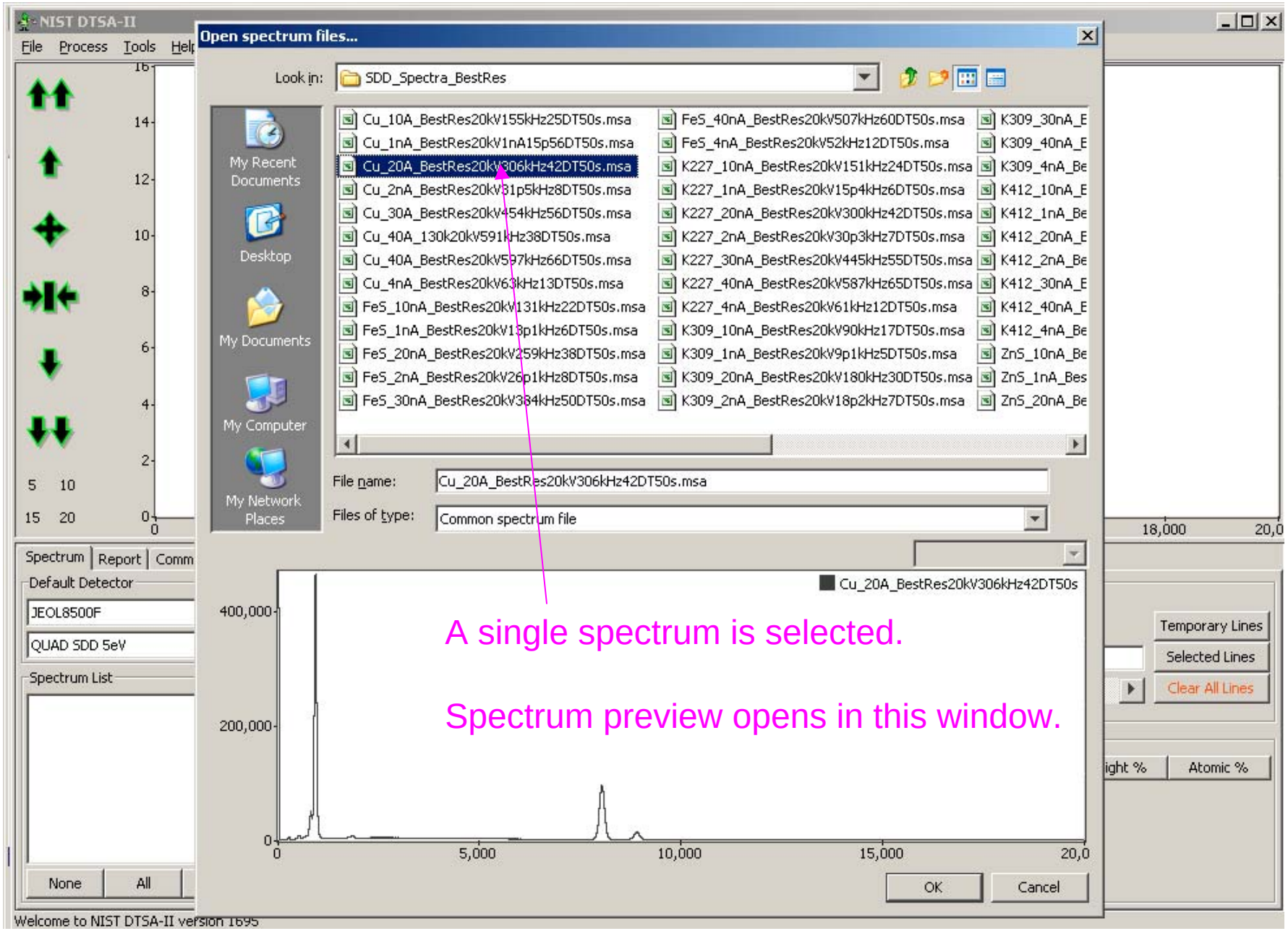
# Basic operations

- Opening and manipulating spectral files

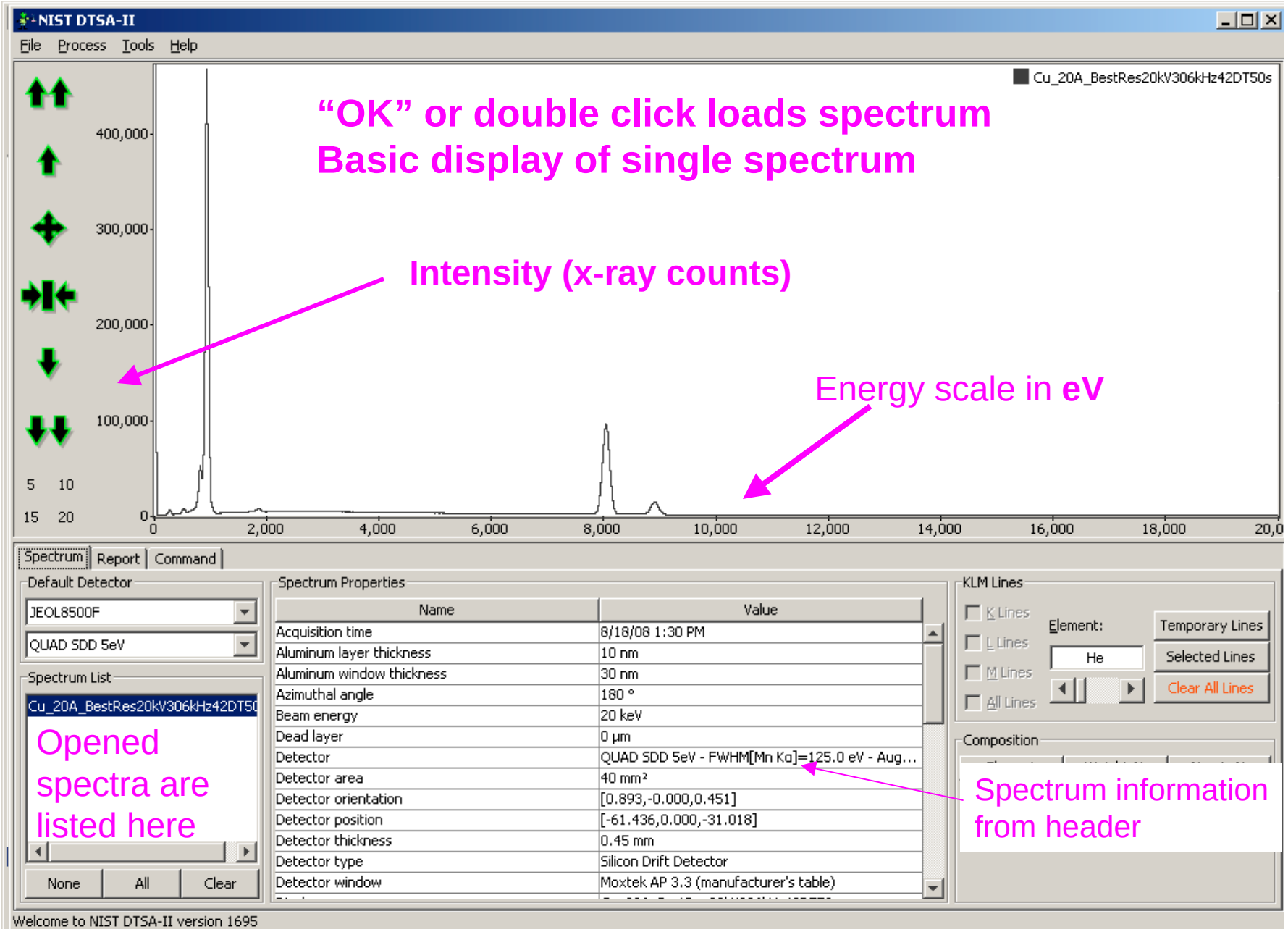
## Display and overlay spectra with various scaling options on linear/log/sqrt axes



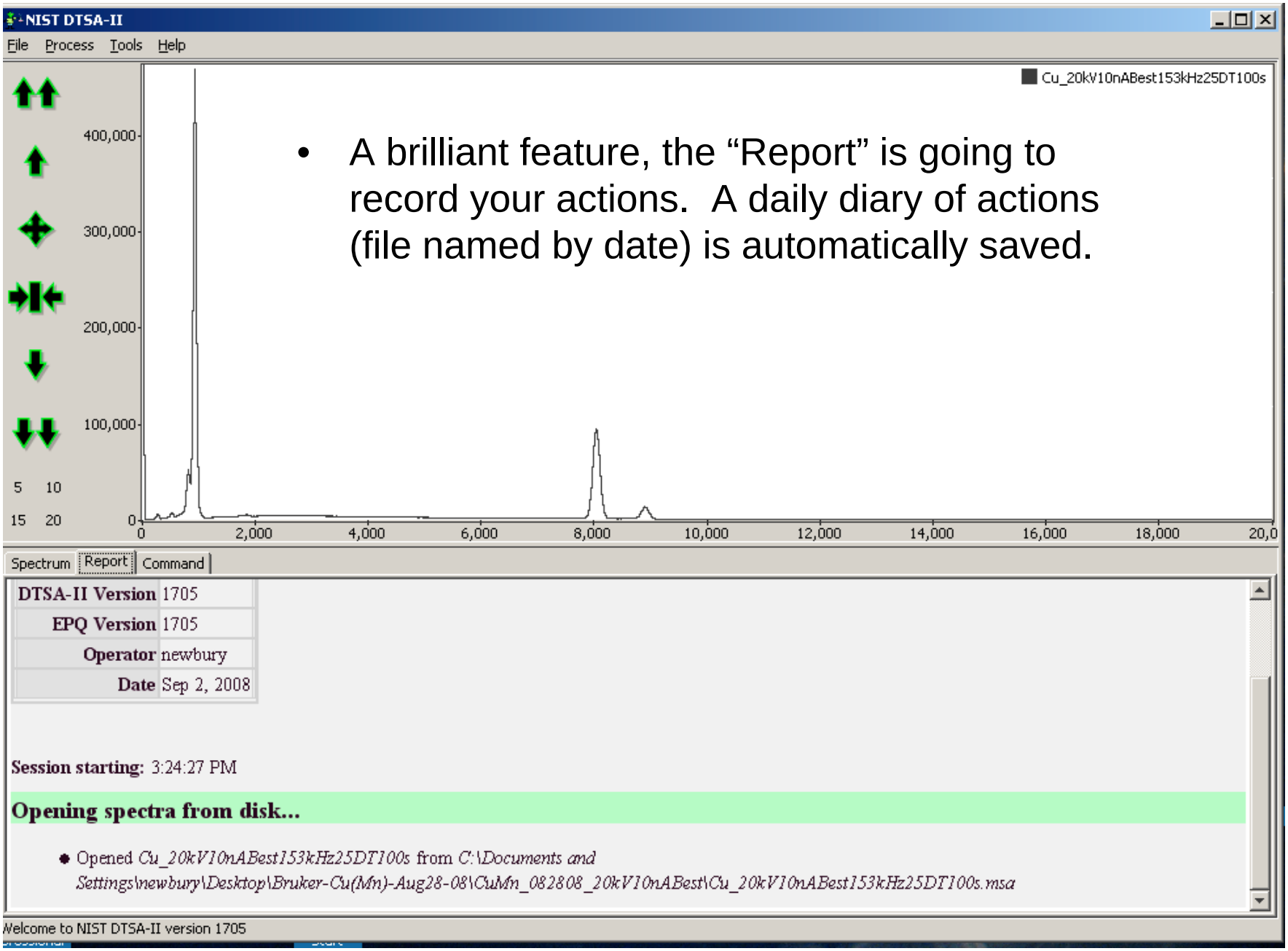

NIST DTSA-II
File Process Tools Help
Open spectrum files...
Look in: SDD_Spectra_BestRes
My Recent Documents
Desktop
My Documents
My Computer
My Network Places
Cu_10A_BestRes20kV155kHz25DT50s.msa
Cu_1nA_BestRes20kV1nA15p56DT50s.msa
Cu_20A_BestRes20kV306kHz42DT50s.msa
Cu_2nA_BestRes20kV31p5kHz8DT50s.msa
Cu_30A_BestRes20kV454kHz56DT50s.msa
Cu_40A_130k20kV591kHz38DT50s.msa
Cu_40A_BestRes20kV597kHz66DT50s.msa
Cu_4nA_BestRes20kV63kHz13DT50s.msa
FeS_10nA_BestRes20kV131kHz22DT50s.msa
FeS_1nA_BestRes20kV13p1kHz6DT50s.msa
FeS_20nA_BestRes20kV259kHz38DT50s.msa
FeS_2nA_BestRes20kV26p1kHz8DT50s.msa
FeS_30nA_BestRes20kV384kHz50DT50s.msa
FeS_40nA_BestRes20kV507kHz60DT50s.msa
FeS_4nA_BestRes20kV52kHz12DT50s.msa
K227_10nA_BestRes20kV151kHz24DT50s.msa
K227_1nA_BestRes20kV15p4kHz6DT50s.msa
K227_20nA_BestRes20kV300kHz42DT50s.msa
K227_2nA_BestRes20kV30p3kHz7DT50s.msa
K227_30nA_BestRes20kV445kHz55DT50s.msa
K227_40nA_BestRes20kV587kHz65DT50s.msa
K227_4nA_BestRes20kV61kHz12DT50s.msa
K309_10nA_BestRes20kV90kHz17DT50s.msa
K309_1nA_BestRes20kV9p1kHz5DT50s.msa
K309_20nA_BestRes20kV180kHz30DT50s.msa
K309_2nA_BestRes20kV18p2kHz7DT50s.msa
K309_30nA_E
K309_40nA_E
K309_4nA_Be
K412_10nA_E
K412_1nA_Be
K412_20nA_E
K412_2nA_Be
K412_30nA_E
K412_40nA_E
K412_4nA_Be
ZnS_10nA_Be
ZnS_1nA_Bes
ZnS_20nA_Be
File name:
Files of type: Common spectrum file
OK
Cancel
Spectrum file selection window
Spectrum Report Comm
Default Detector
JEOL8500F
QUAD SDD 5eV
Spectrum List
None All
Temporary Lines
Selected Lines
Clear All Lines
Atomic %
Welcome to NIST DTSA-II version 1695


NIST DTSA-II
File Process Tools Help
Open spectrum files...
Look in: SDD_Spectra_BestRes
My Recent Documents
Desktop
My Documents
My Computer
My Network Places
Cu_10A_BestRes20kV155kHz25DT50s.msa
Cu_1nA_BestRes20kV1nA15p56DT50s.msa
Cu_20A_BestRes20kV306kHz42DT50s.msa
Cu_2nA_BestRes20kV31p5kHz8DT50s.msa
Cu_30A_BestRes20kV454kHz56DT50s.msa
Cu_40A_130k20kV591kHz38DT50s.msa
Cu_40A_BestRes20kV597kHz66DT50s.msa
Cu_4nA_BestRes20kV63kHz13DT50s.msa
FeS_10nA_BestRes20kV131kHz22DT50s.msa
FeS_1nA_BestRes20kV13p1kHz6DT50s.msa
FeS_20nA_BestRes20kV259kHz38DT50s.msa
FeS_2nA_BestRes20kV26p1kHz8DT50s.msa
FeS_30nA_BestRes20kV384kHz50DT50s.msa
FeS_40nA_BestRes20kV507kHz60DT50s.msa
FeS_4nA_BestRes20kV52kHz12DT50s.msa
K227_10nA_BestRes20kV151kHz24DT50s.msa
K227_1nA_BestRes20kV15p4kHz6DT50s.msa
K227_20nA_BestRes20kV300kHz42DT50s.msa
K227_2nA_BestRes20kV30p3kHz7DT50s.msa
K227_30nA_BestRes20kV445kHz55DT50s.msa
K227_40nA_BestRes20kV587kHz65DT50s.msa
K227_4nA_BestRes20kV61kHz12DT50s.msa
K309_10nA_BestRes20kV90kHz17DT50s.msa
K309_1nA_BestRes20kV9p1kHz5DT50s.msa
K309_20nA_BestRes20kV180kHz30DT50s.msa
K309_2nA_BestRes20kV18p2kHz7DT50s.msa
K309_30nA_E
K309_40nA_E
K309_4nA_Be
K412_10nA_E
K412_1nA_Be
K412_20nA_E
K412_2nA_Be
K412_30nA_E
K412_40nA_E
K412_4nA_Be
ZnS_10nA_Be
ZnS_1nA_Bes
ZnS_20nA_Be
File name: Cu_20A_BestRes20kV306kHz42DT50s.msa
Files of type: Common spectrum file
Cu_20A_BestRes20kV306kHz42DT50s
400,000
200,000
0
0
5,000
10,000
15,000
20,0
A single spectrum is selected.
Spectrum preview opens in this window.
OK
Cancel
Spectrum
Report
Default Detector
JEOL8500F
QUAD SDD 5eV
Spectrum List
None
All
Temporary Lines
Selected Lines
Clear All Lines
Atomic %
18,000
20,0
Welcome to NIST DTSA-II version 1695

# Display and overlay spectra with various scaling options on linear/log/sqrt axes



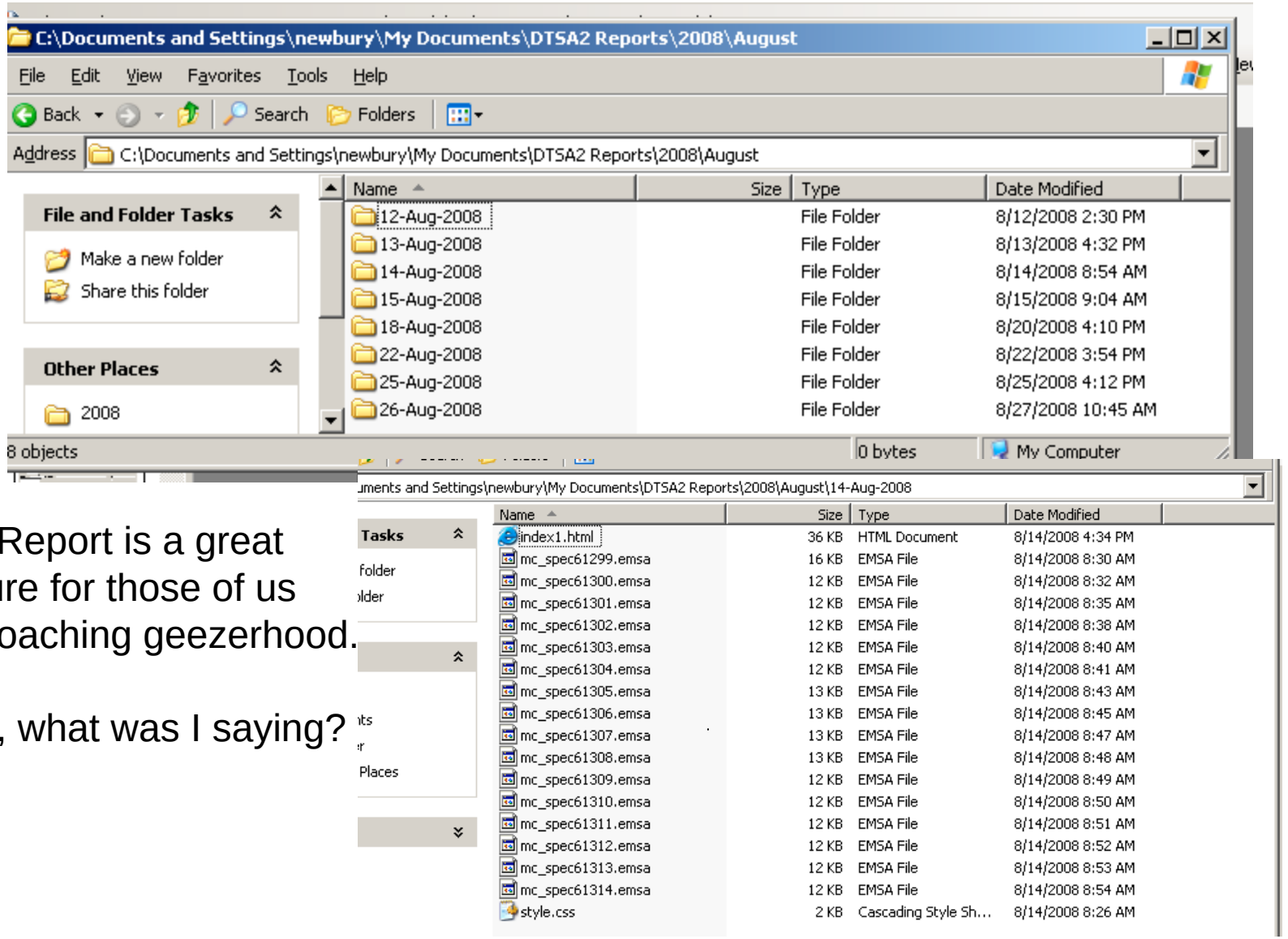
# But wait!




- A brilliant feature, the “Report” is going to record your actions. A daily diary of actions (file named by date) is automatically saved.

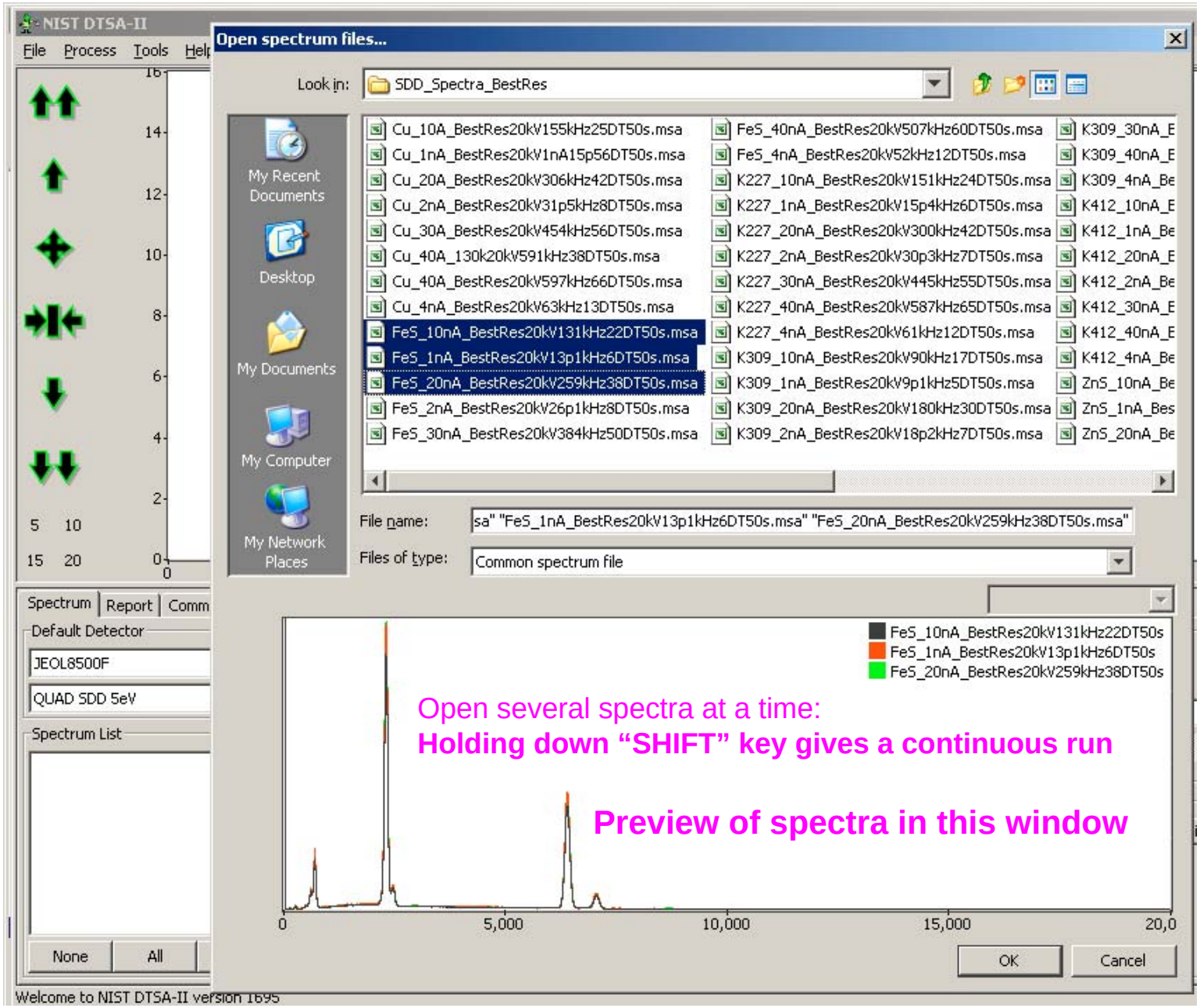
# But wait!

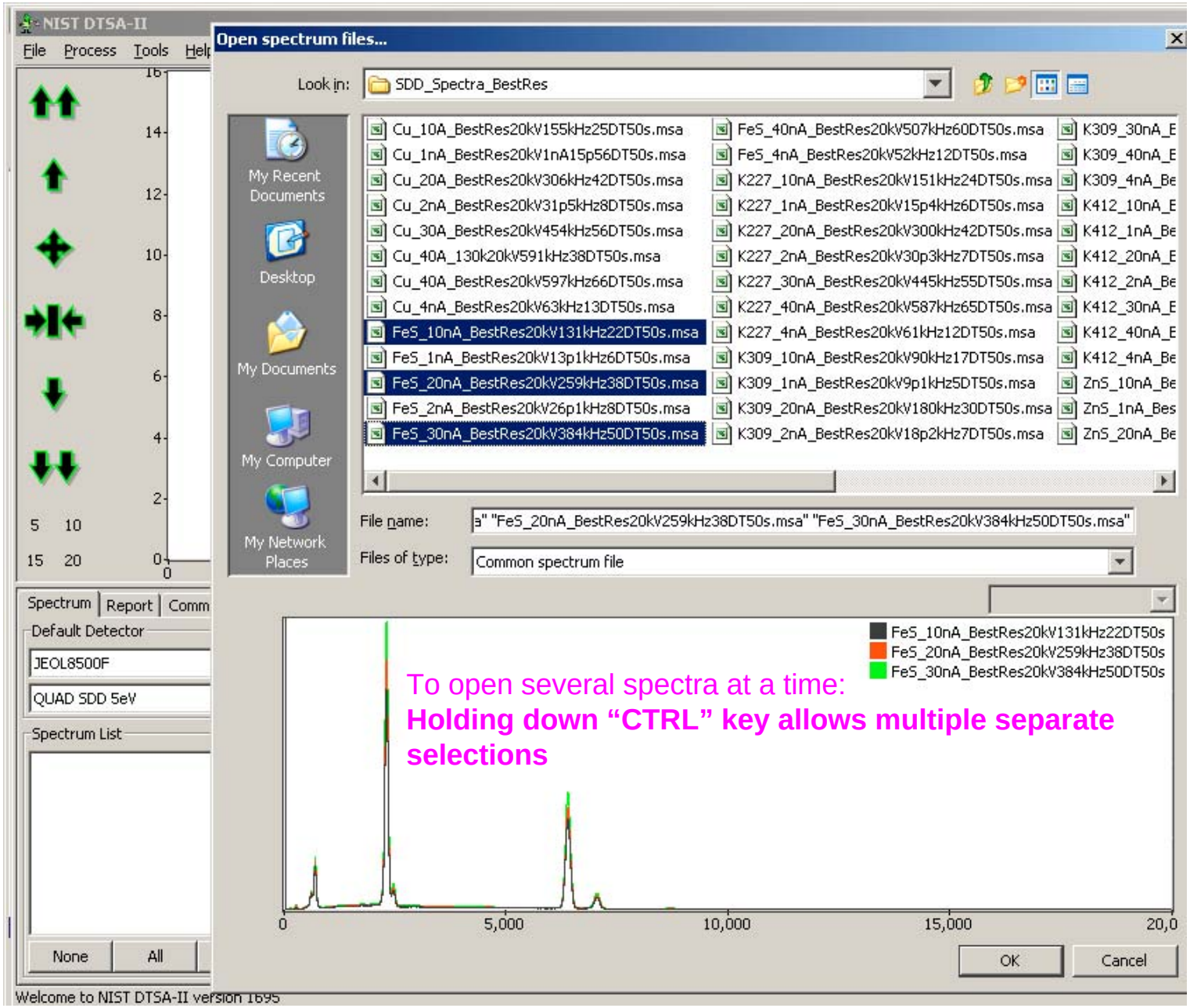
- A brilliant feature, the “Report” is going to record your actions. A daily diary of actions (file named by date) is automatically saved.

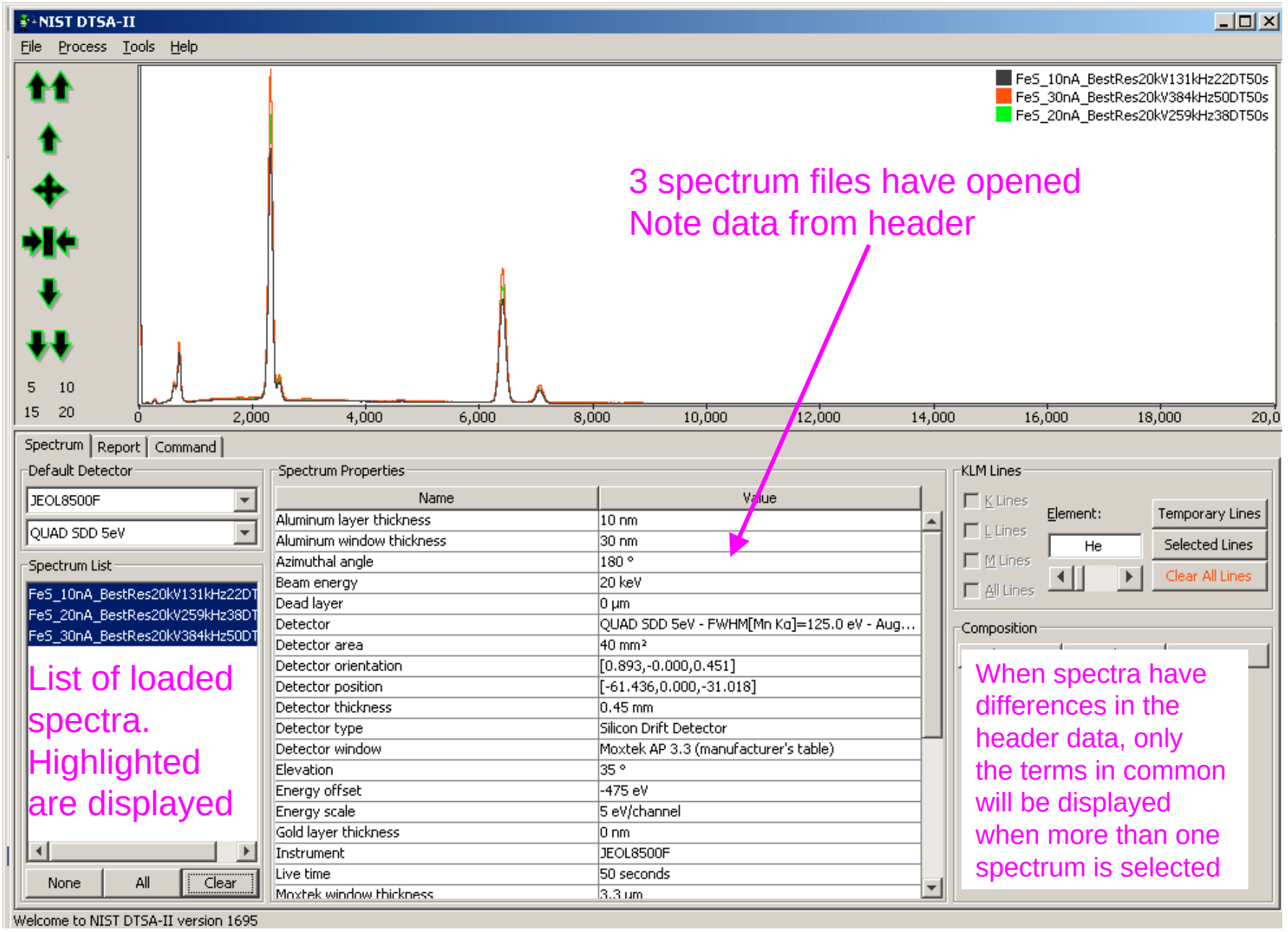



The Report is a great feature for those of us approaching geezerhood.

Now, what was I saying?


NIST DTSA-II
File Process Tools Help
Open spectrum files...
Look in: SDD_Spectra_BestRes
My Recent Documents
Desktop
My Documents
My Computer
My Network Places
Cu_10A_BestRes20kV155kHz25DT50s.msa
Cu_1nA_BestRes20kV1nA15p56DT50s.msa
Cu_20A_BestRes20kV306kHz42DT50s.msa
Cu_2nA_BestRes20kV31p5kHz8DT50s.msa
Cu_30A_BestRes20kV454kHz56DT50s.msa
Cu_40A_130k20kV591kHz38DT50s.msa
Cu_40A_BestRes20kV597kHz66DT50s.msa
Cu_4nA_BestRes20kV63kHz13DT50s.msa
FeS_10nA_BestRes20kV131kHz22DT50s.msa
FeS_1nA_BestRes20kV13p1kHz6DT50s.msa
FeS_20nA_BestRes20kV259kHz38DT50s.msa
FeS_2nA_BestRes20kV26p1kHz8DT50s.msa
FeS_30nA_BestRes20kV384kHz50DT50s.msa
FeS_40nA_BestRes20kV507kHz60DT50s.msa
FeS_4nA_BestRes20kV52kHz12DT50s.msa
K227_10nA_BestRes20kV151kHz24DT50s.msa
K227_1nA_BestRes20kV15p4kHz6DT50s.msa
K227_20nA_BestRes20kV300kHz42DT50s.msa
K227_2nA_BestRes20kV30p3kHz7DT50s.msa
K227_30nA_BestRes20kV445kHz55DT50s.msa
K227_40nA_BestRes20kV587kHz65DT50s.msa
K227_4nA_BestRes20kV61kHz12DT50s.msa
K309_10nA_BestRes20kV90kHz17DT50s.msa
K309_1nA_BestRes20kV9p1kHz5DT50s.msa
K309_20nA_BestRes20kV180kHz30DT50s.msa
K309_2nA_BestRes20kV18p2kHz7DT50s.msa
K309_30nA_E
K309_40nA_E
K309_4nA_Be
K412_10nA_E
K412_1nA_Be
K412_20nA_E
K412_2nA_Be
K412_30nA_E
K412_40nA_E
K412_4nA_Be
ZnS_10nA_Be
ZnS_1nA_Bes
ZnS_20nA_Be
File name: sa" "FeS_1nA_BestRes20kV13p1kHz6DT50s.msa" "FeS_20nA_BestRes20kV259kHz38DT50s.msa"
Files of type: Common spectrum file
FeS_10nA_BestRes20kV131kHz22DT50s
FeS_1nA_BestRes20kV13p1kHz6DT50s
FeS_20nA_BestRes20kV259kHz38DT50s
Open several spectra at a time:
Holding down “SHIFT” key gives a continuous run
Preview of spectra in this window
0
5,000
10,000
15,000
20,0
OK
Cancel
Spectrum Report Comm
Default Detector
JEOL8500F
QUAD SDD 5eV
Spectrum List
None
All
Welcome to NIST DTSA-II version 1695

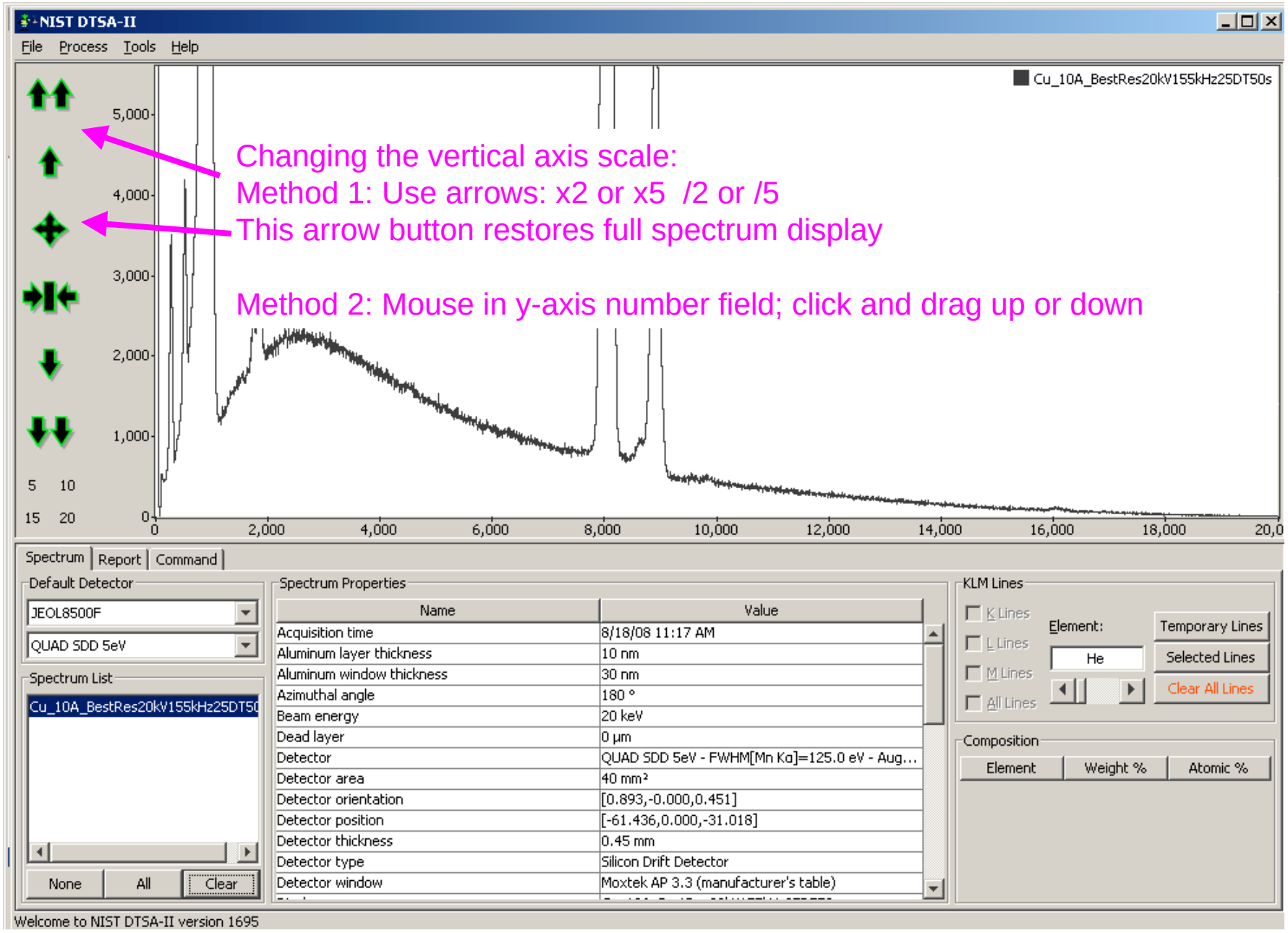

NIST DTSA-II
File Process Tools Help
Open spectrum files...
Look in: SDD_Spectra_BestRes
My Recent Documents
Desktop
My Documents
My Computer
My Network Places
Cu_10A_BestRes20kV155kHz25DT50s.msa
Cu_1nA_BestRes20kV1nA15p56DT50s.msa
Cu_20A_BestRes20kV306kHz42DT50s.msa
Cu_2nA_BestRes20kV31p5kHz8DT50s.msa
Cu_30A_BestRes20kV454kHz56DT50s.msa
Cu_40A_130k20kV591kHz38DT50s.msa
Cu_40A_BestRes20kV597kHz66DT50s.msa
Cu_4nA_BestRes20kV63kHz13DT50s.msa
FeS_10nA_BestRes20kV131kHz22DT50s.msa
FeS_1nA_BestRes20kV13p1kHz6DT50s.msa
FeS_20nA_BestRes20kV259kHz38DT50s.msa
FeS_2nA_BestRes20kV26p1kHz8DT50s.msa
FeS_30nA_BestRes20kV384kHz50DT50s.msa
FeS_40nA_BestRes20kV507kHz60DT50s.msa
FeS_4nA_BestRes20kV52kHz12DT50s.msa
K227_10nA_BestRes20kV151kHz24DT50s.msa
K227_1nA_BestRes20kV15p4kHz6DT50s.msa
K227_20nA_BestRes20kV300kHz42DT50s.msa
K227_2nA_BestRes20kV30p3kHz7DT50s.msa
K227_30nA_BestRes20kV445kHz55DT50s.msa
K227_40nA_BestRes20kV587kHz65DT50s.msa
K227_4nA_BestRes20kV61kHz12DT50s.msa
K309_10nA_BestRes20kV90kHz17DT50s.msa
K309_1nA_BestRes20kV9p1kHz5DT50s.msa
K309_20nA_BestRes20kV180kHz30DT50s.msa
K309_2nA_BestRes20kV18p2kHz7DT50s.msa
K309_30nA_E
K309_40nA_E
K309_4nA_Be
K412_10nA_E
K412_1nA_Be
K412_20nA_E
K412_2nA_Be
K412_30nA_E
K412_40nA_E
K412_4nA_Be
ZnS_10nA_Be
ZnS_1nA_Bes
ZnS_20nA_Be
File name: s" "FeS_20nA_BestRes20kV259kHz38DT50s.msa" "FeS_30nA_BestRes20kV384kHz50DT50s.msa"
Files of type: Common spectrum file
FeS_10nA_BestRes20kV131kHz22DT50s
FeS_20nA_BestRes20kV259kHz38DT50s
FeS_30nA_BestRes20kV384kHz50DT50s
To open several spectra at a time:
Holding down "CTRL" key allows multiple separate selections
0
5,000
10,000
15,000
20,0
OK
Cancel
Spectrum Report Comm
Default Detector
JEOL8500F
QUAD SDD 5eV
Spectrum List
None
All
Welcome to NIST DTSA-II version 1695


NIST DTSA-II
File Process Tools Help
FeS_10nA_BestRes20kV131kHz22DT50s
FeS_30nA_BestRes20kV384kHz50DT50s
FeS_20nA_BestRes20kV259kHz38DT50s
3 spectrum files have opened
Note data from header
0 2,000 4,000 6,000 8,000 10,000 12,000 14,000 16,000 18,000 20,0
Spectrum Report Command
Default Detector
JEOL8500F
QUAD SDD 5eV
Spectrum List
FeS_10nA_BestRes20kV131kHz22DT
FeS_20nA_BestRes20kV259kHz38DT
FeS_30nA_BestRes20kV384kHz50DT
List of loaded spectra. Highlighted are displayed
None All Clear
Spectrum Properties
Name Value
Aluminum layer thickness 10 nm
Aluminum window thickness 30 nm
Azimuthal angle 180 °
Beam energy 20 keV
Dead layer 0 µm
Detector QUAD SDD 5eV - FWHM[Mn Kα]=125.0 eV - Aug...
Detector area 40 mm²
Detector orientation [0.893,-0.000,0.451]
Detector position [-61.436,0.000,-31.018]
Detector thickness 0.45 mm
Detector type Silicon Drift Detector
Detector window Moxtek AP 3.3 (manufacturer's table)
Elevation 35 °
Energy offset -475 eV
Energy scale 5 eV/channel
Gold layer thickness 0 nm
Instrument JEOL8500F
Live time 50 seconds
Moxtek window thickness 3.3 µm
KLM Lines
K Lines
L Lines
M Lines
All Lines
Element:
He
Temporary Lines
Selected Lines
Clear All Lines
Composition
When spectra have differences in the header data, only the terms in common will be displayed when more than one spectrum is selected
Welcome to NIST DTSA-II version 1695

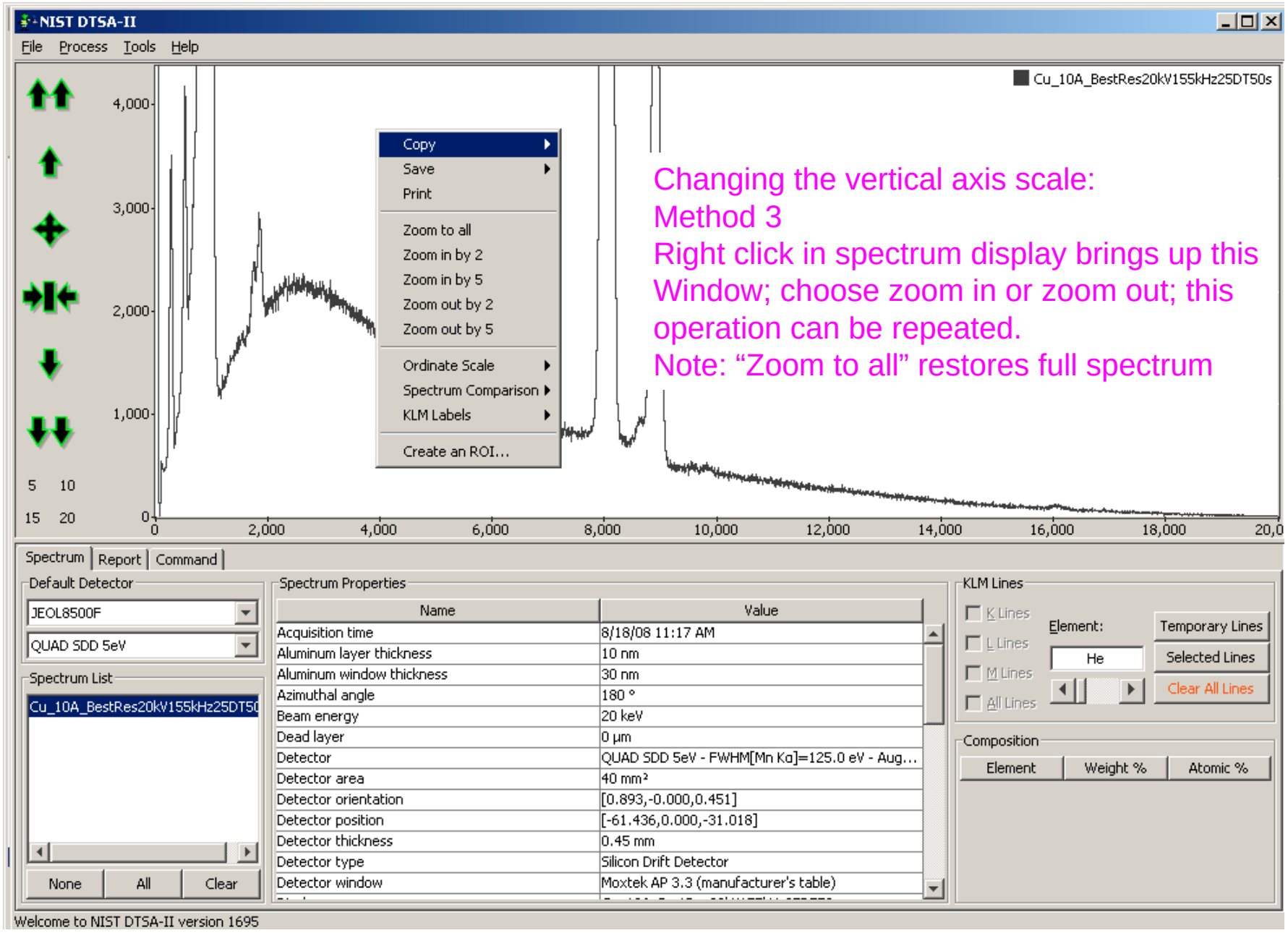
# Basic operations

- Opening and manipulating spectral files
- Display of spectra

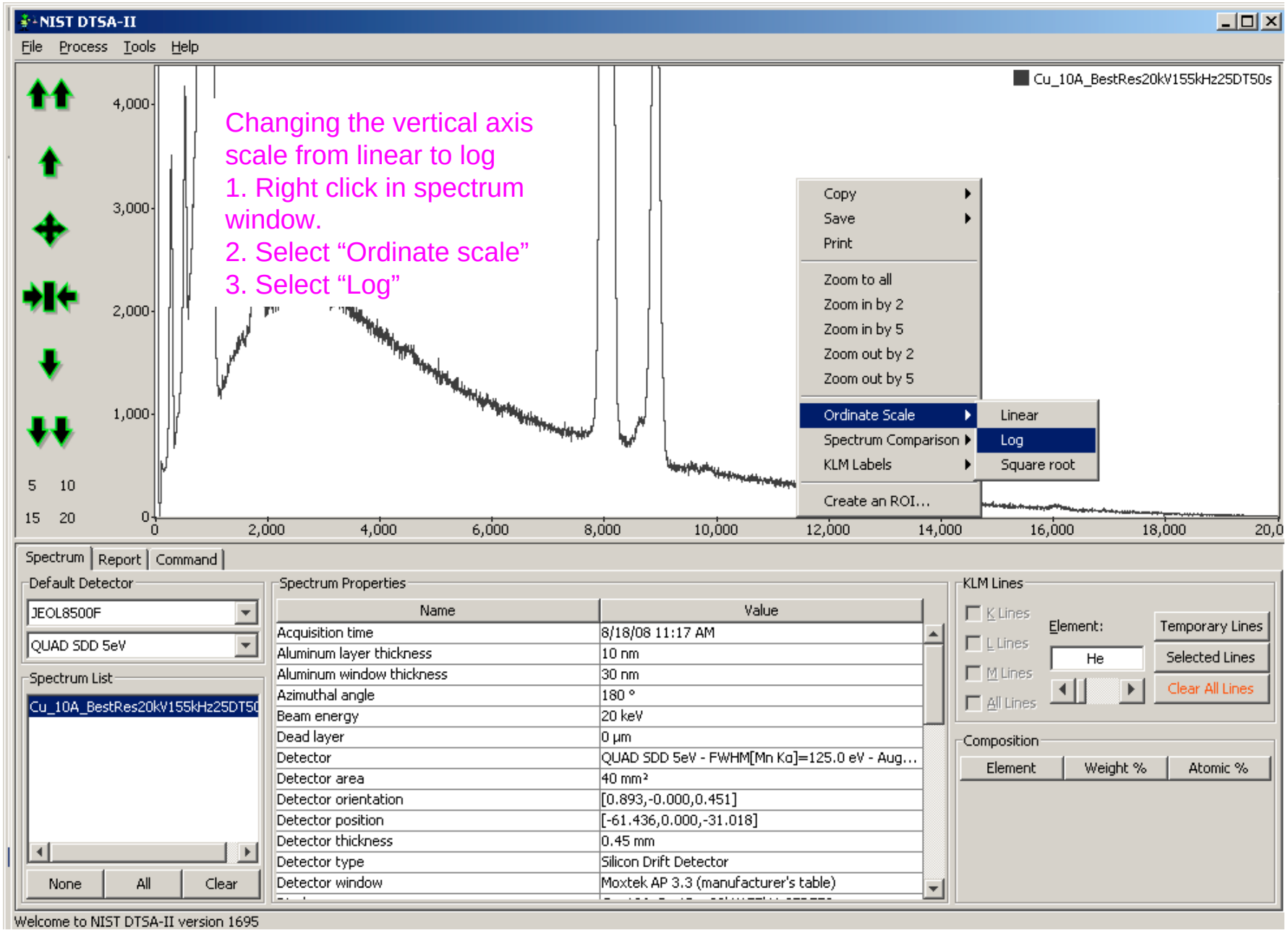
# Basic display of single spectrum



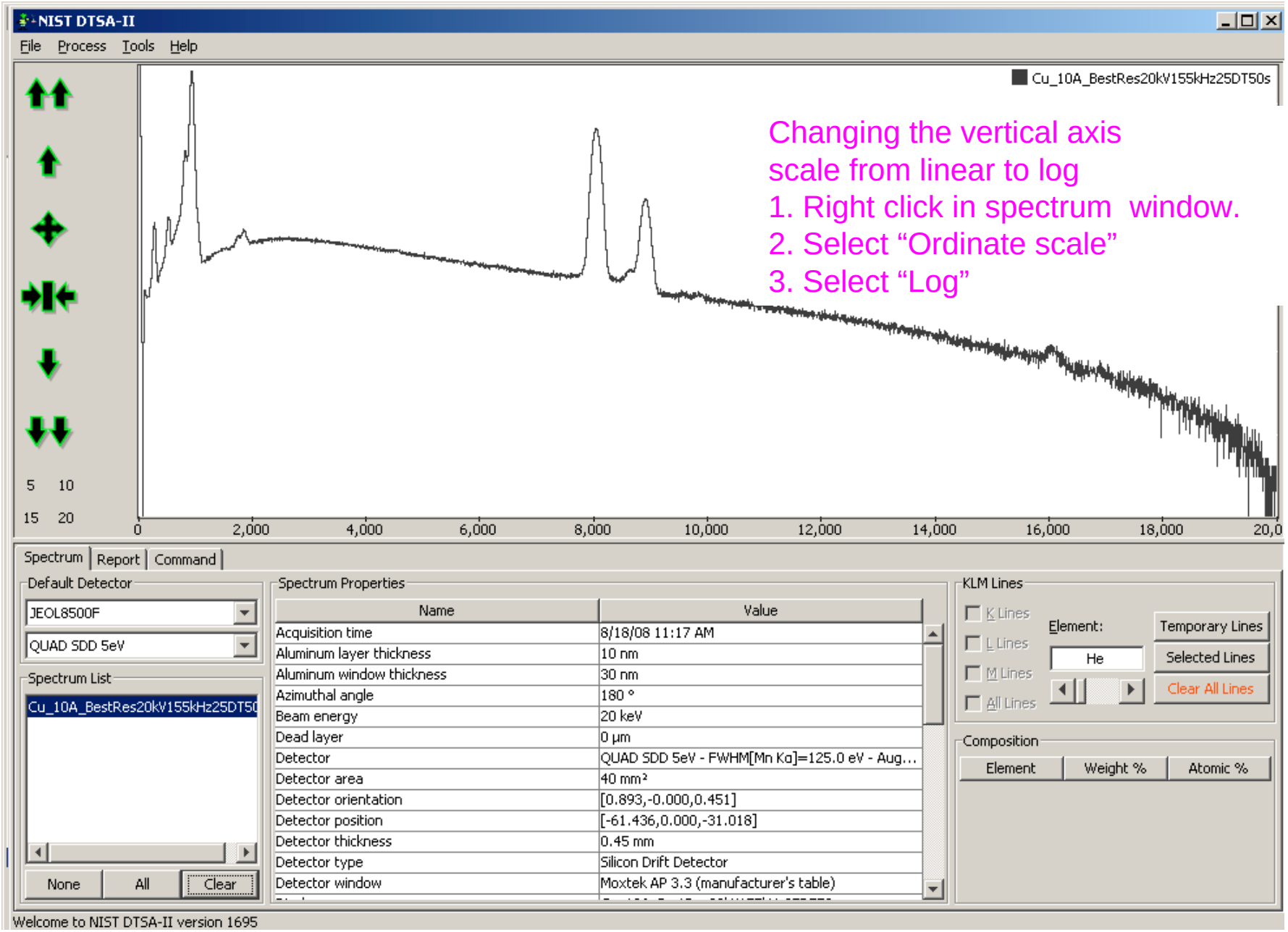
# Basic display of single spectrum



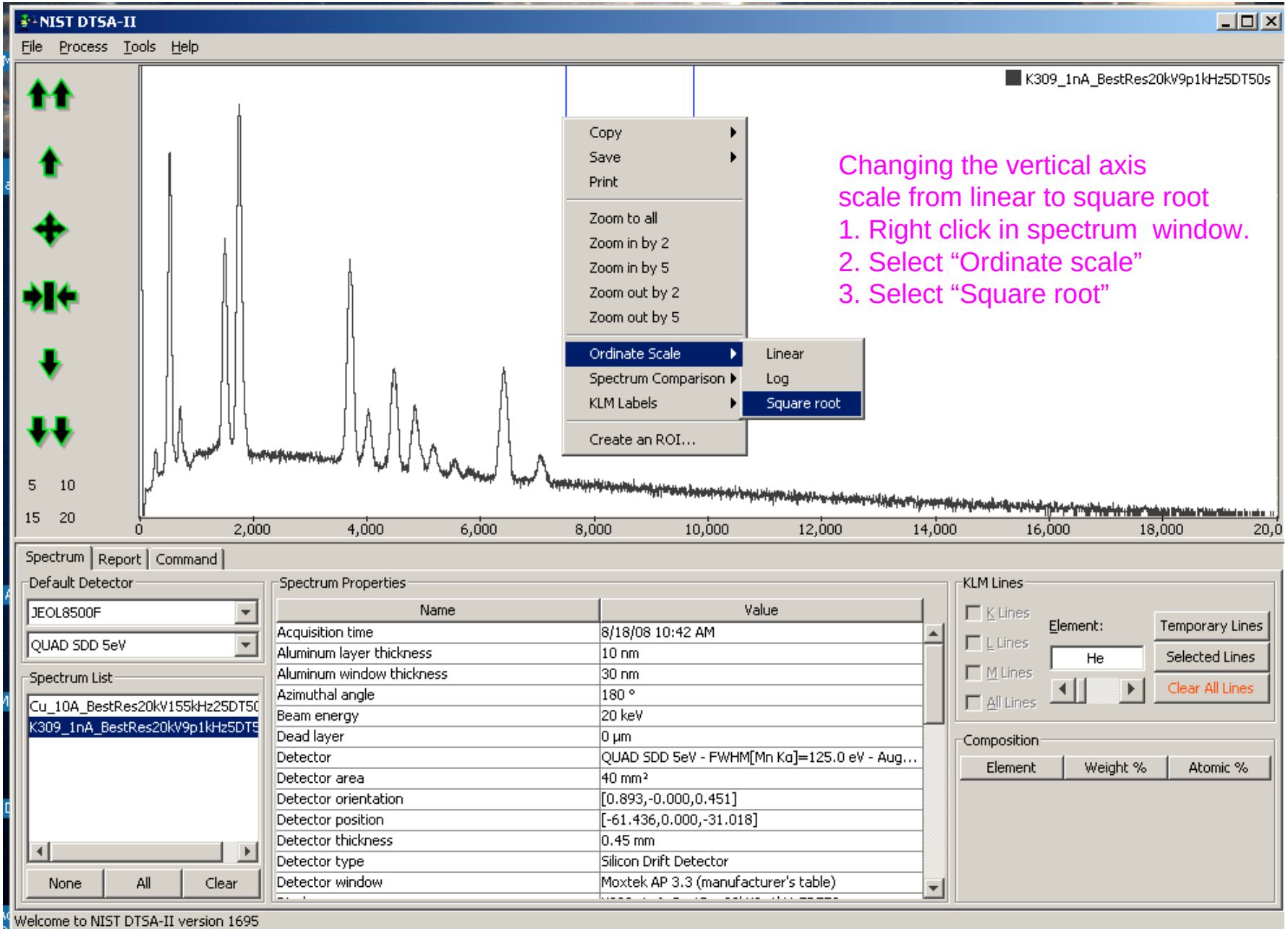
# Basic display of single spectrum



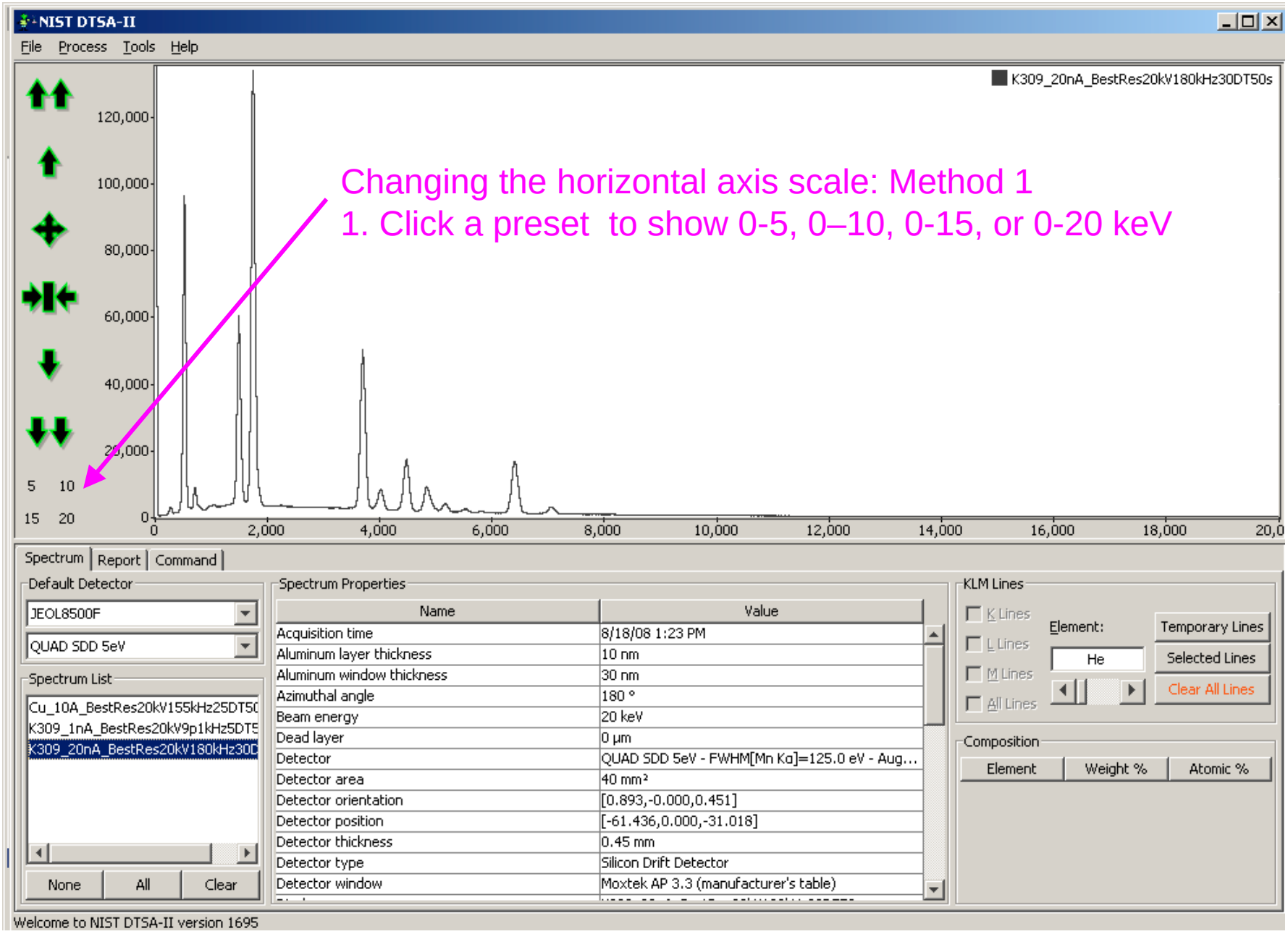
# Basic display of single spectrum



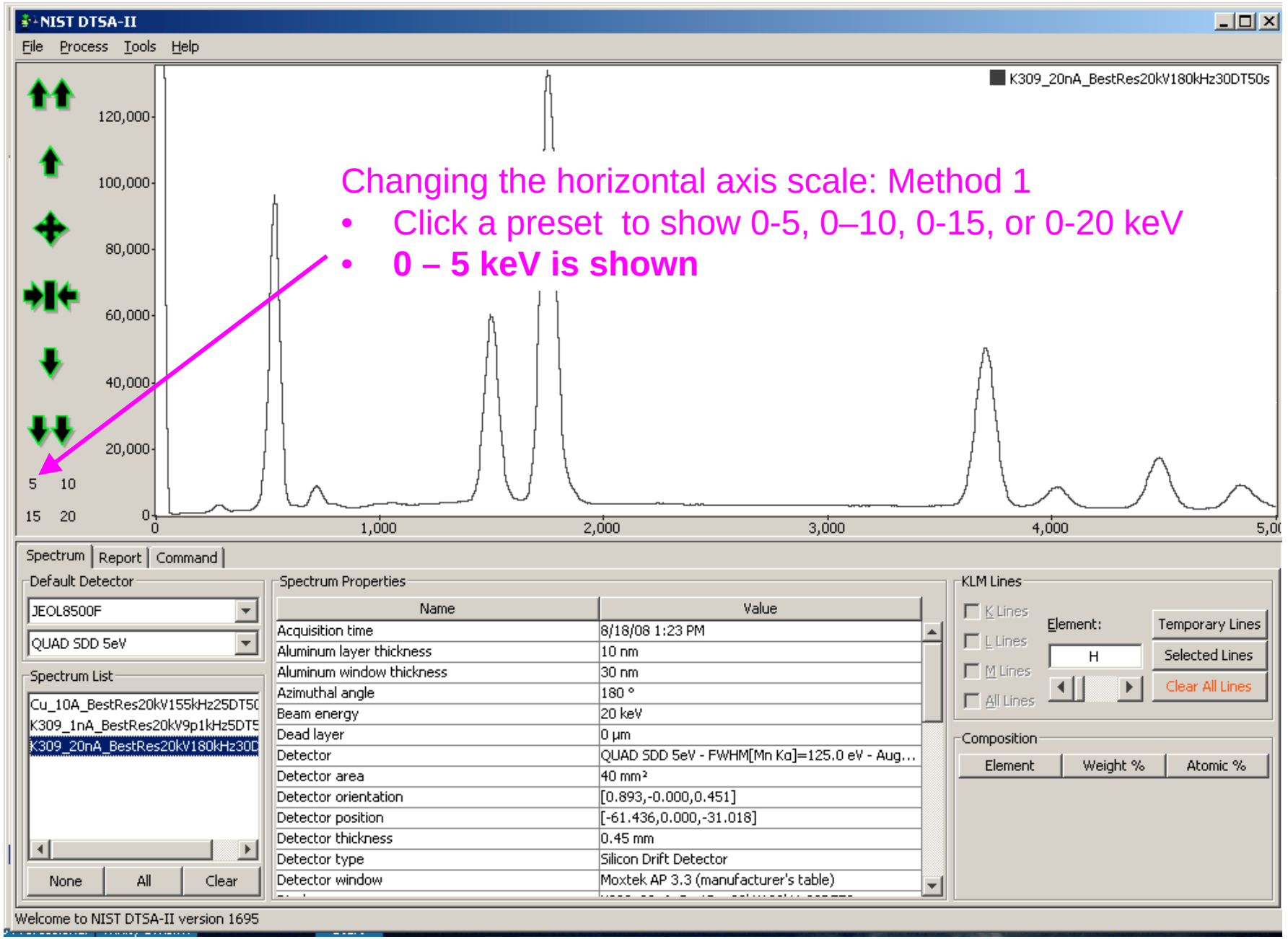
# Basic display of single spectrum



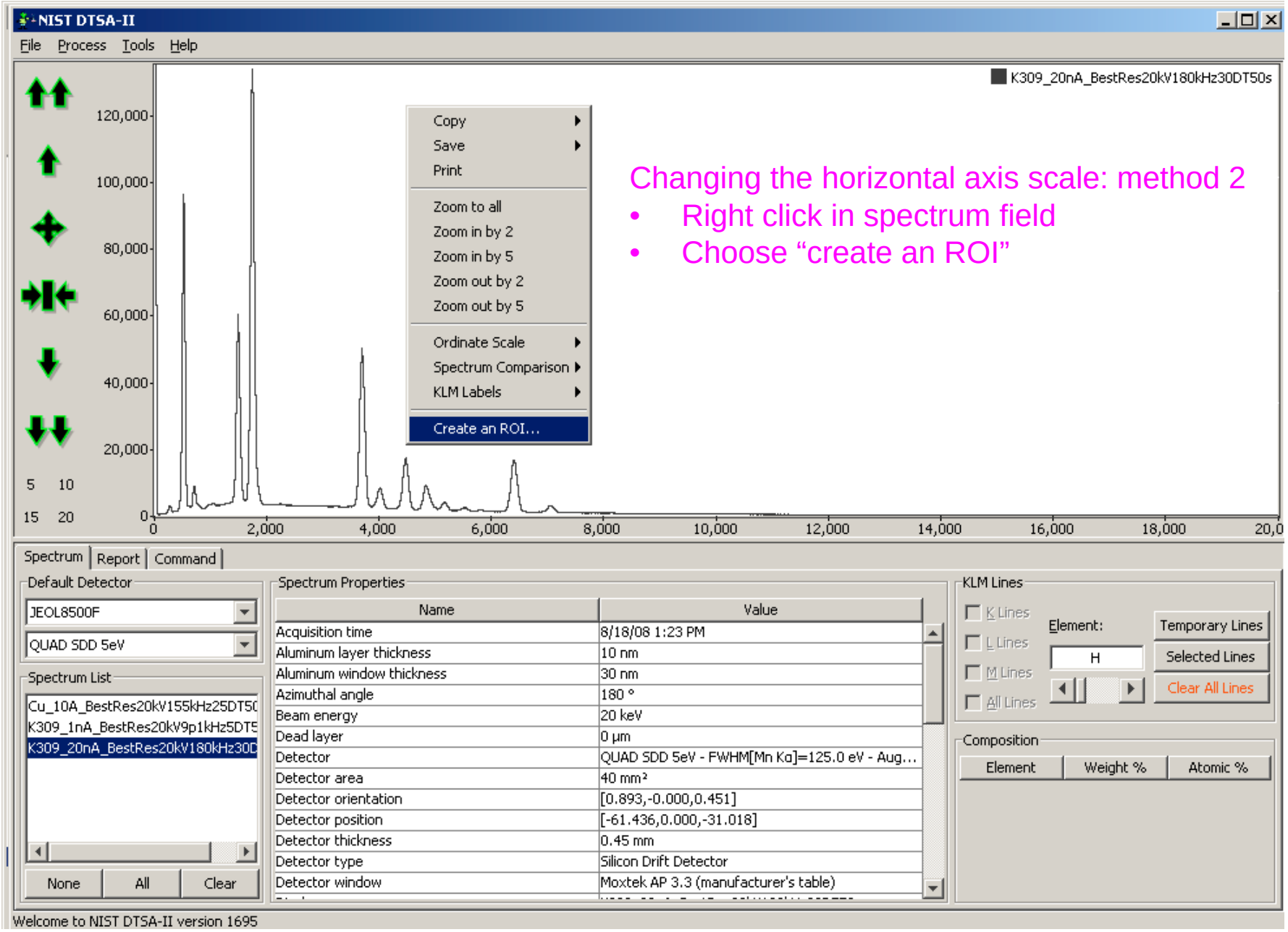
# Basic display of single spectrum



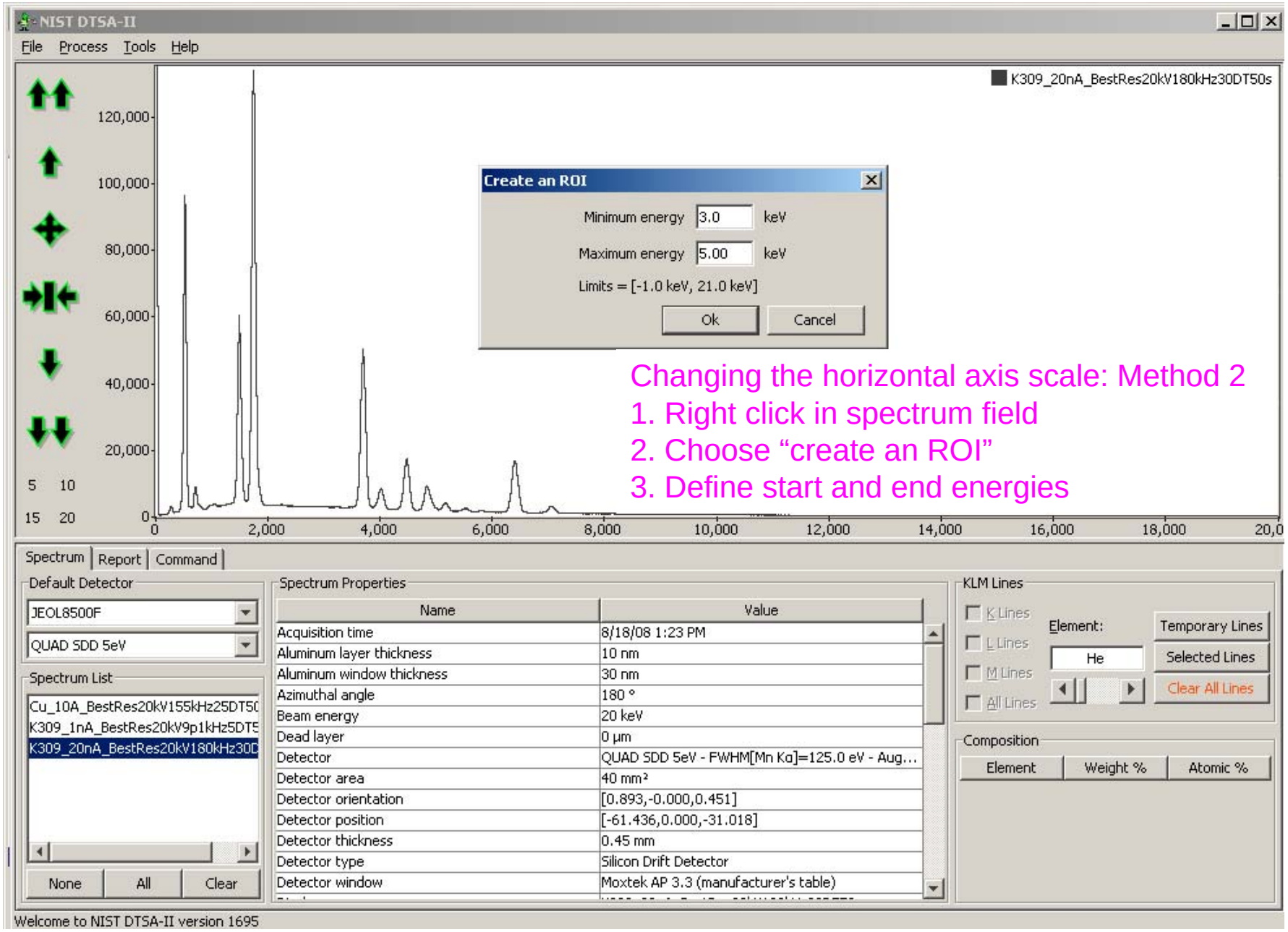
# Basic display of single spectrum



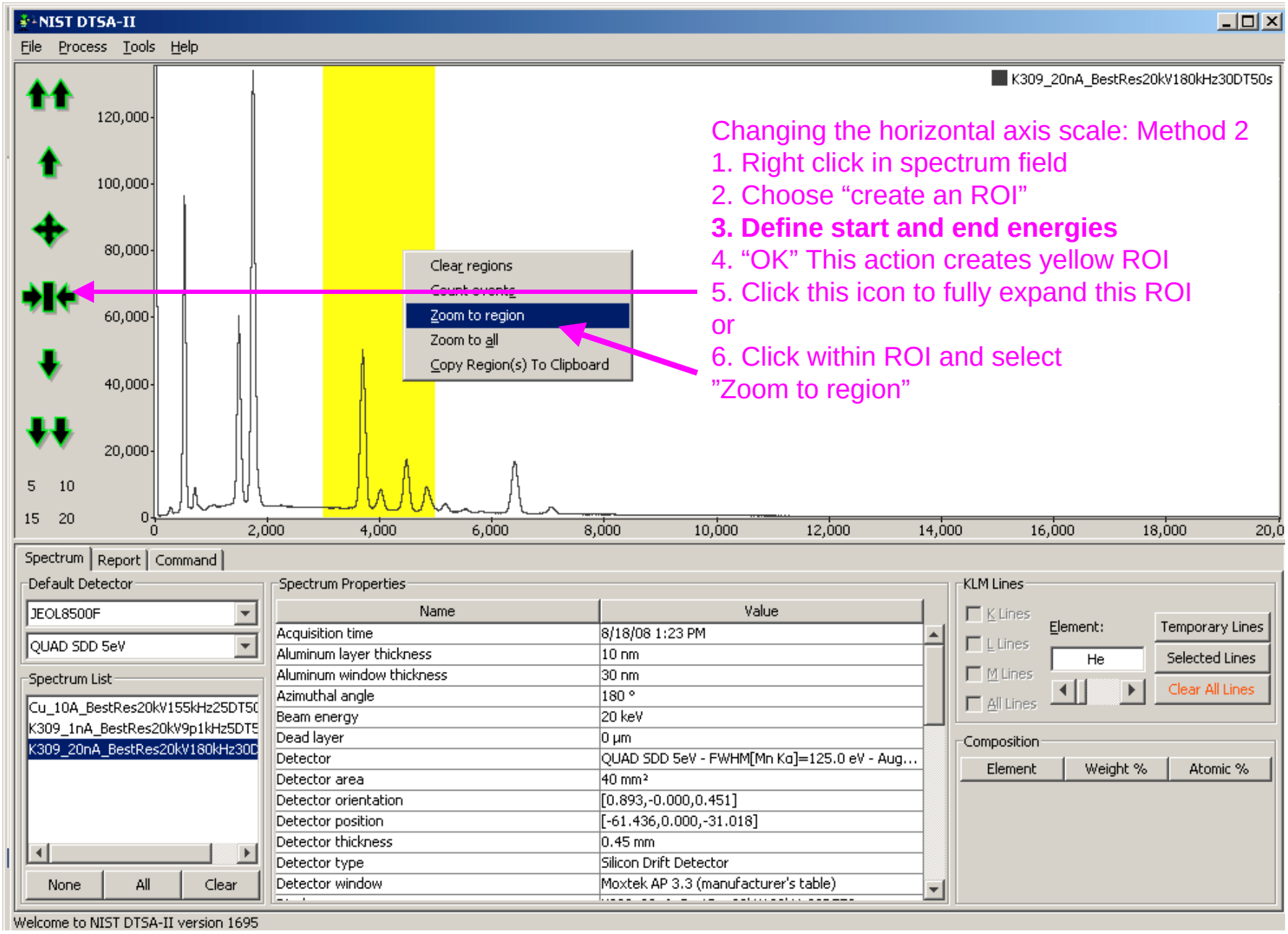
# Basic display of single spectrum



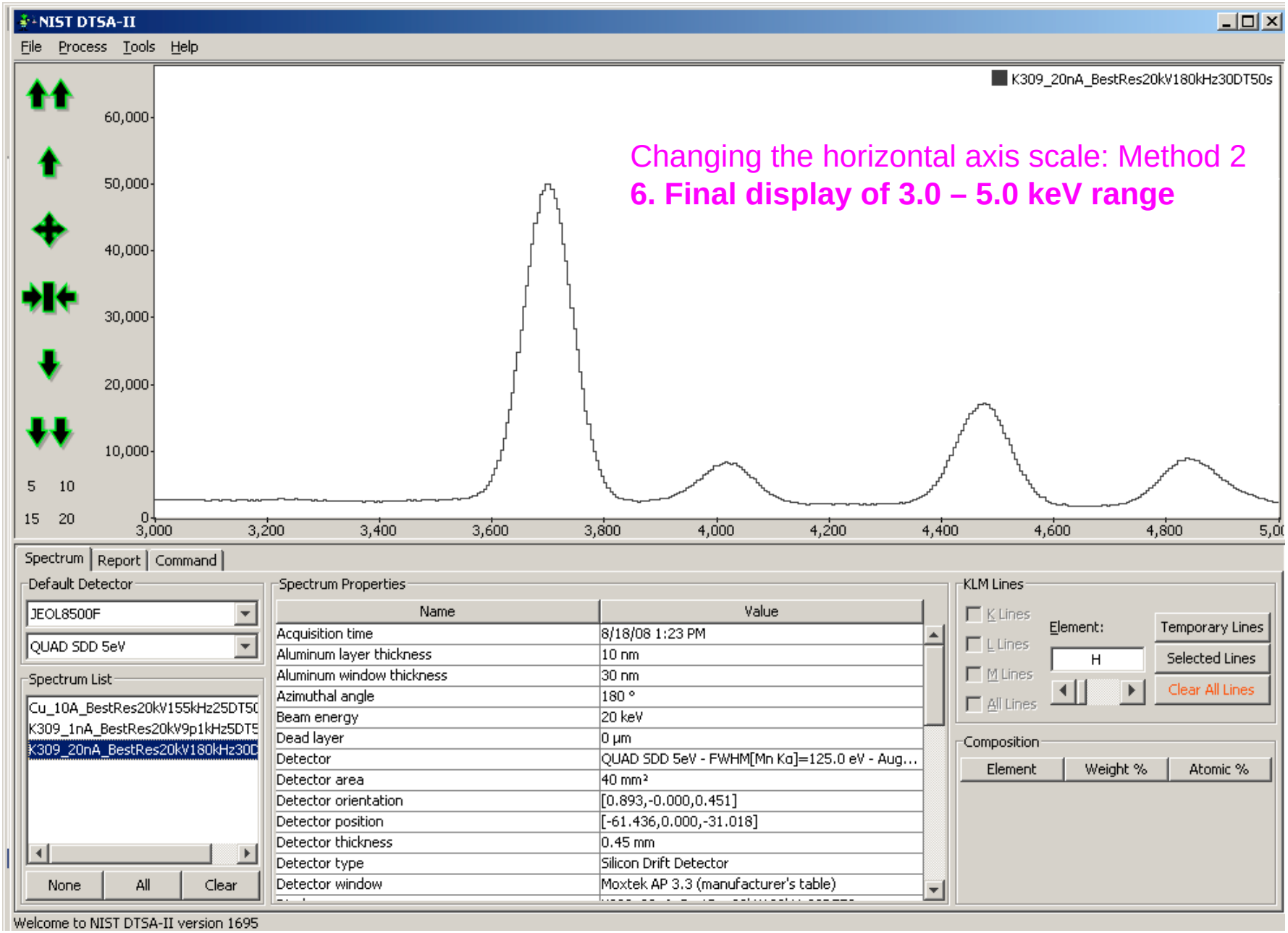
# Basic display of single spectrum



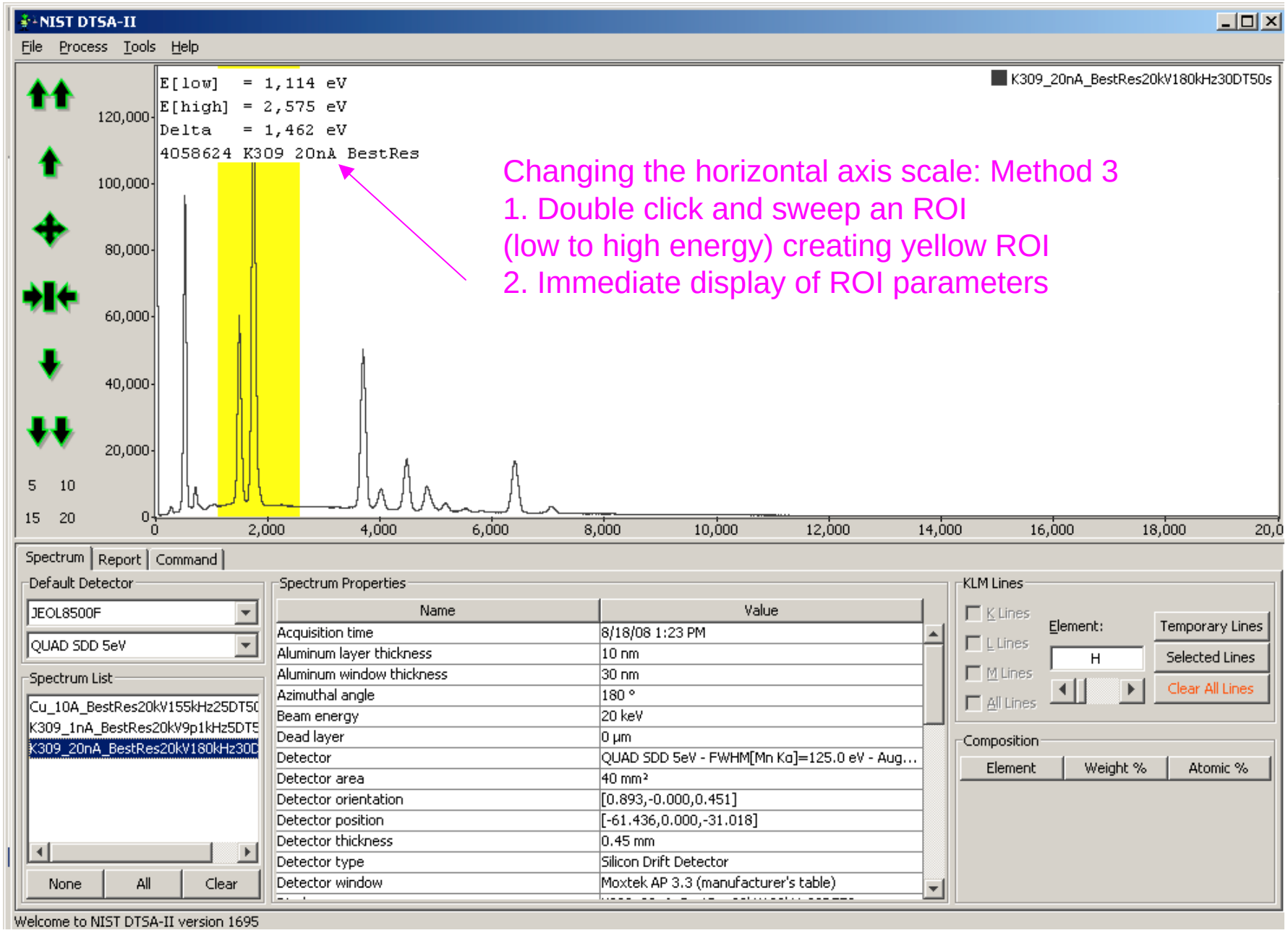
# Basic display of single spectrum



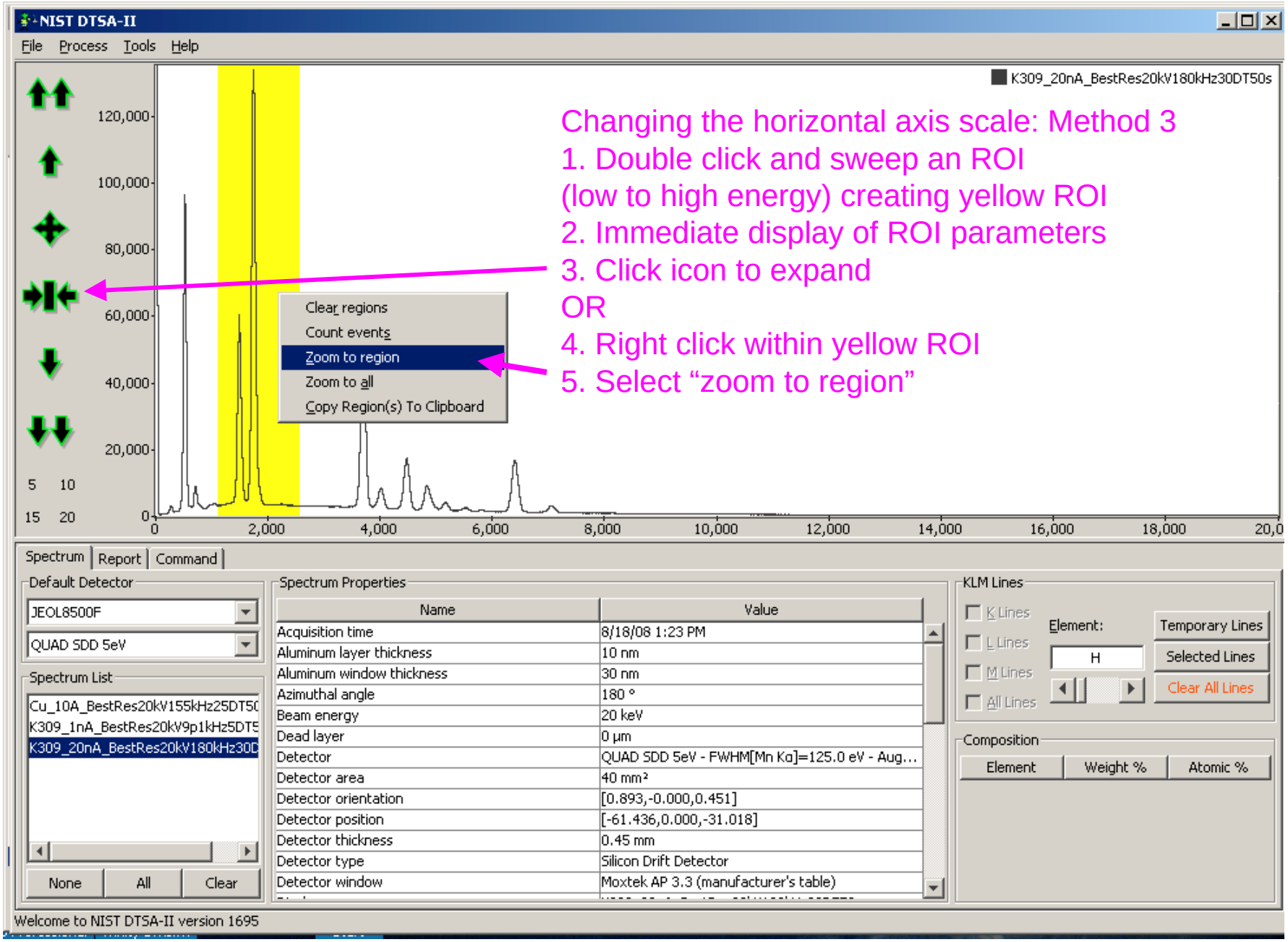
# Basic display of single spectrum



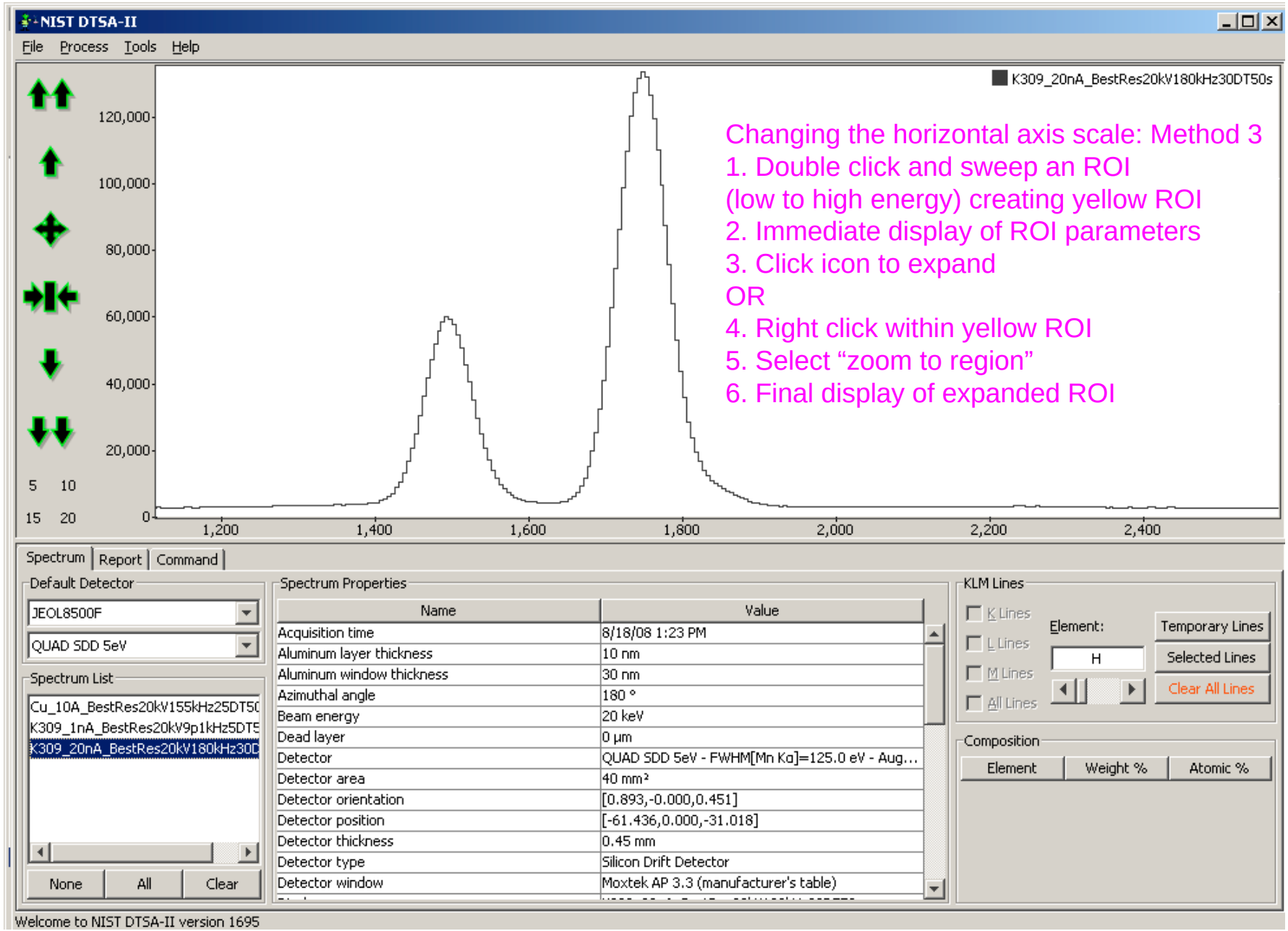
# Basic display of single spectrum



# Basic display of single spectrum



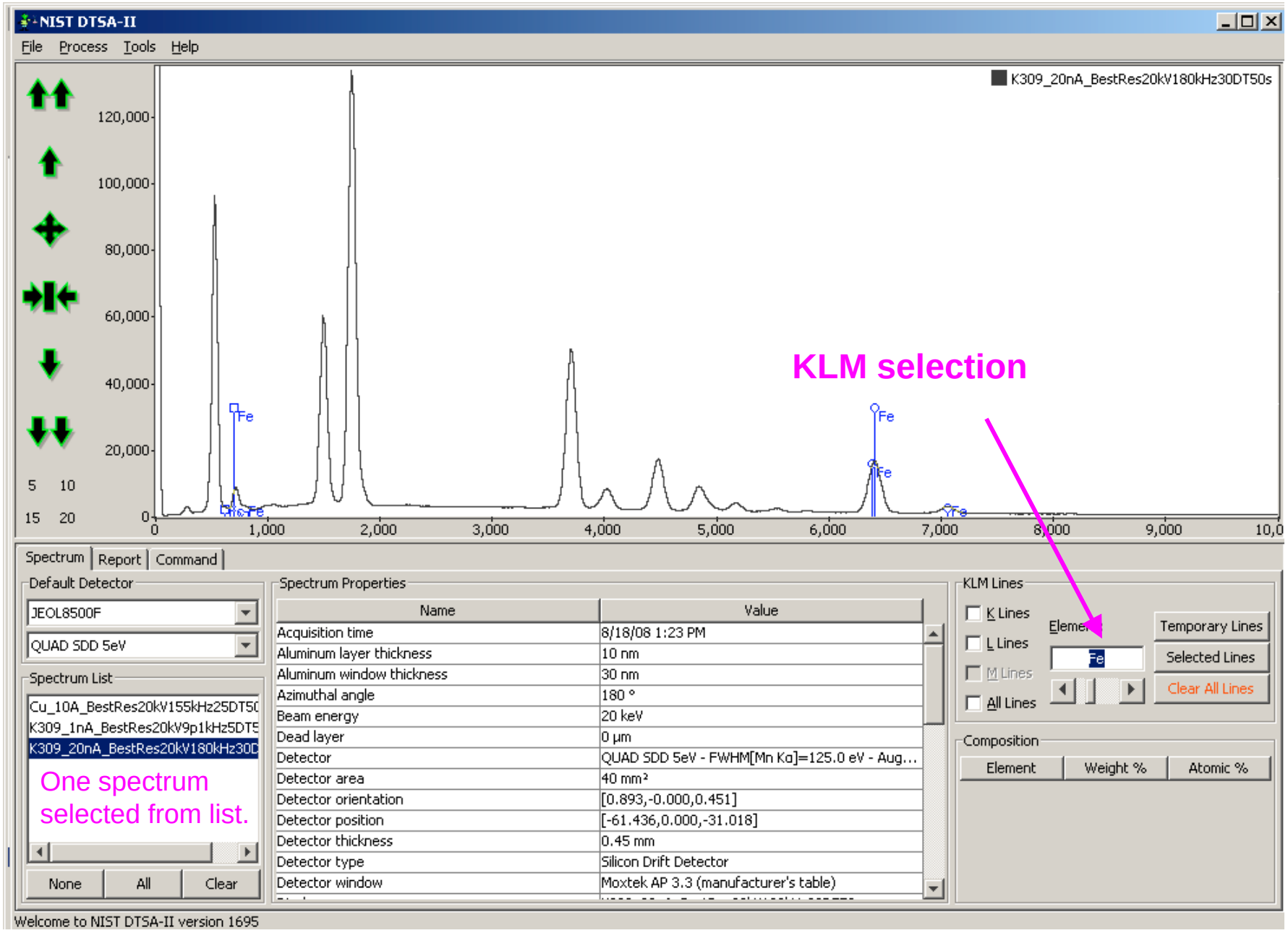
# Basic display of single spectrum



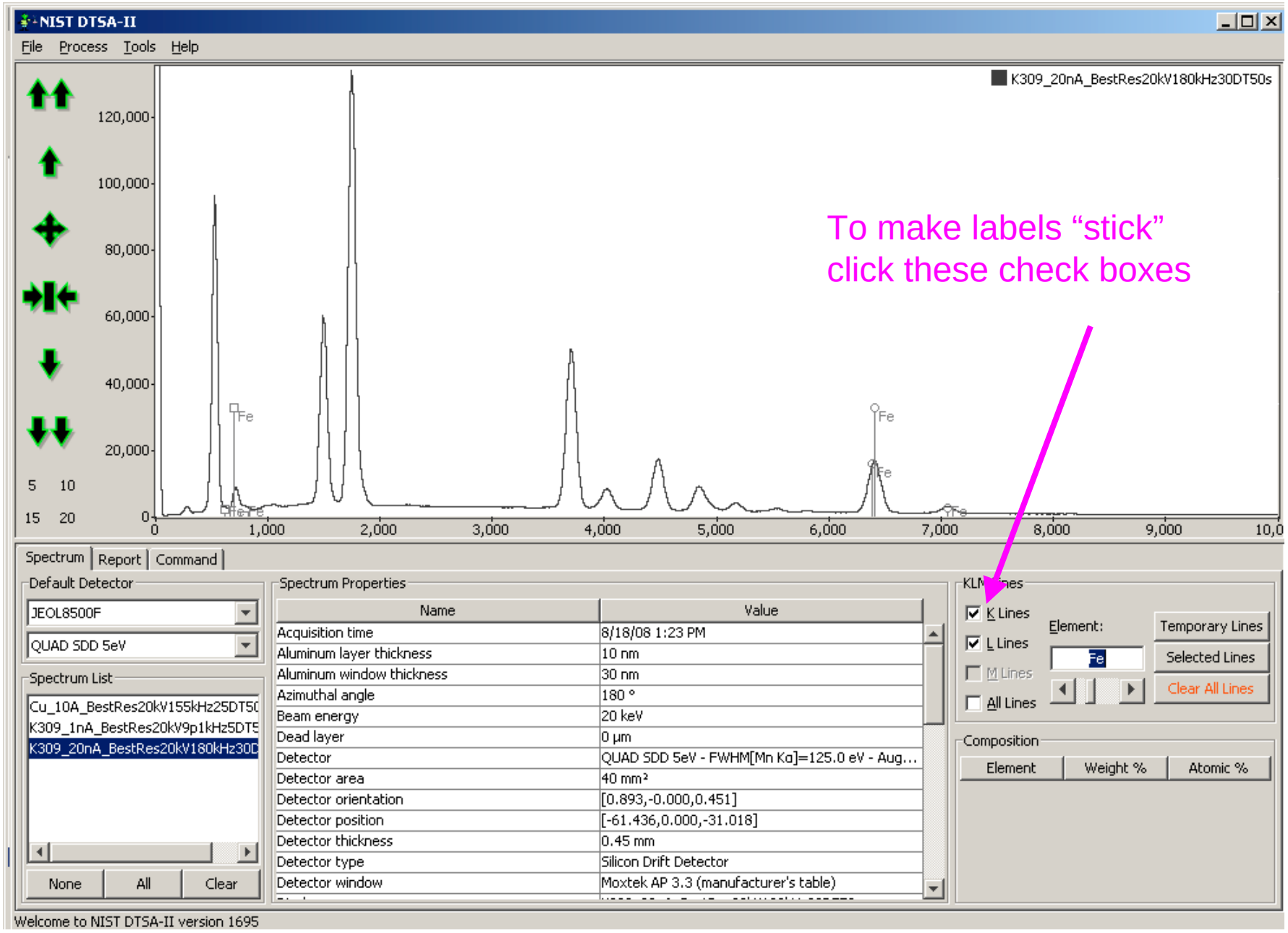
# Basic operations

- Opening and manipulating spectral files
- Display of spectra
- Peak labeling (manual only)

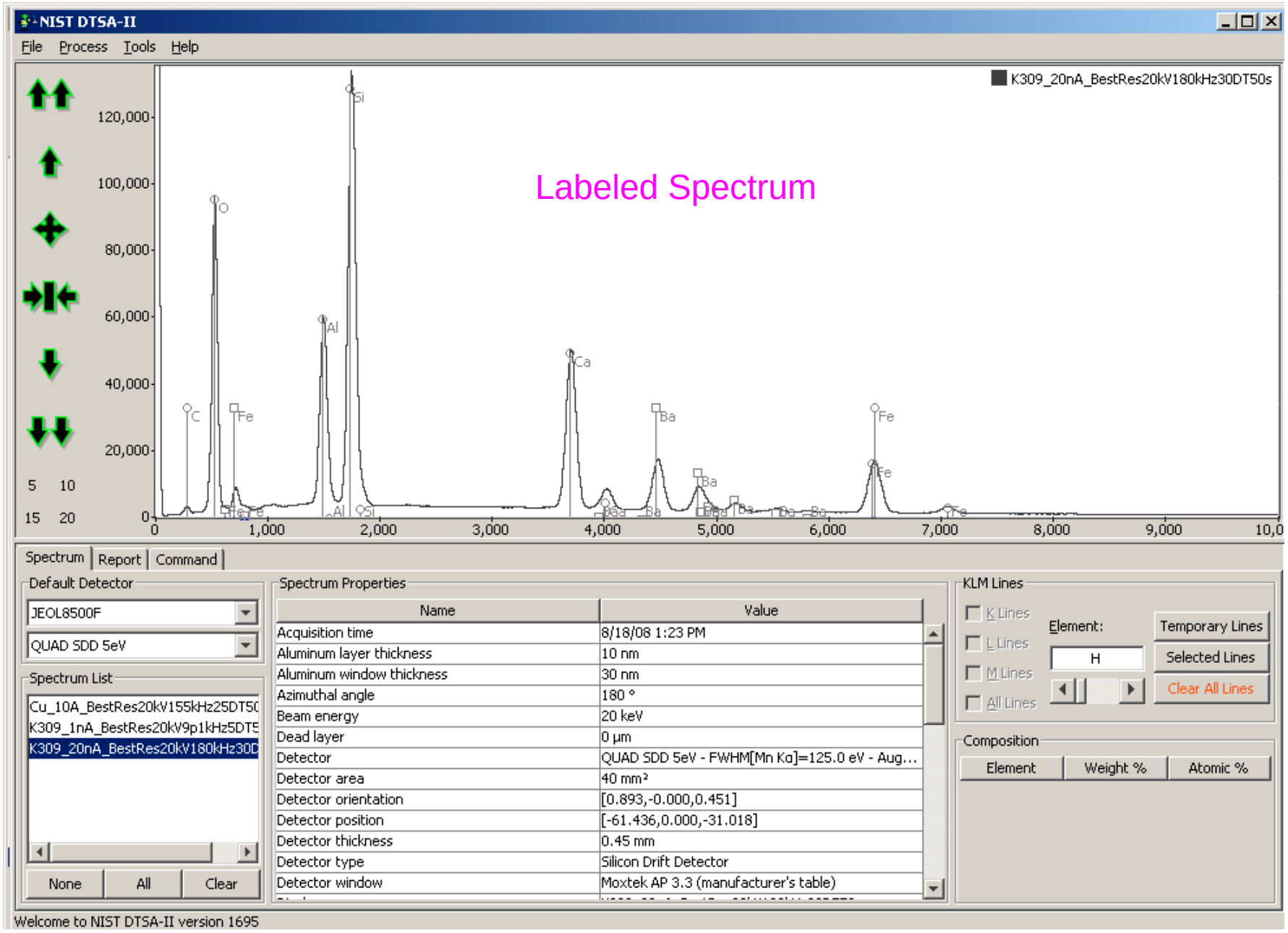
# Peak Labeling



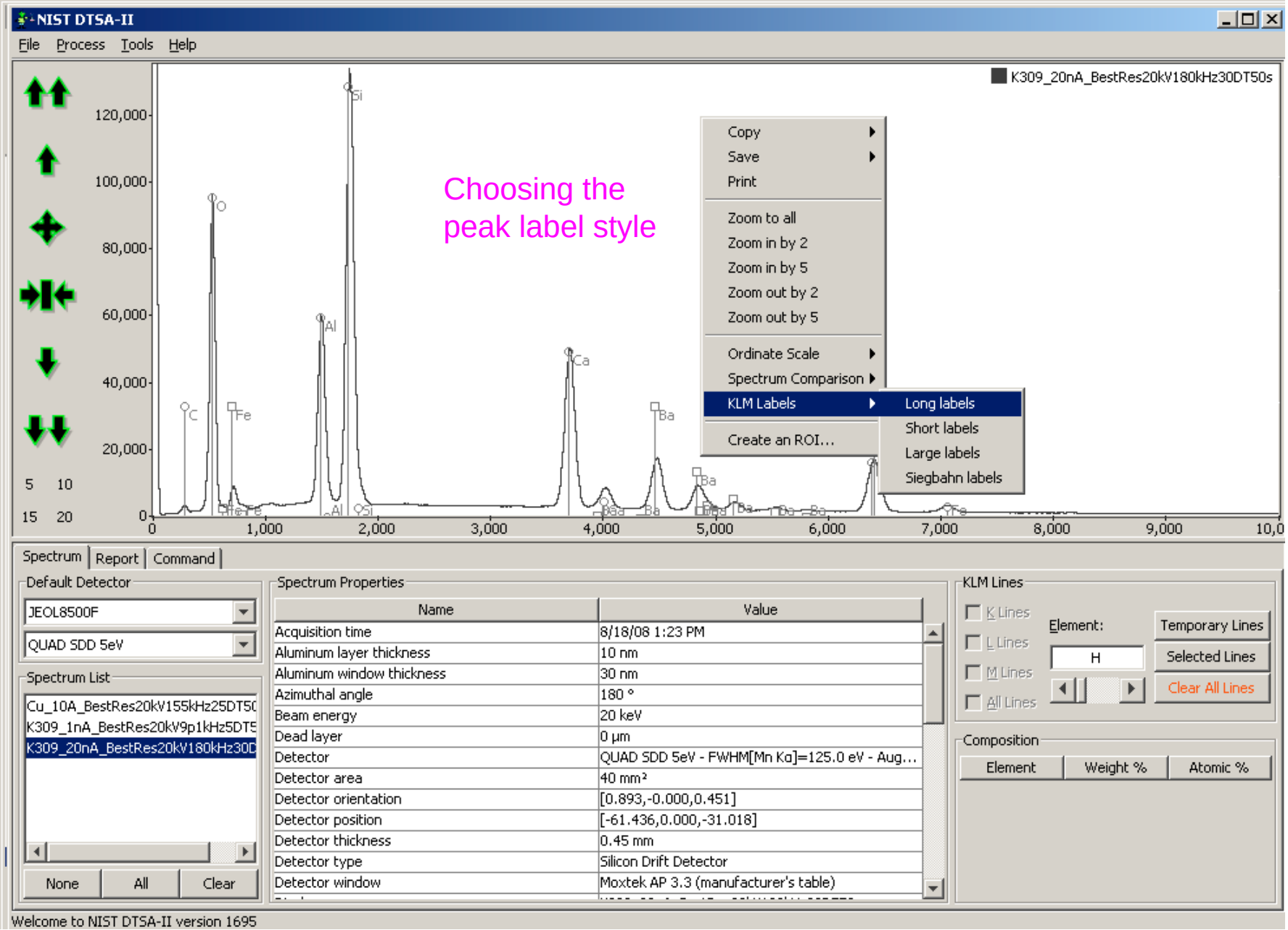
# Peak Labeling



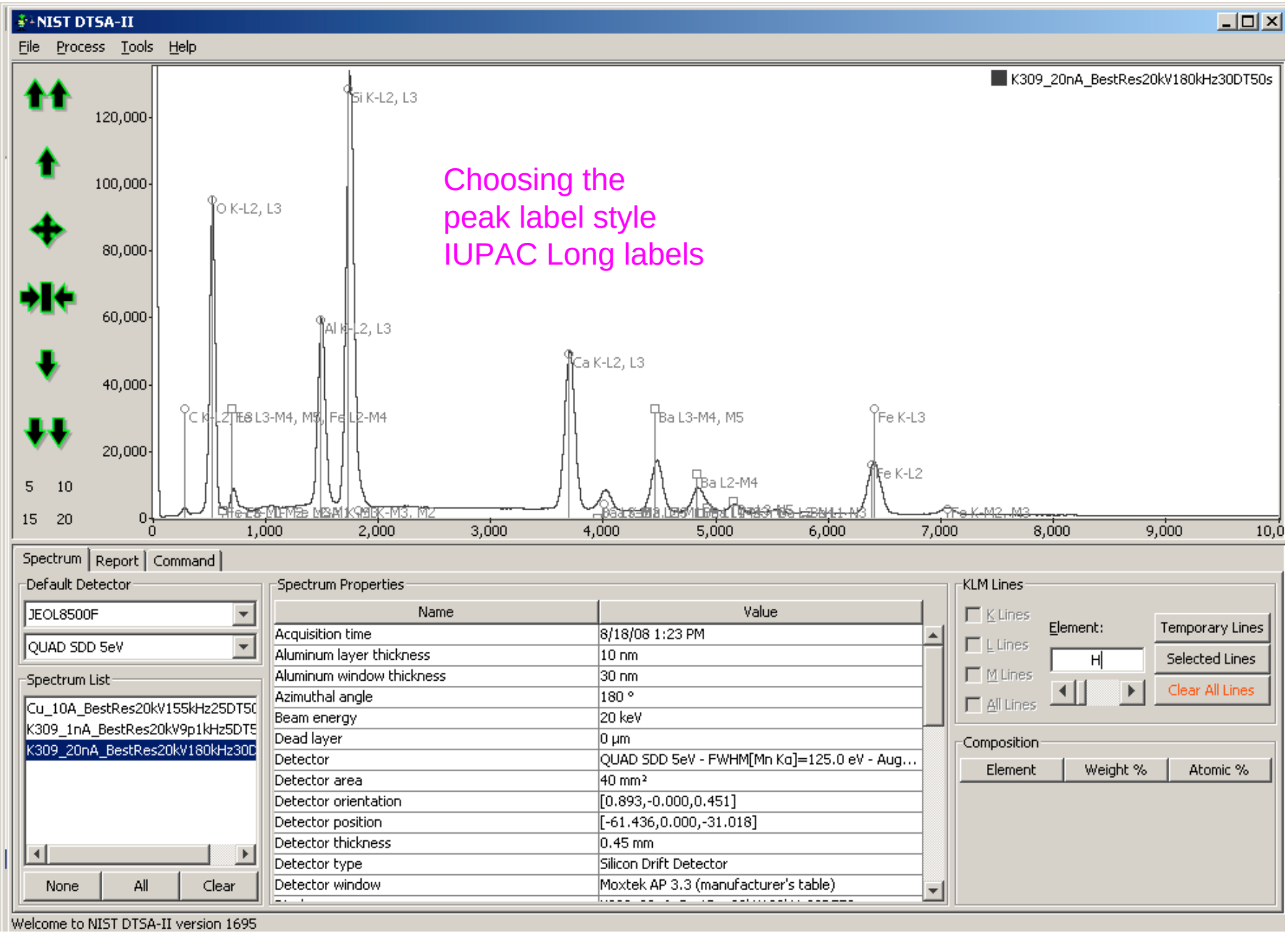
# Peak Labeling



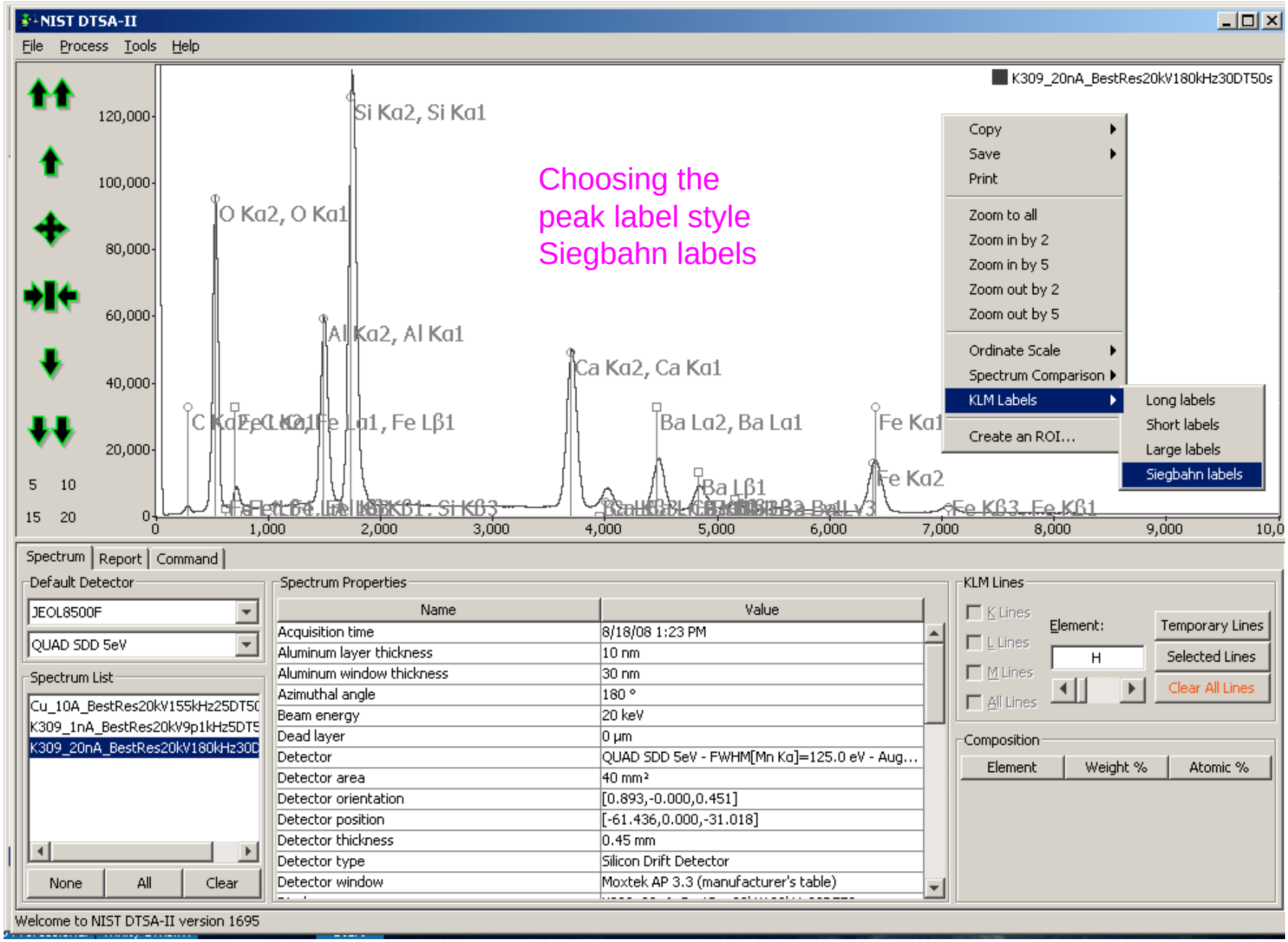
# Peak Labeling



# Peak Labeling



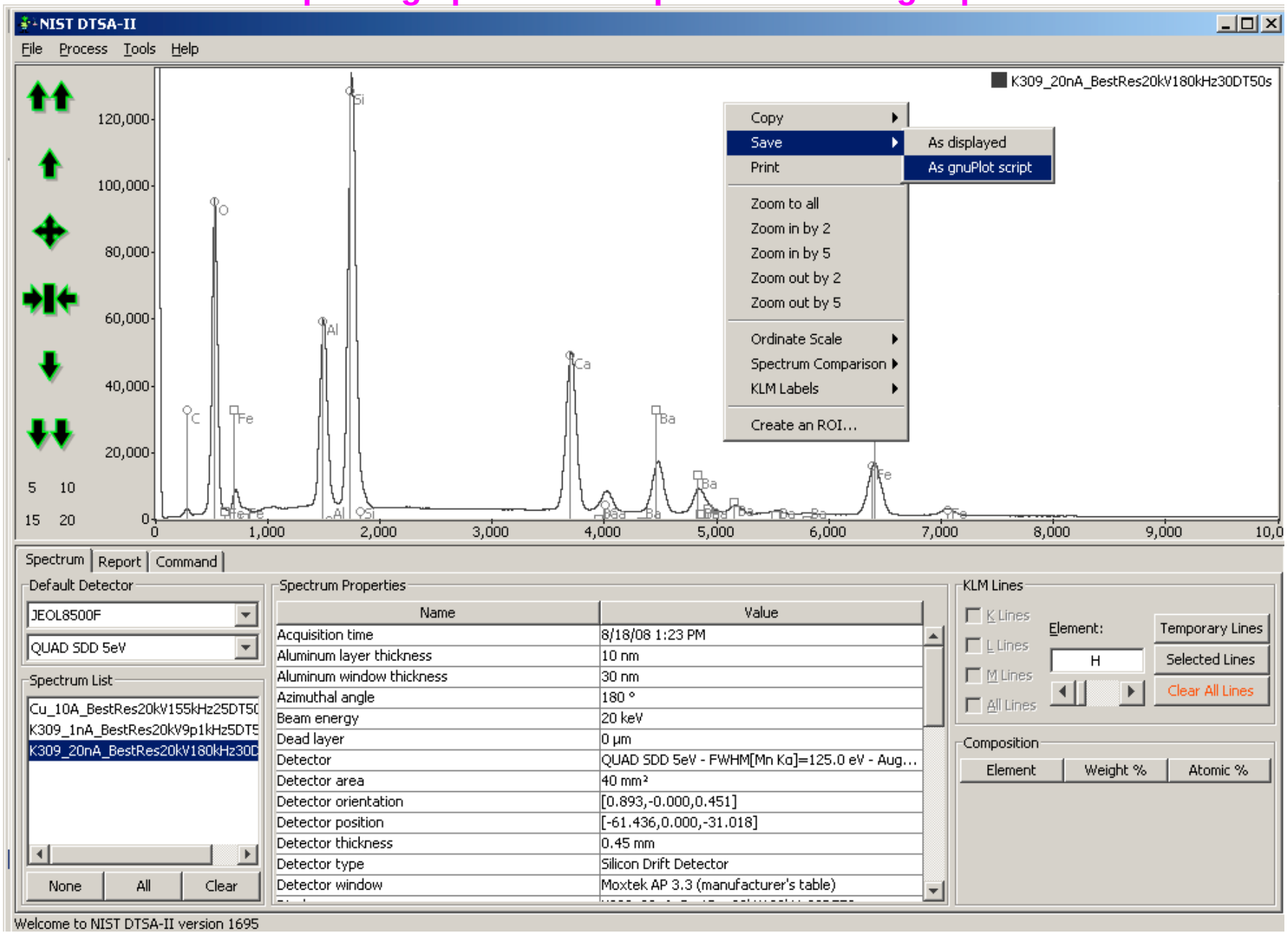
# Peak Labeling



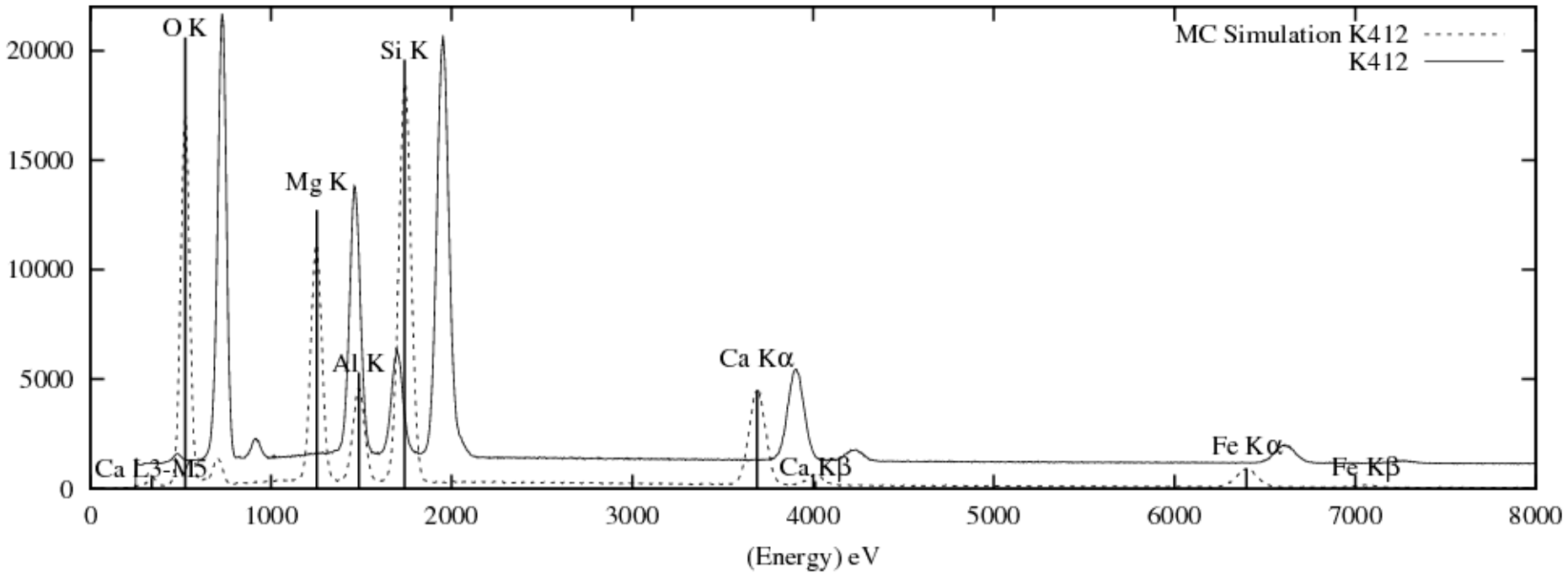
# Basic operations

- Opening and manipulating spectral files
- Peak labeling (manual only)
- Exporting spectra for publication (Gnuplot)

# Exporting spectrum for publication as gnuplot



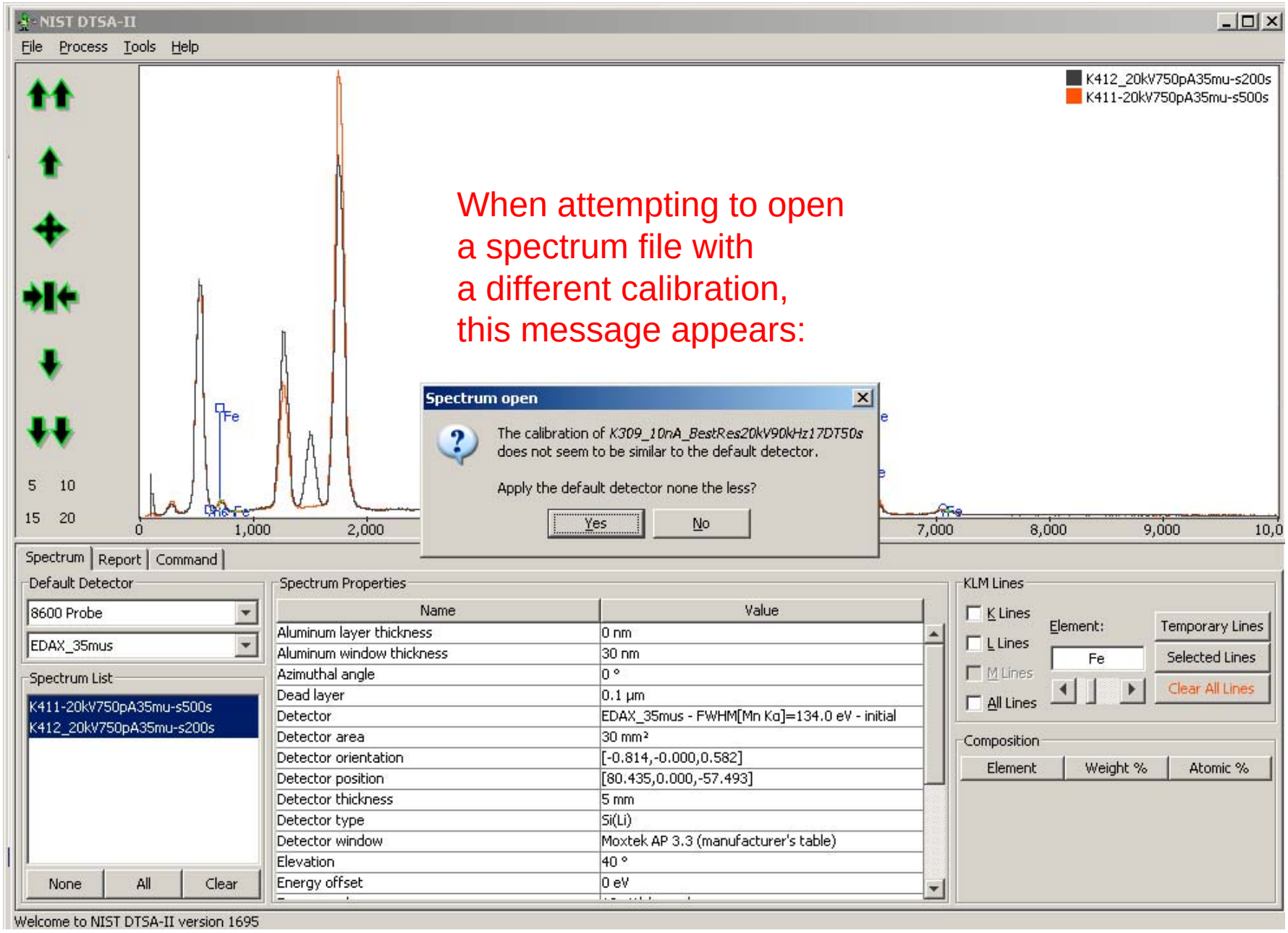
Publication-quality graphics from Gnuplot



# Comparing spectra from different EDS spectrometers, or from different dates from the same EDS: The issue of EDS calibration

- A spectrum is recorded with calibration data: eV/channel, zero offset, number of channels (depending on manufacturer, this data may or may not be embedded in the .msa header).
- When a spectrum is read into DTSA-II, the calibration information is checked against the current calibration.  If there is a mismatch, a message prompts the analyst.

# Spectrum Calibration



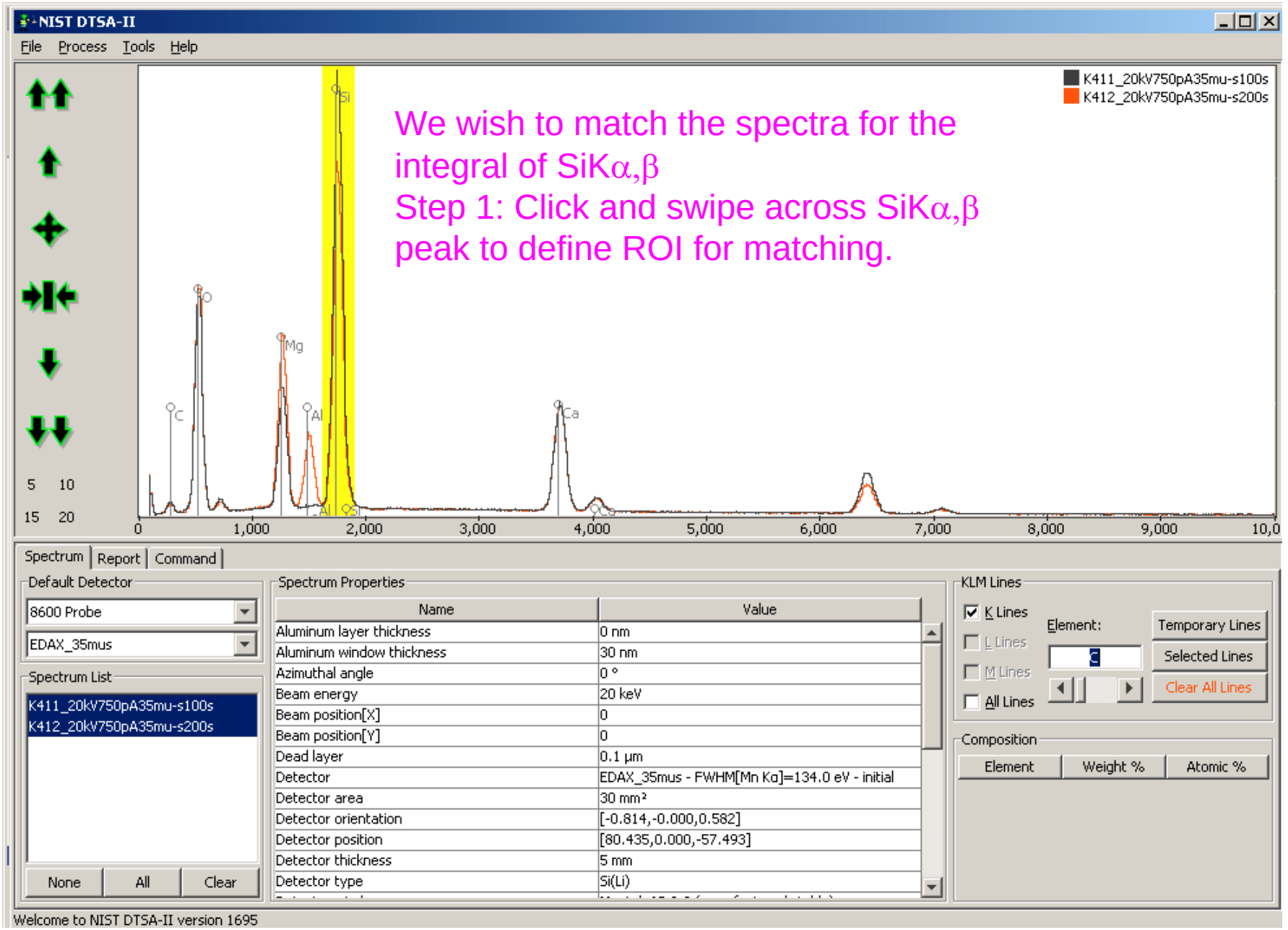
# The issue of EDS calibration

- A spectrum is recorded with calibration data: eV/channel, zero offset, number of channels (depending on manufacturer, this data may or may not be embedded in the .msa header).
- When a spectrum is read into DTSA-II, the calibration information is checked against the current calibration. If there is a mismatch, a message prompts the analyst.
- The analyst then has two choices:
  - 1. Change the detector selection to match the incoming spectrum
  - 2. Accept the incoming spectrum but display it according to the current calibration information. (Note: the incoming spectrum will retain its calibration data so that when it is the only spectrum being displayed, its own calibration will be applied.)

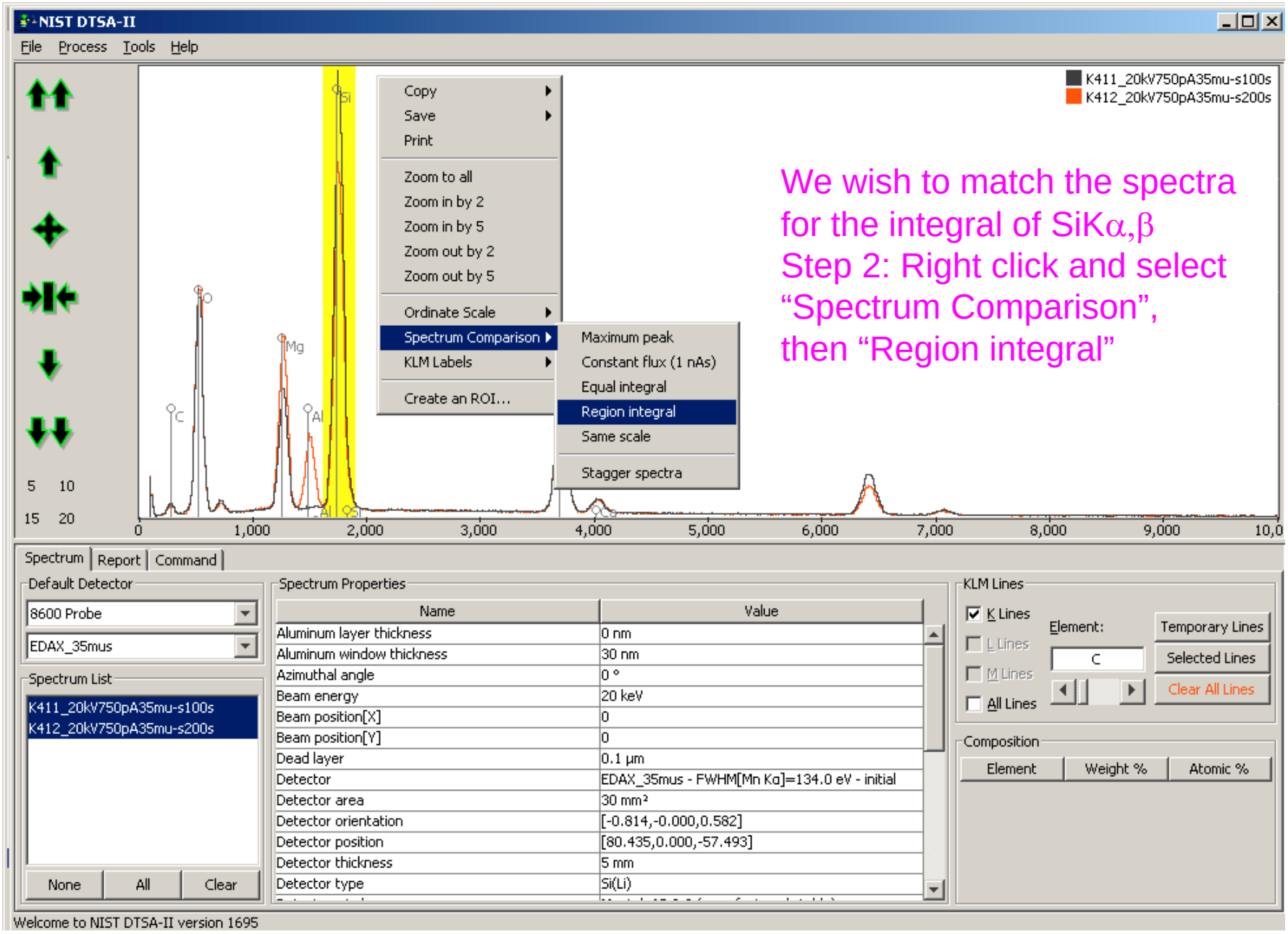
# Comparing multiple spectra

- Matching to a particular ROI

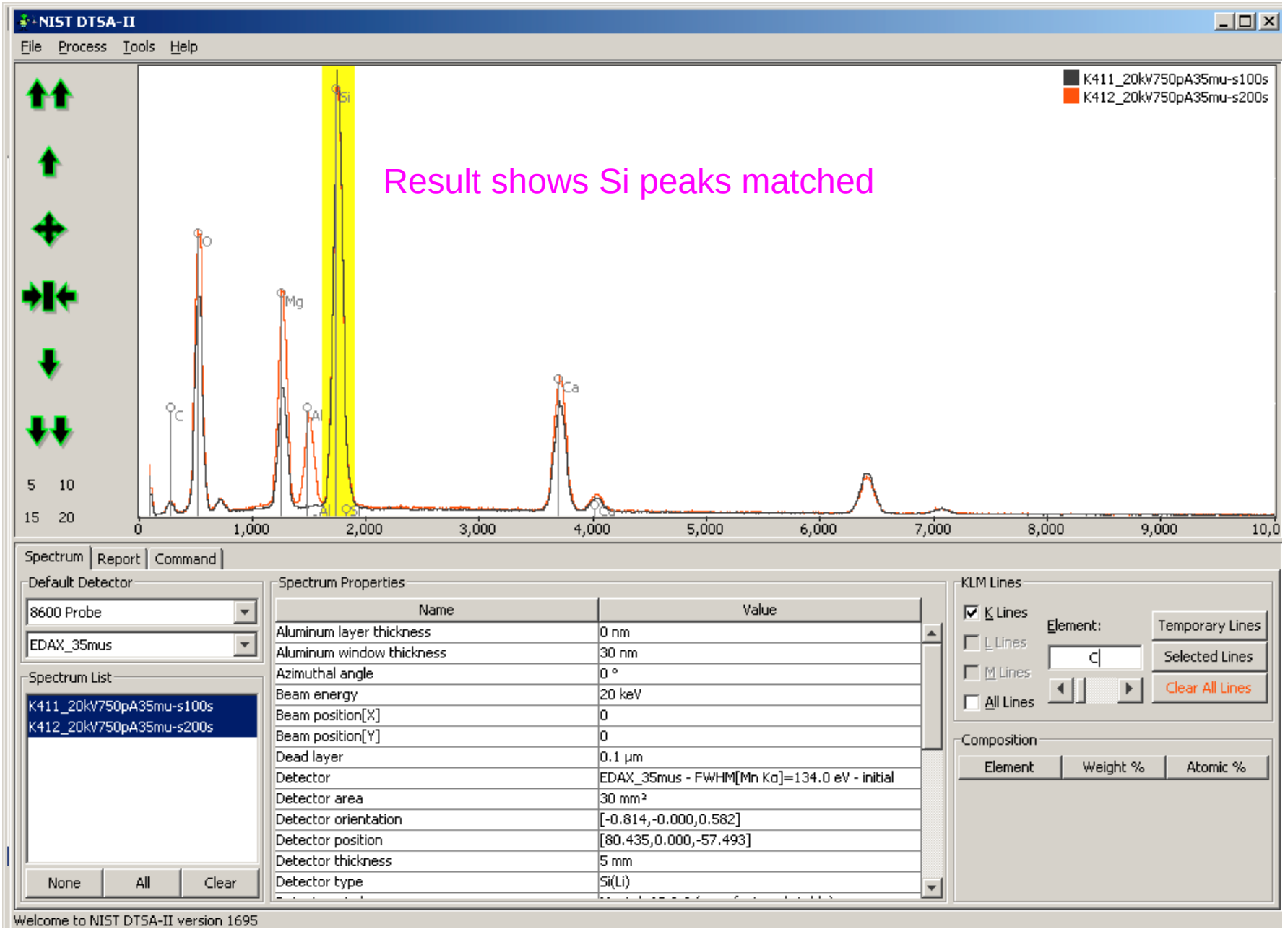
# Comparing multiple spectra



# Comparing multiple spectra



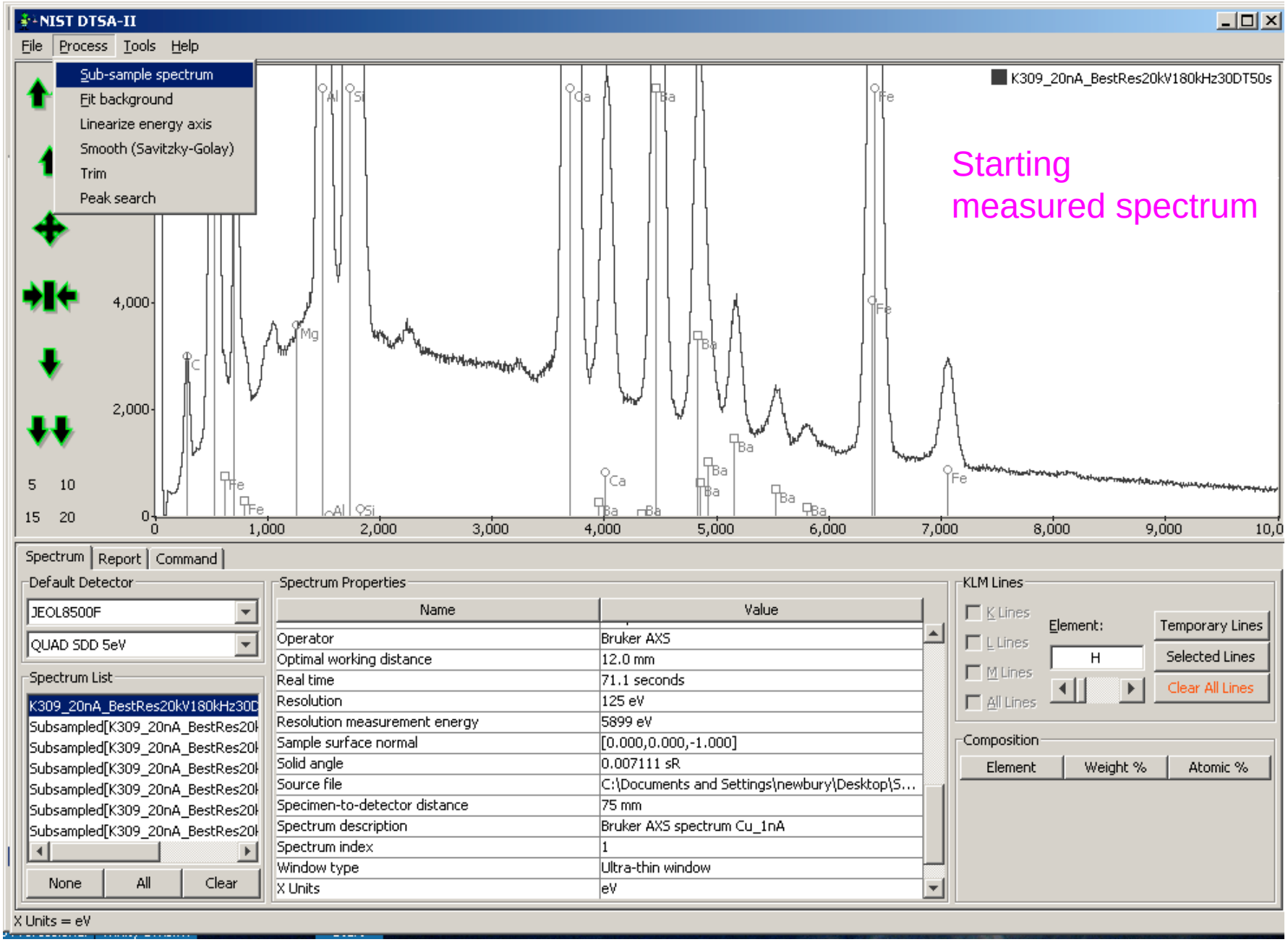
# Comparing multiple spectra



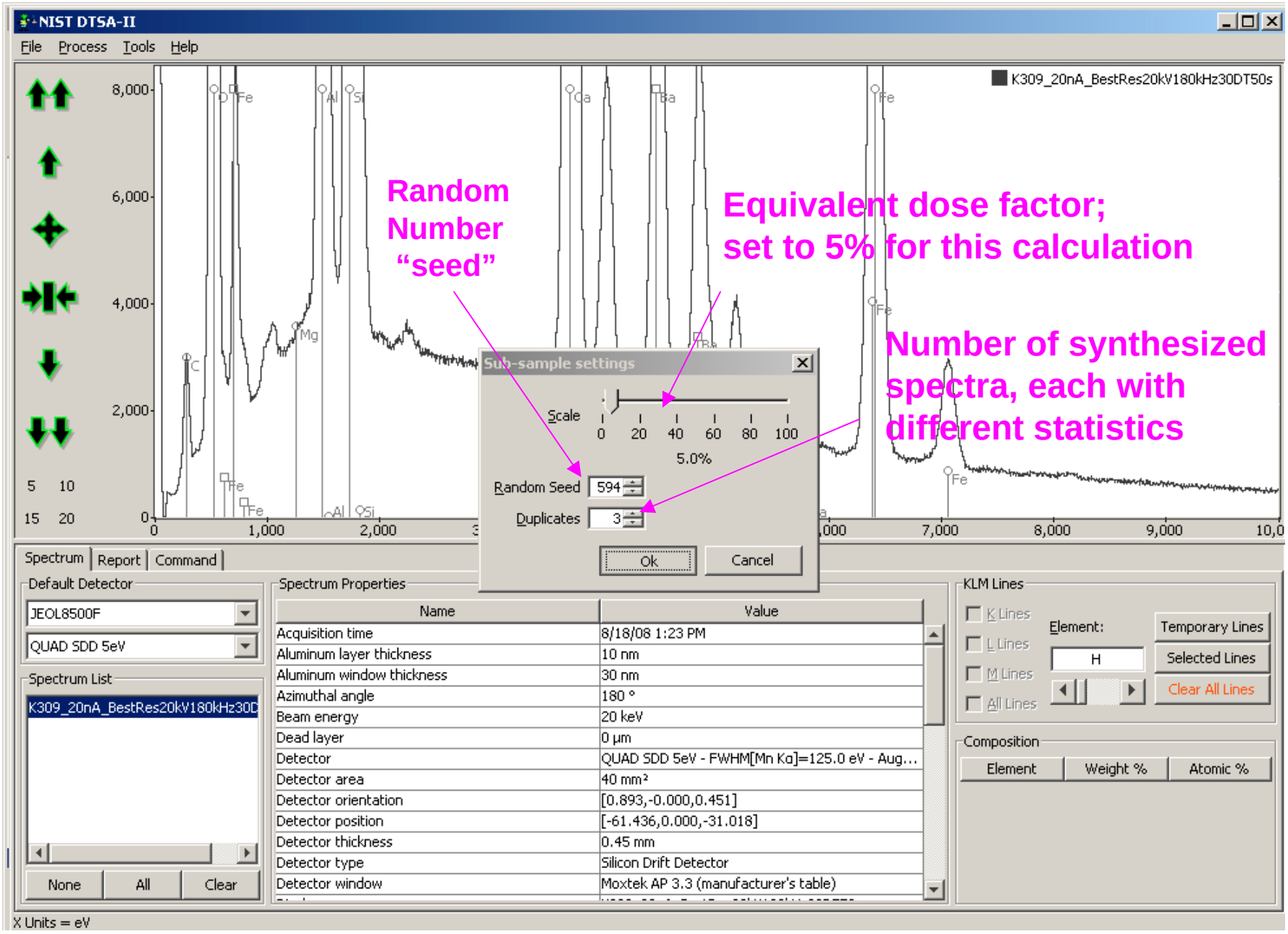
# Spectrum sub-sampling tool

- Take an experimentally measured spectrum and create one or more “sub-samples”, that is, equivalent spectra that would have been collected at lower dose.
- Sub-sampled spectra are useful for statistical studies. e.g., how does detection limit vary with dose.

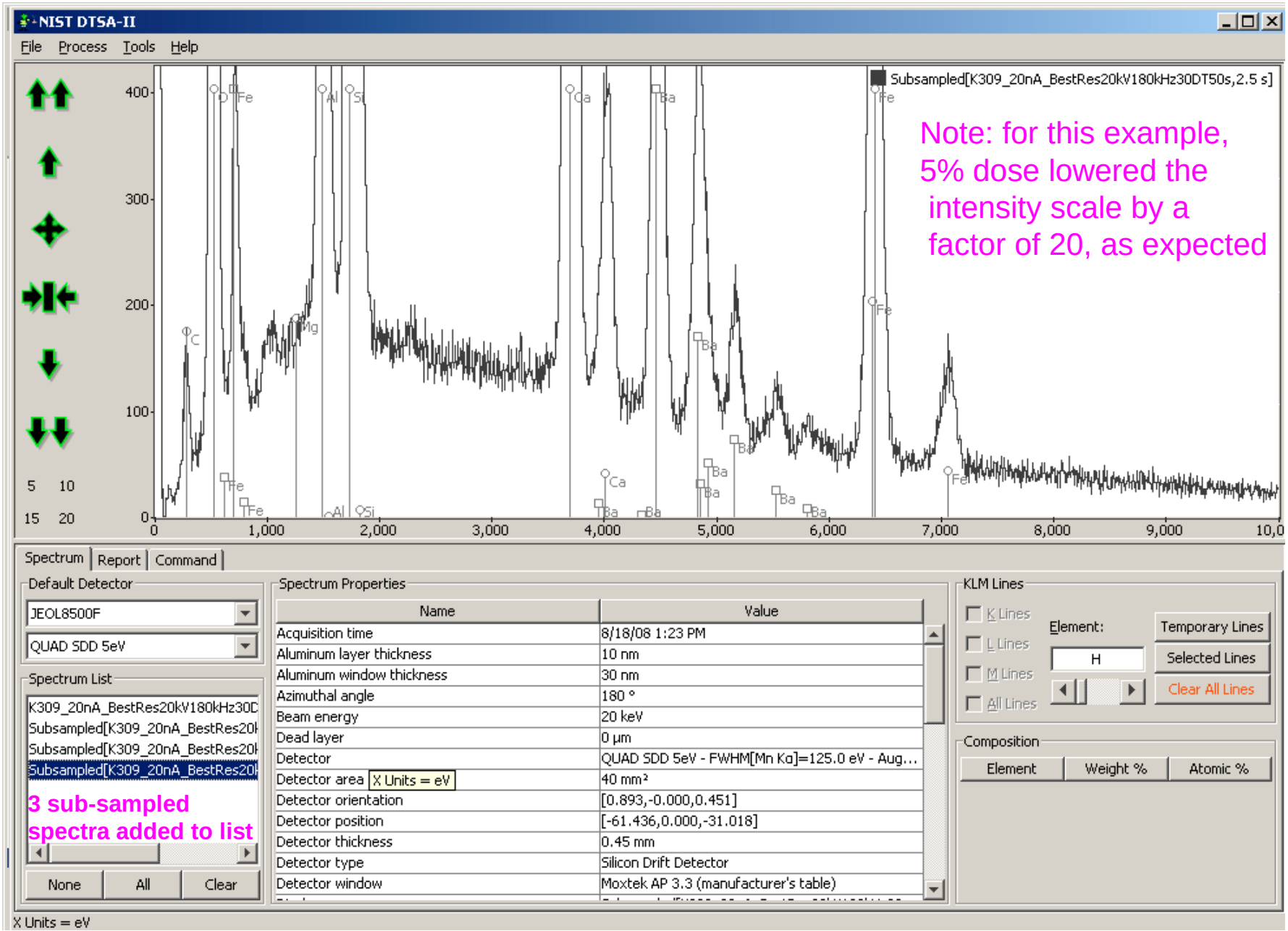
# Spectrum “sub-sampling”: creating equivalent spectra for other doses



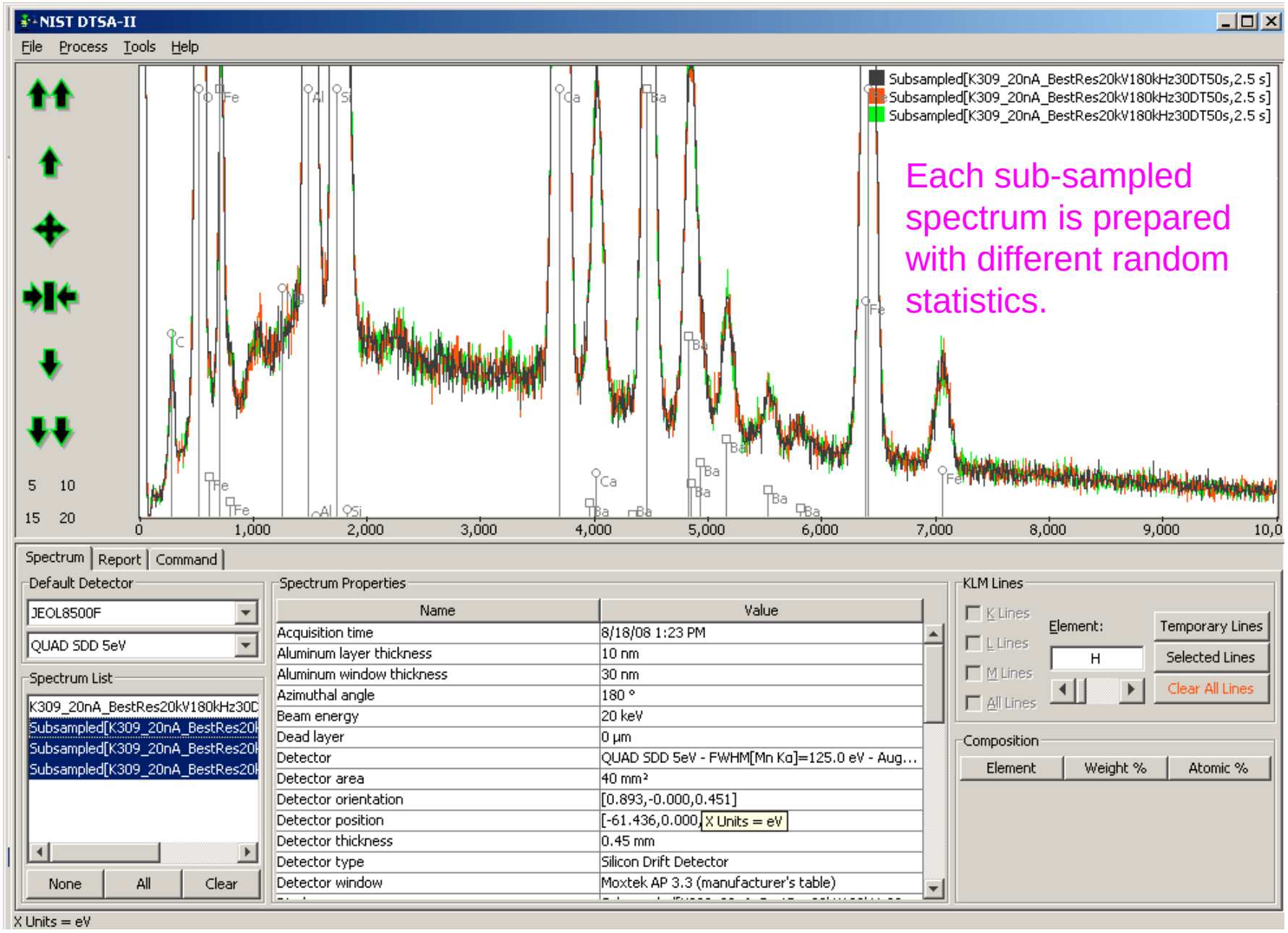
# Spectrum “sub-sampling”: creating equivalent spectra for other doses



# Spectrum “sub-sampling”: creating equivalent spectra for other doses

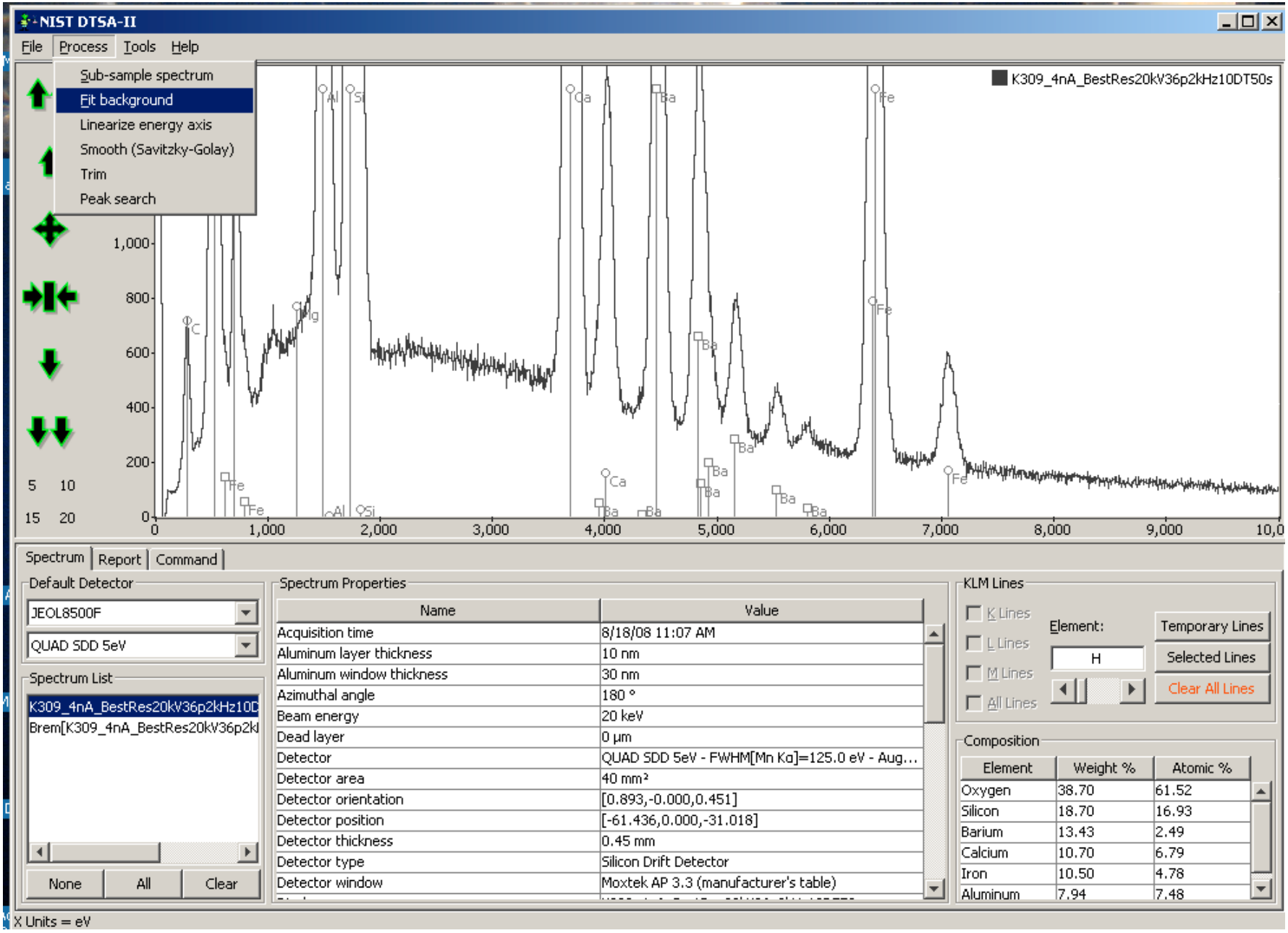


# Spectrum “sub-sampling”: creating equivalent spectra for other doses

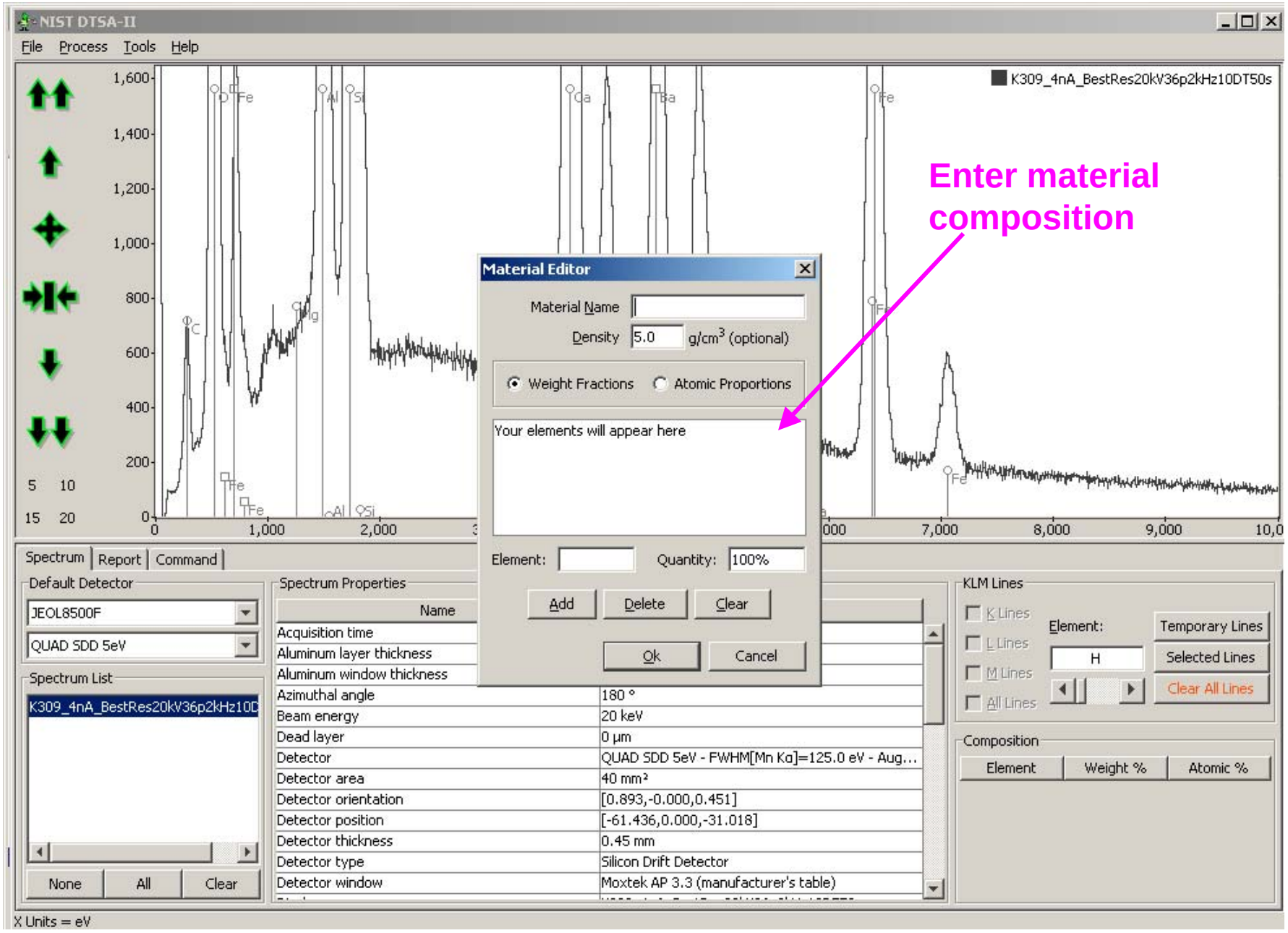


# Background fitting tool

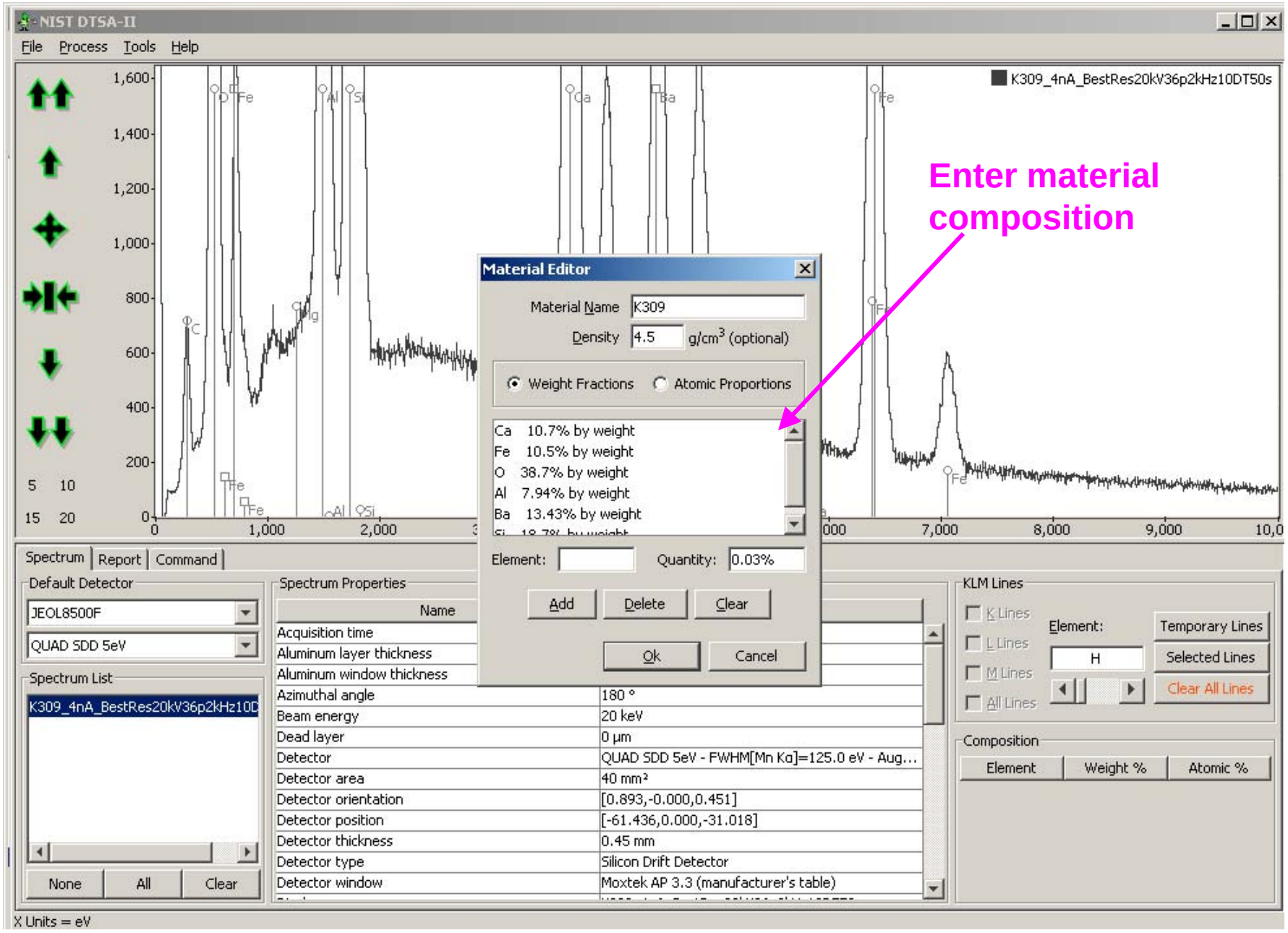
# Background Fitting



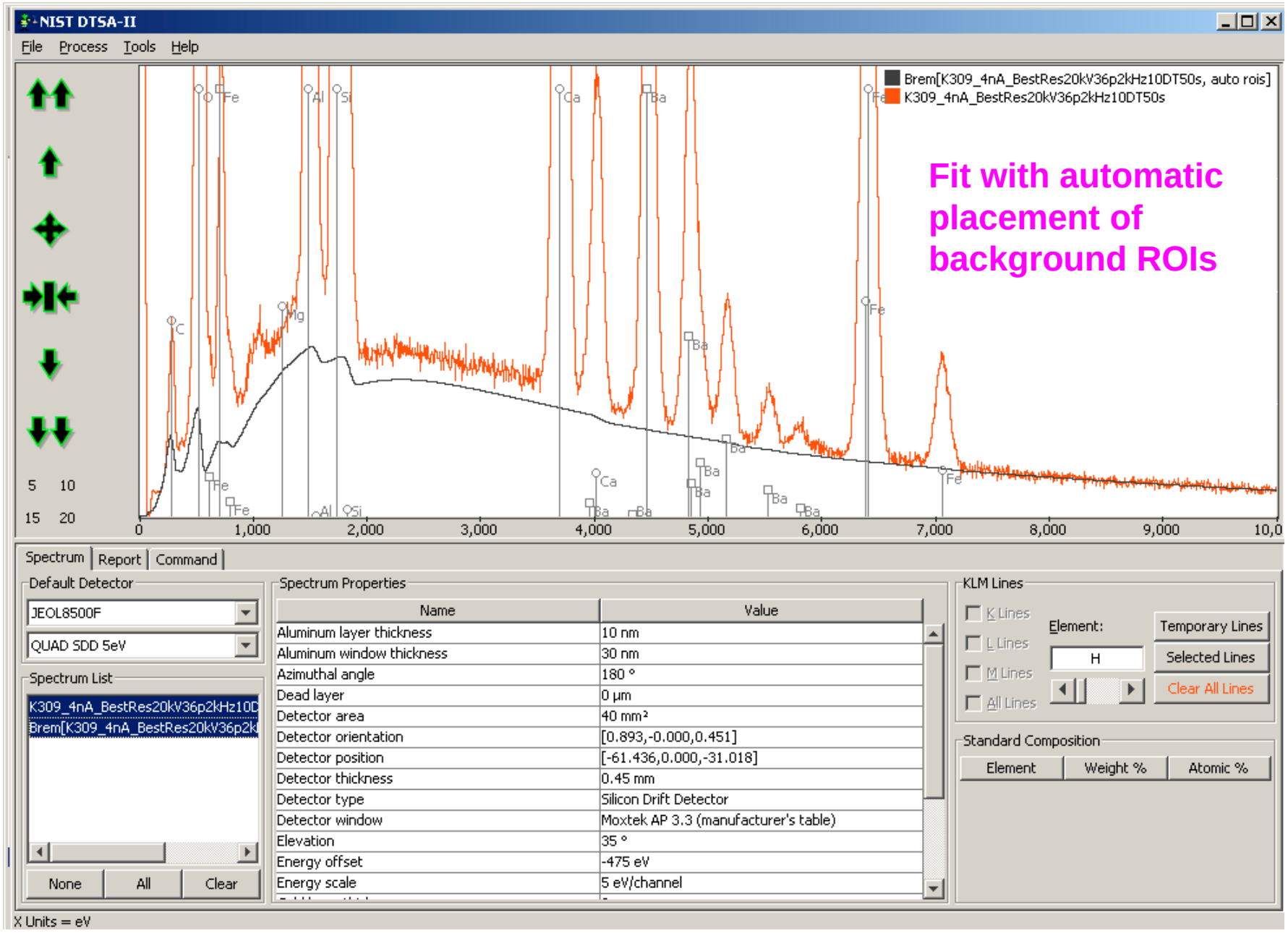
# Background Fitting



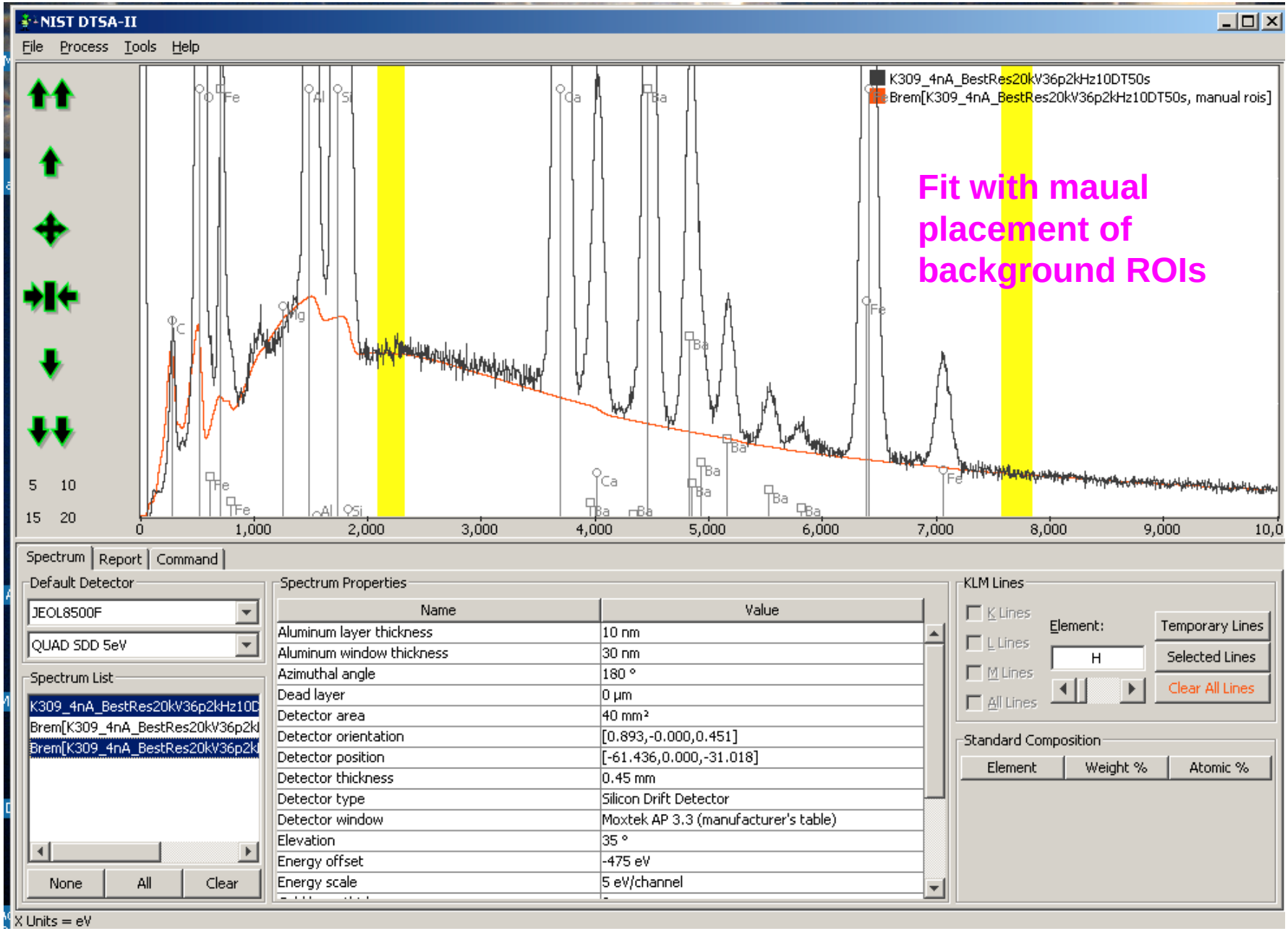
# Background Fitting



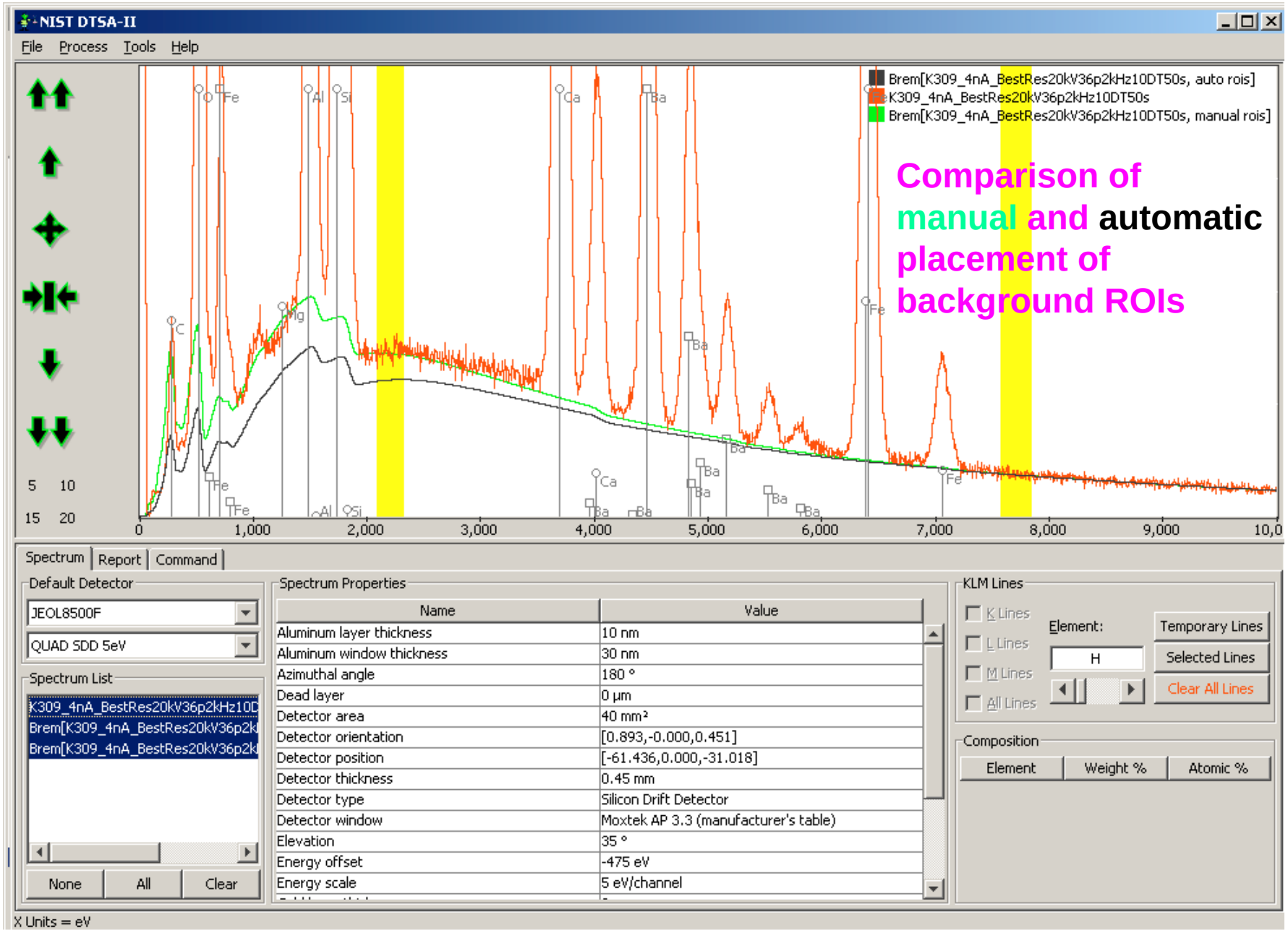
# Background Fitting



# Background Fitting



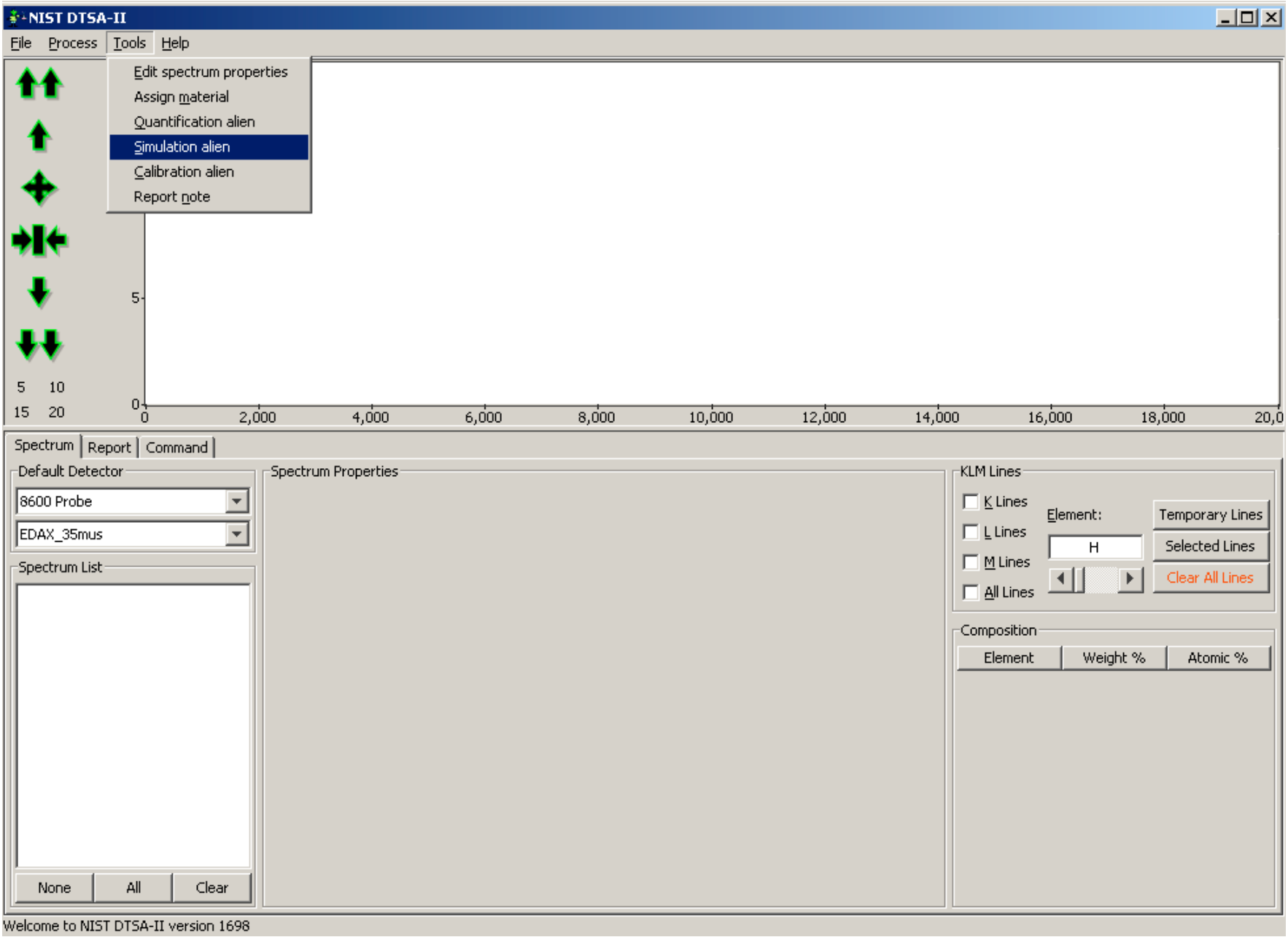
# Background Fitting



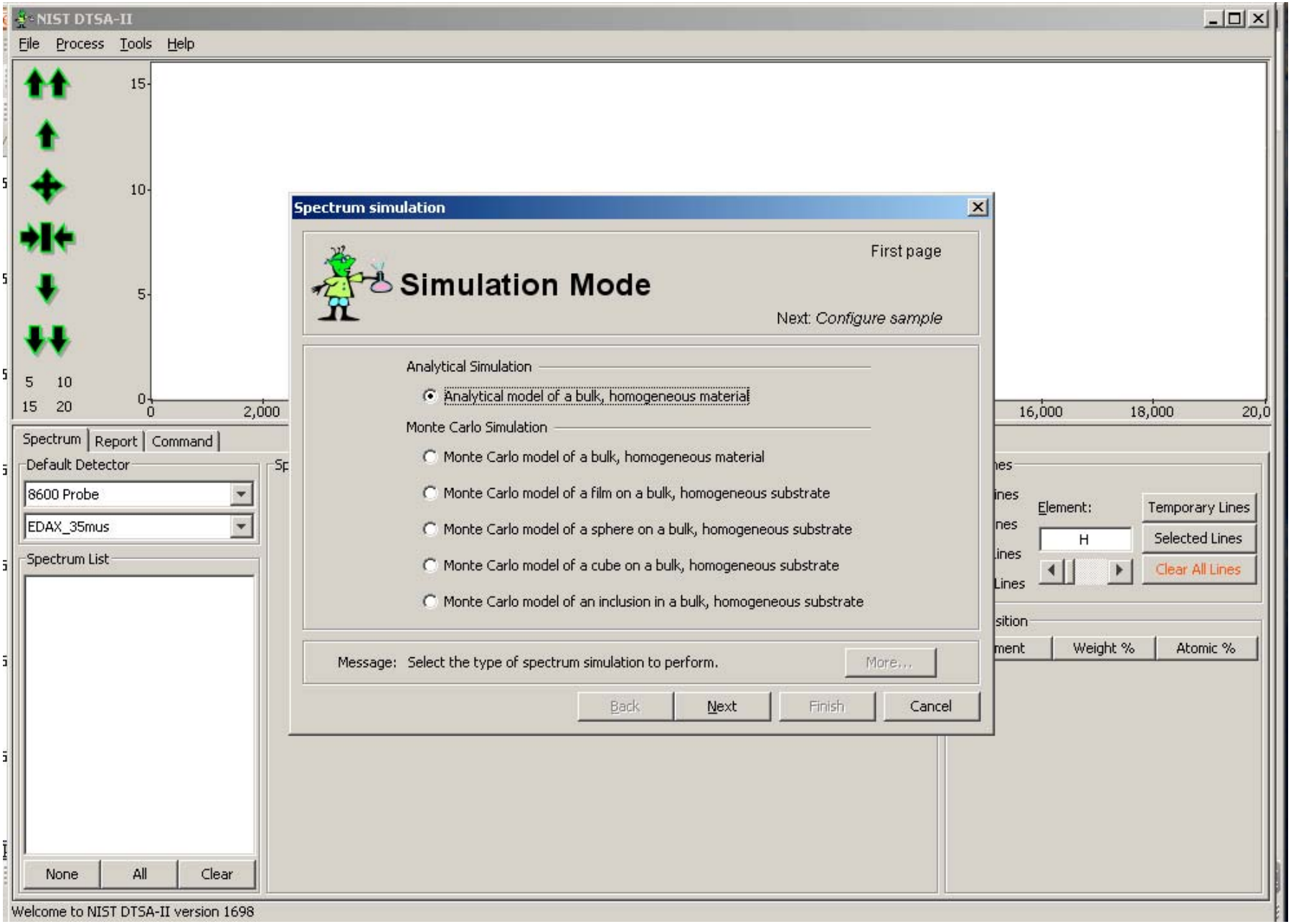
# DTSA-II Simulation Mode

- EDS spectra calculated from
  - 1. First principles, using best available cross sections and physical data (flat, bulk target only)

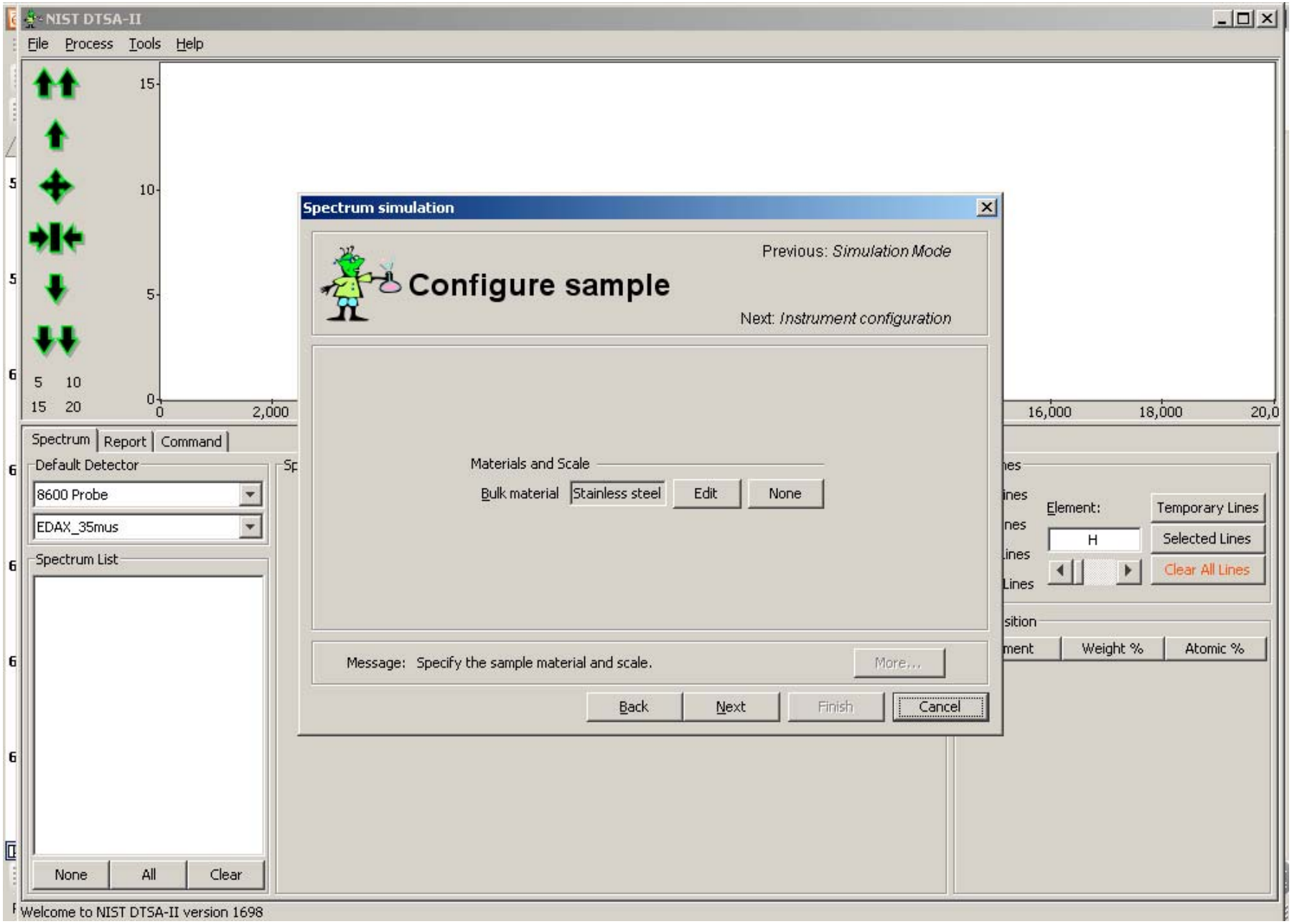
# Simulation Alien



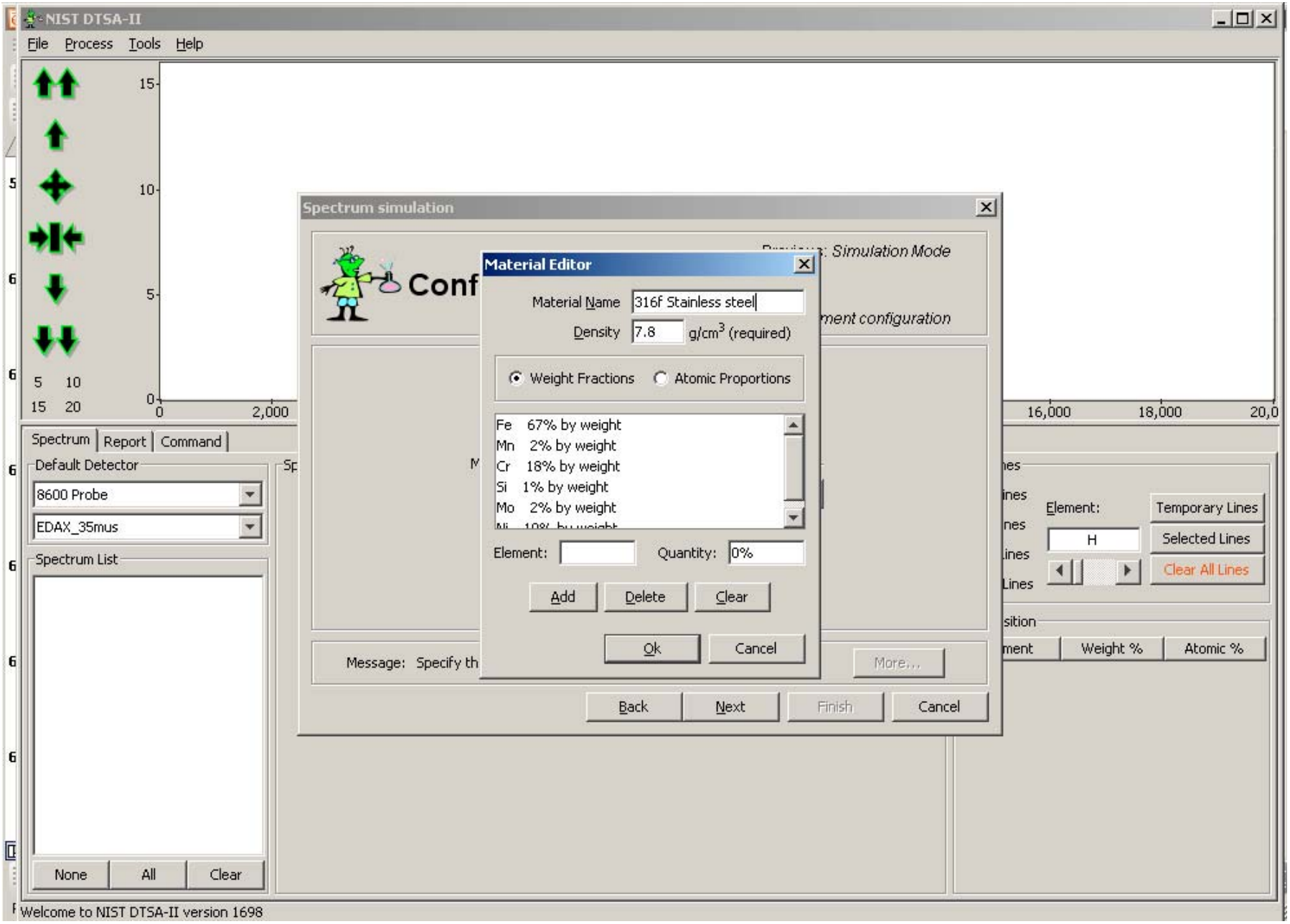
# Simulation Alien: selecting Analytical Simulation



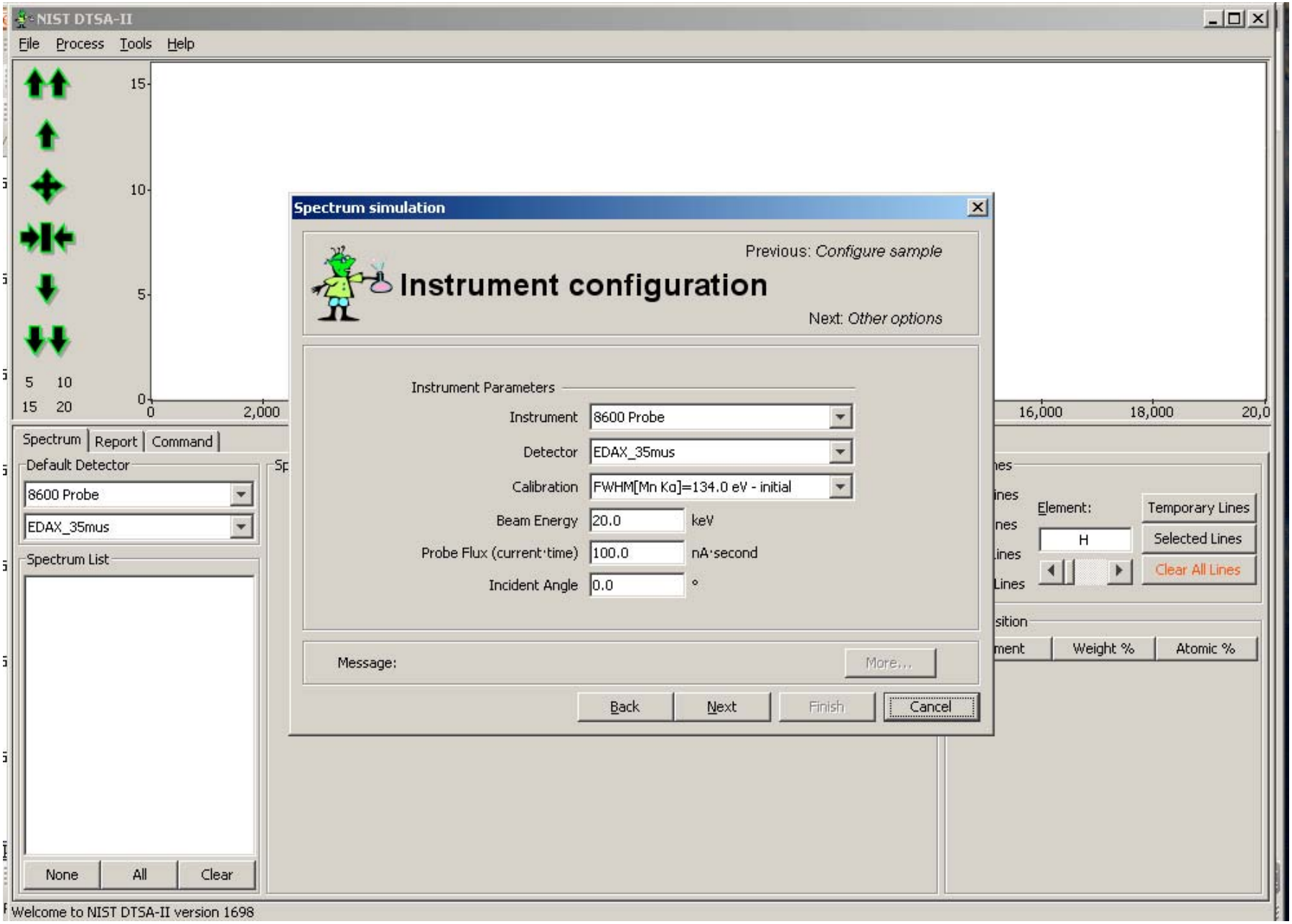
# Simulation Alien: specifying composition



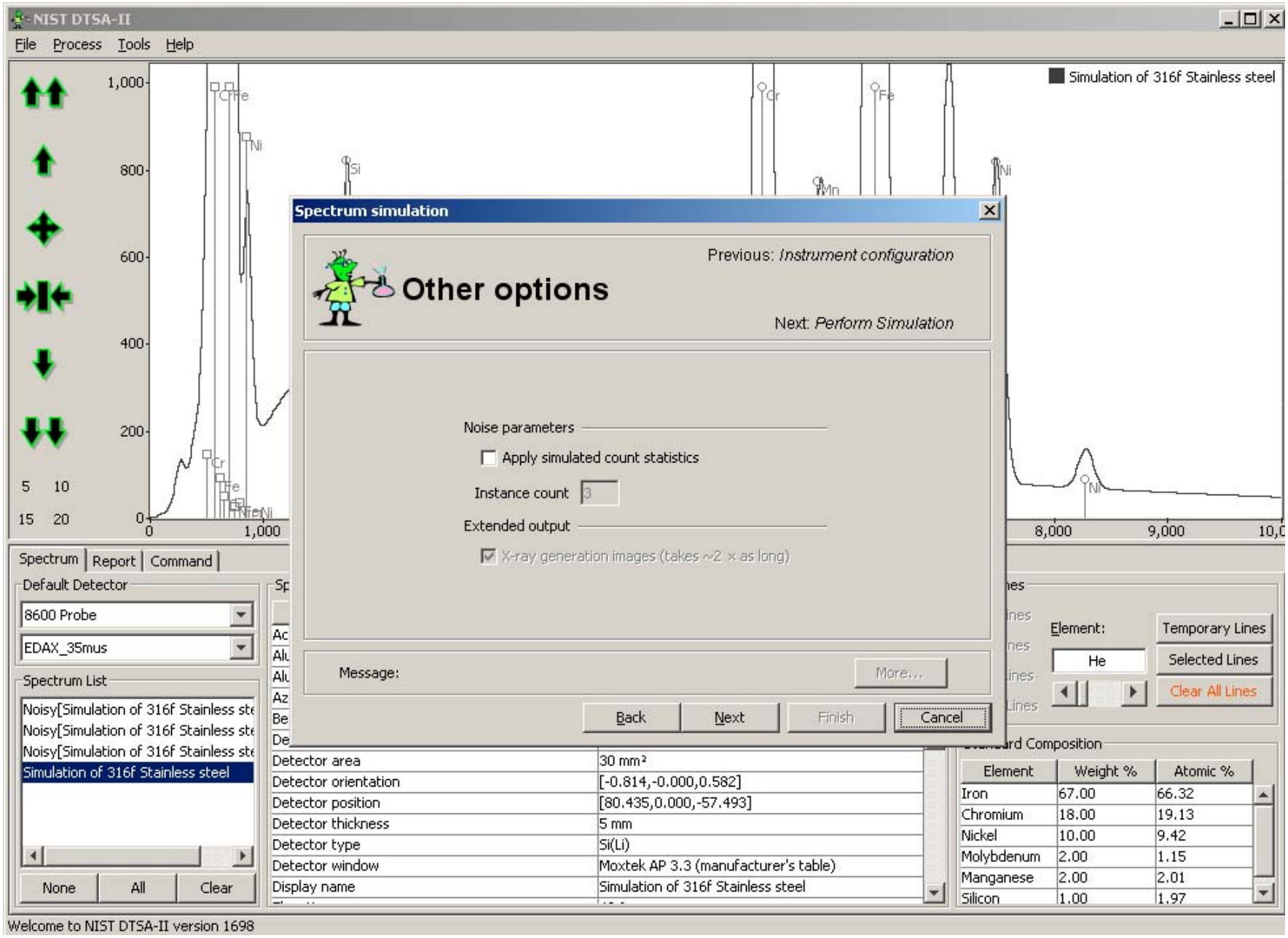
# Simulation Alien: target composition



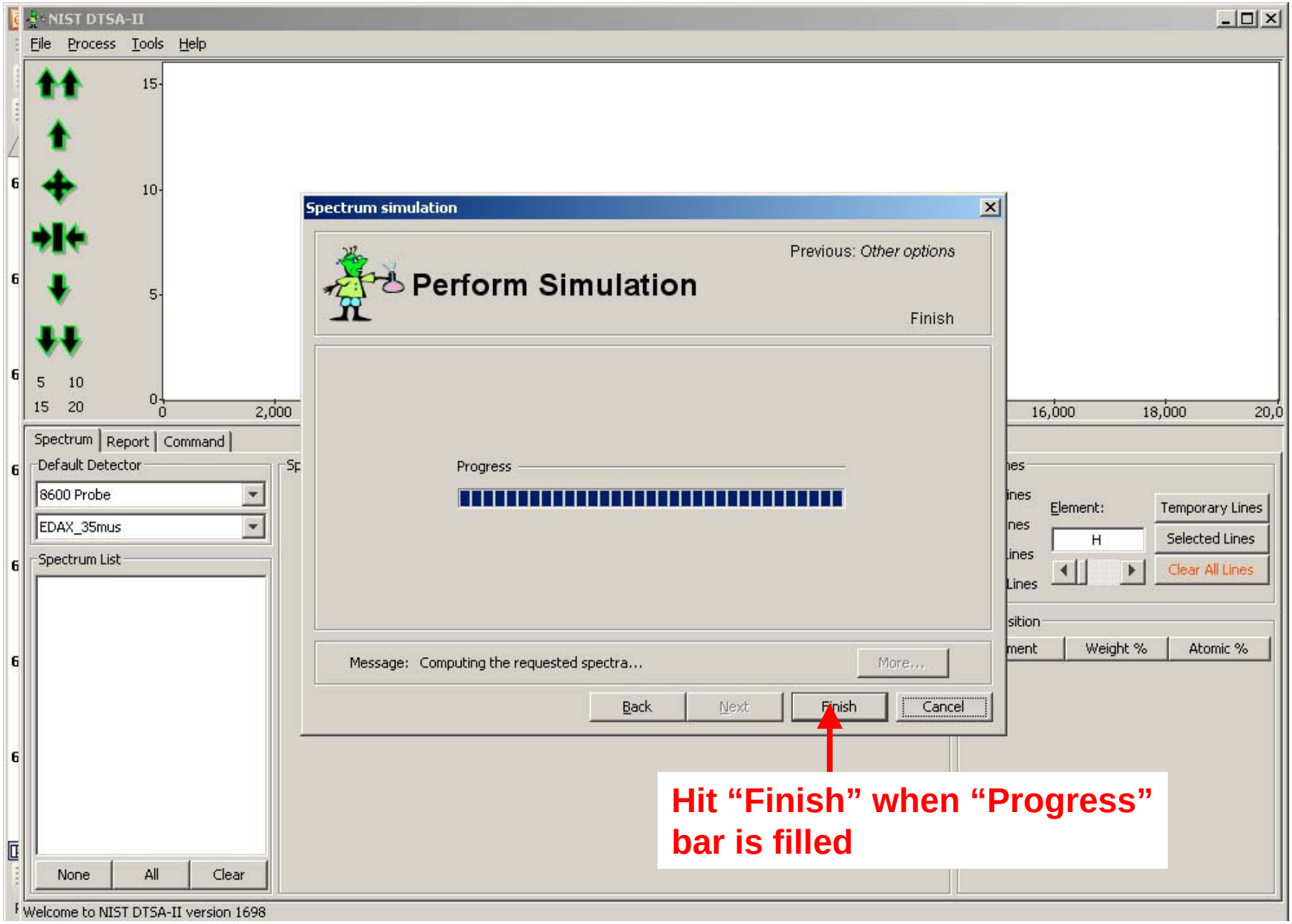
# Simulation Alien: instrument configuration



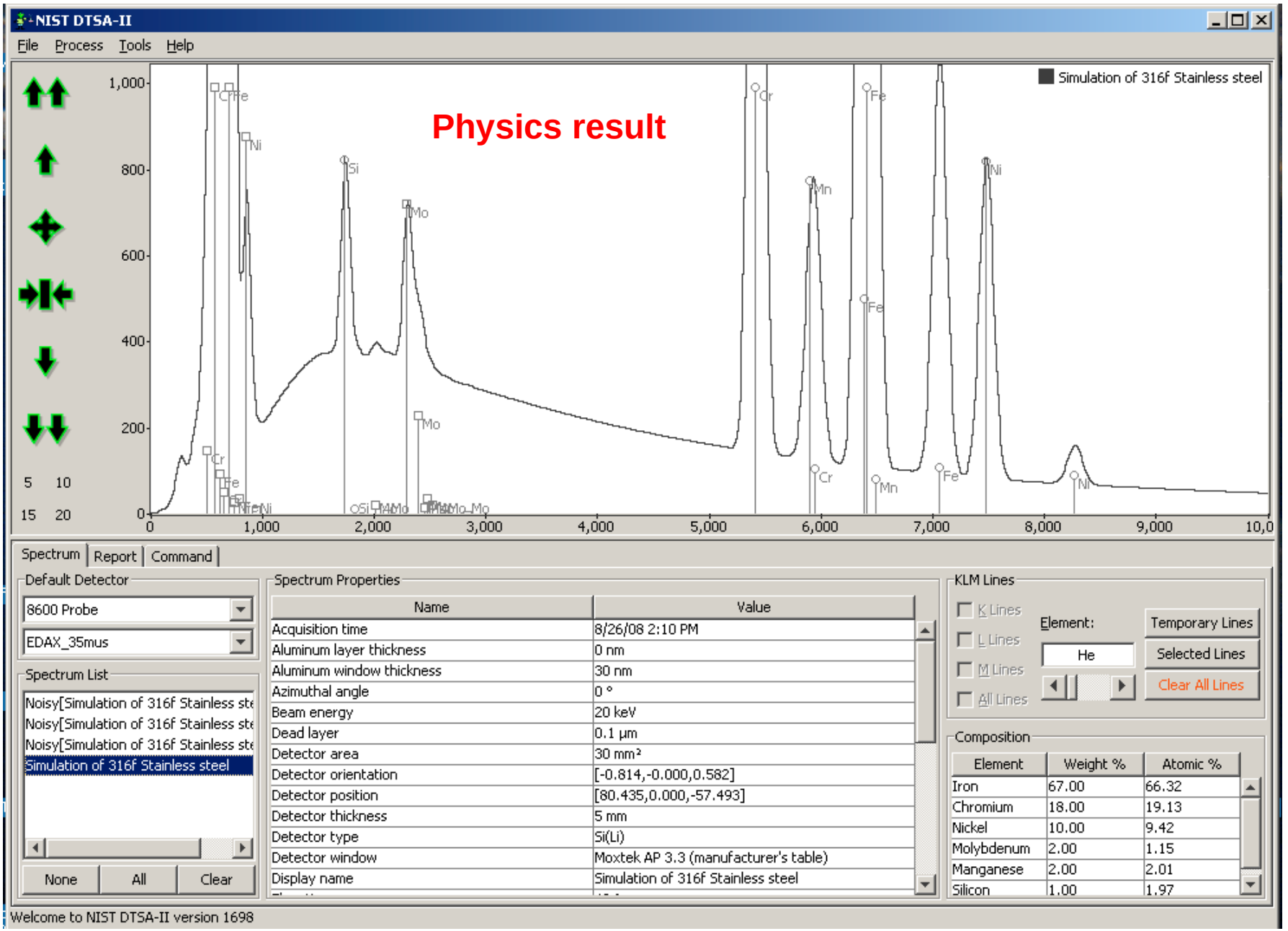
# Simulation Alien: Other options not invoked



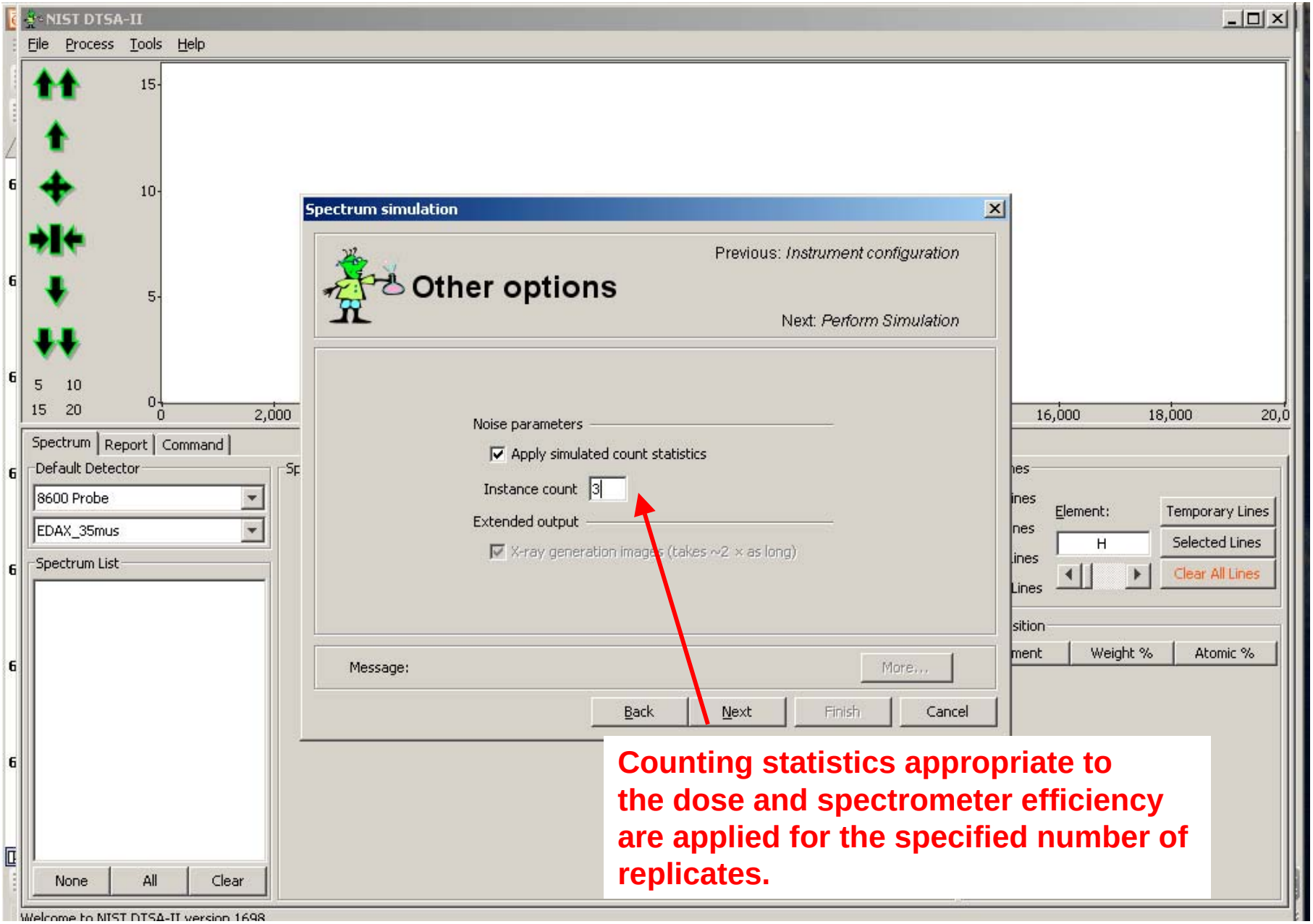
# Simulation Alien



# Simulation Alien

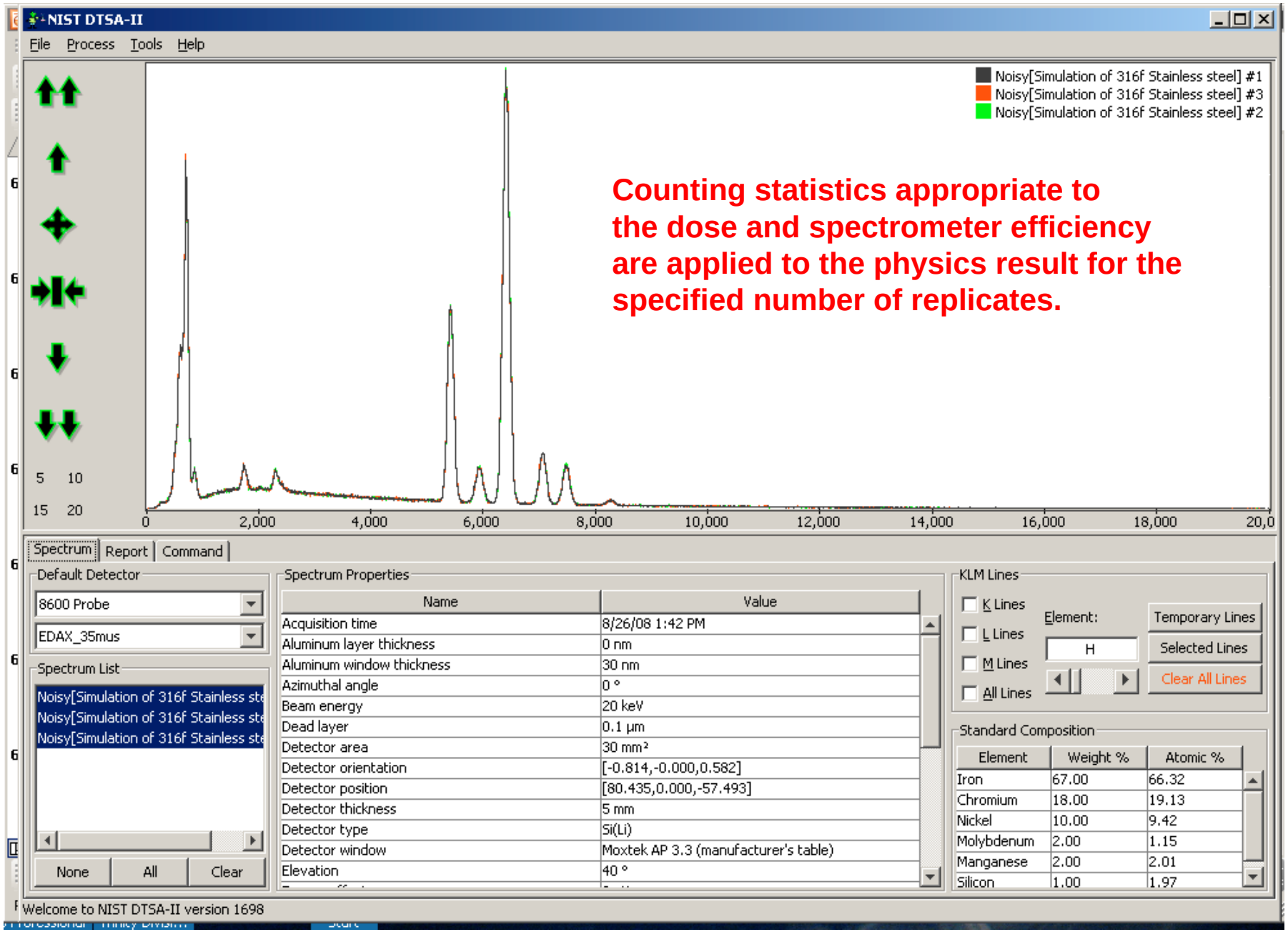


# Simulation Alien: Other options invoked

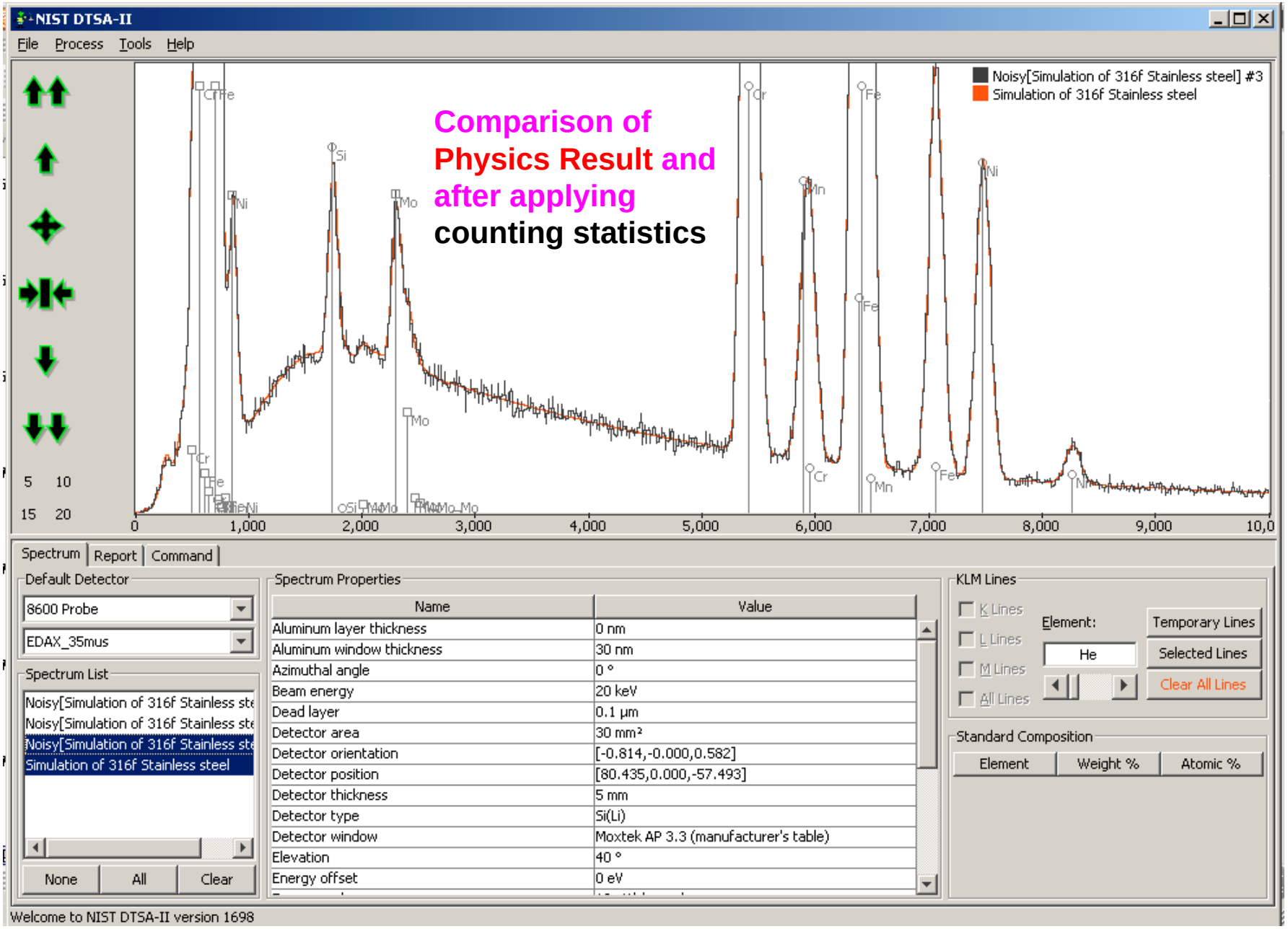



**Counting statistics appropriate to the dose and spectrometer efficiency are applied for the specified number of replicates.**

# Simulation Alien



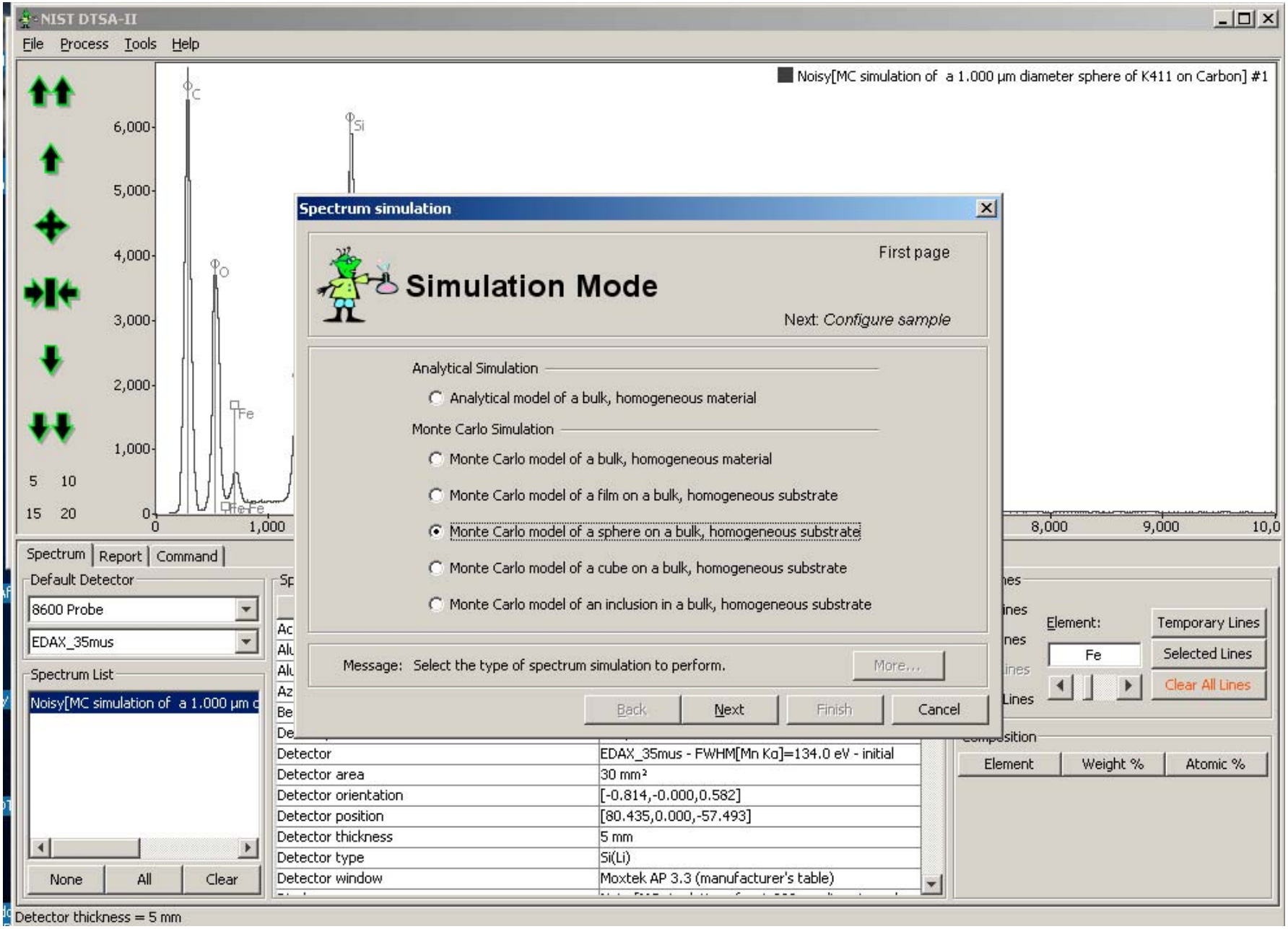
# Simulation Alien



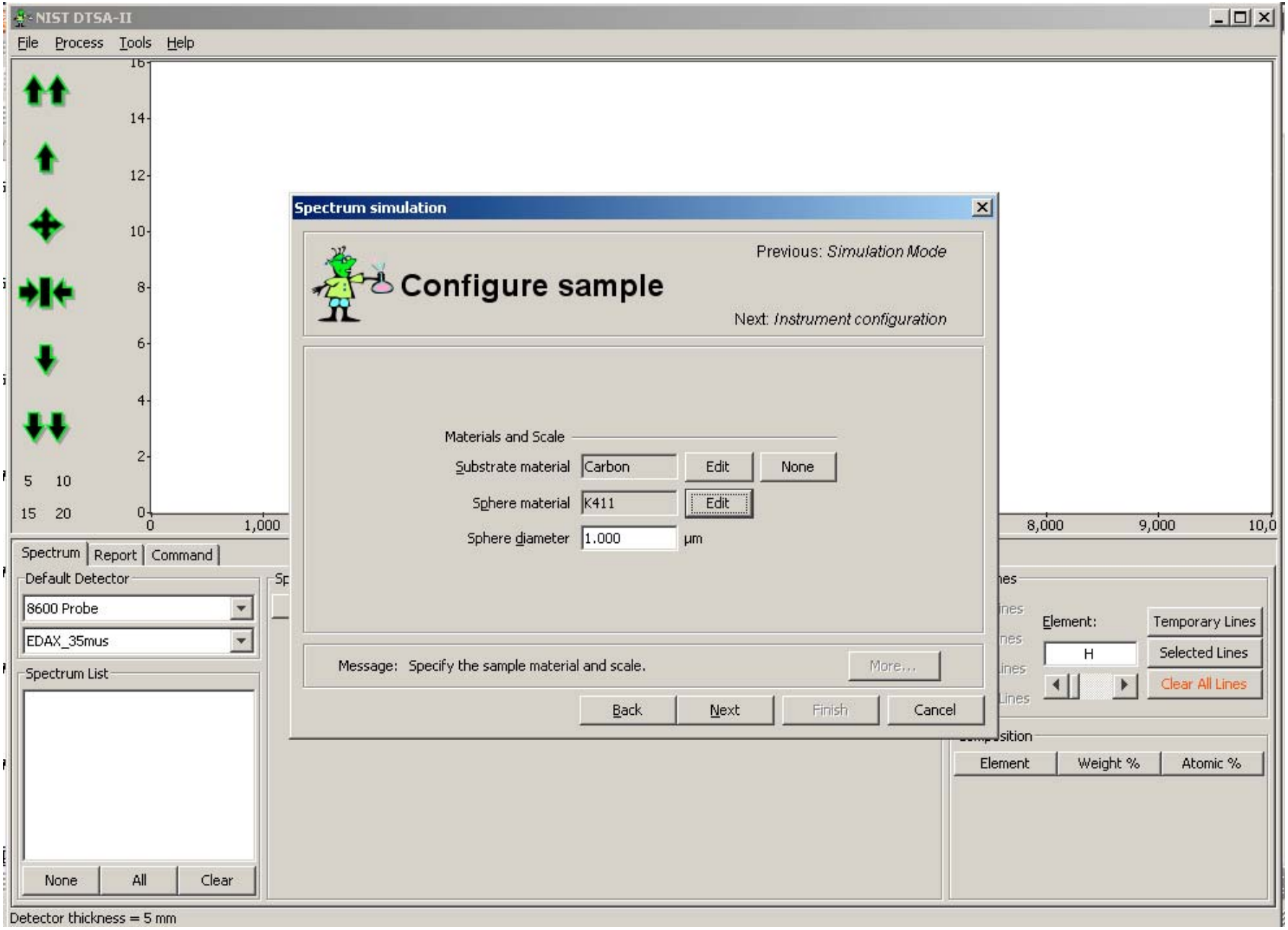
# DTSA-II Simulation Mode

- EDS spectra calculated from
  - 1. First principles, using best available cross sections and physical data (flat, bulk target only)
  - 2. Monte Carlo electron trajectory simulation for various specimen configurations:
    - 1. Flat, bulk
    - 2. Layer on bulk
    - 3. Inclusion (hemisphere) embedded in bulk
    - **4. Spherical particle on substrate**
    - 5. Cubic particle on substrate

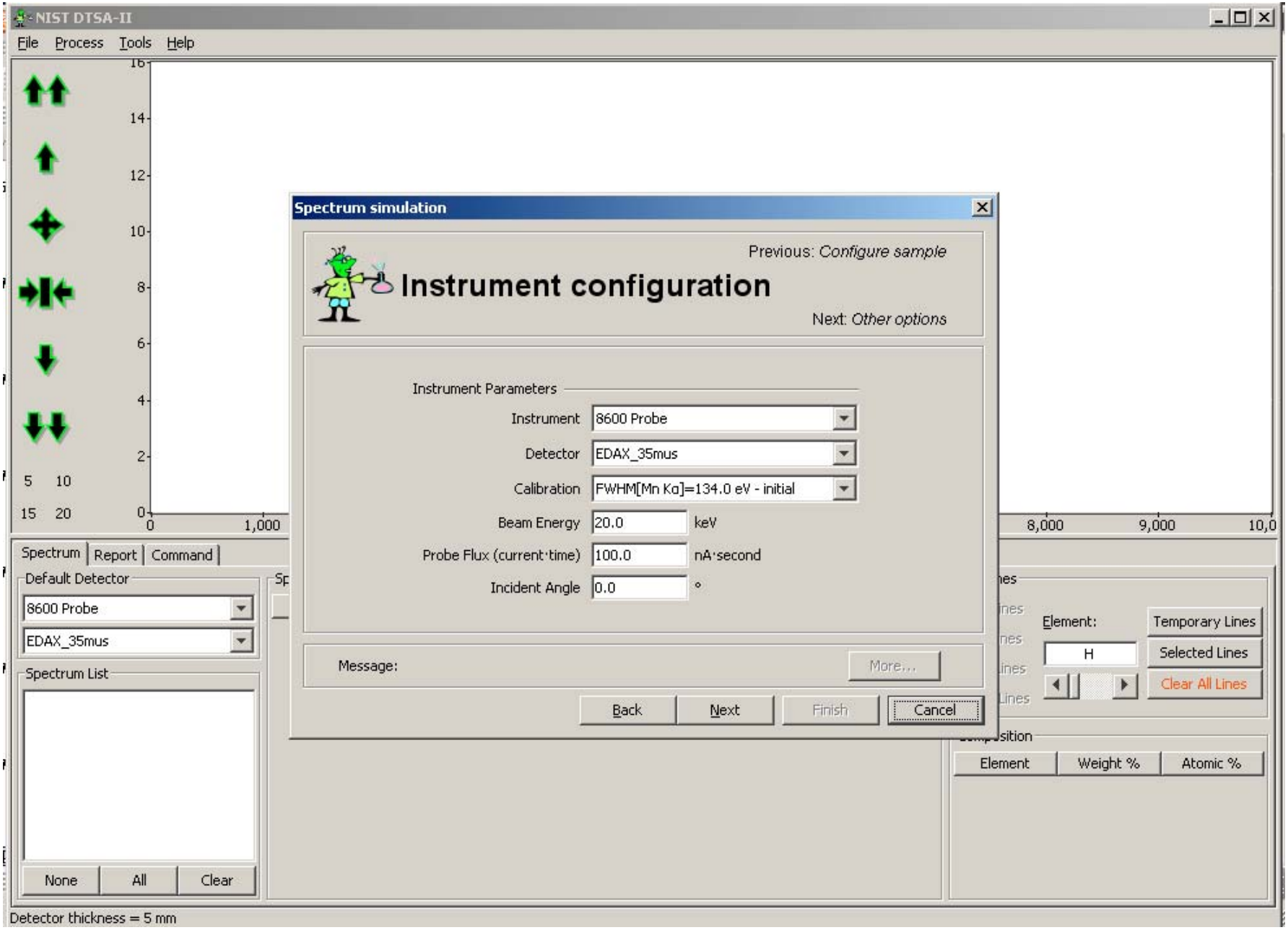
# Simulation Alien: Monte Carlo simulation of a 1 μm K411 glass sphere on a C substrate



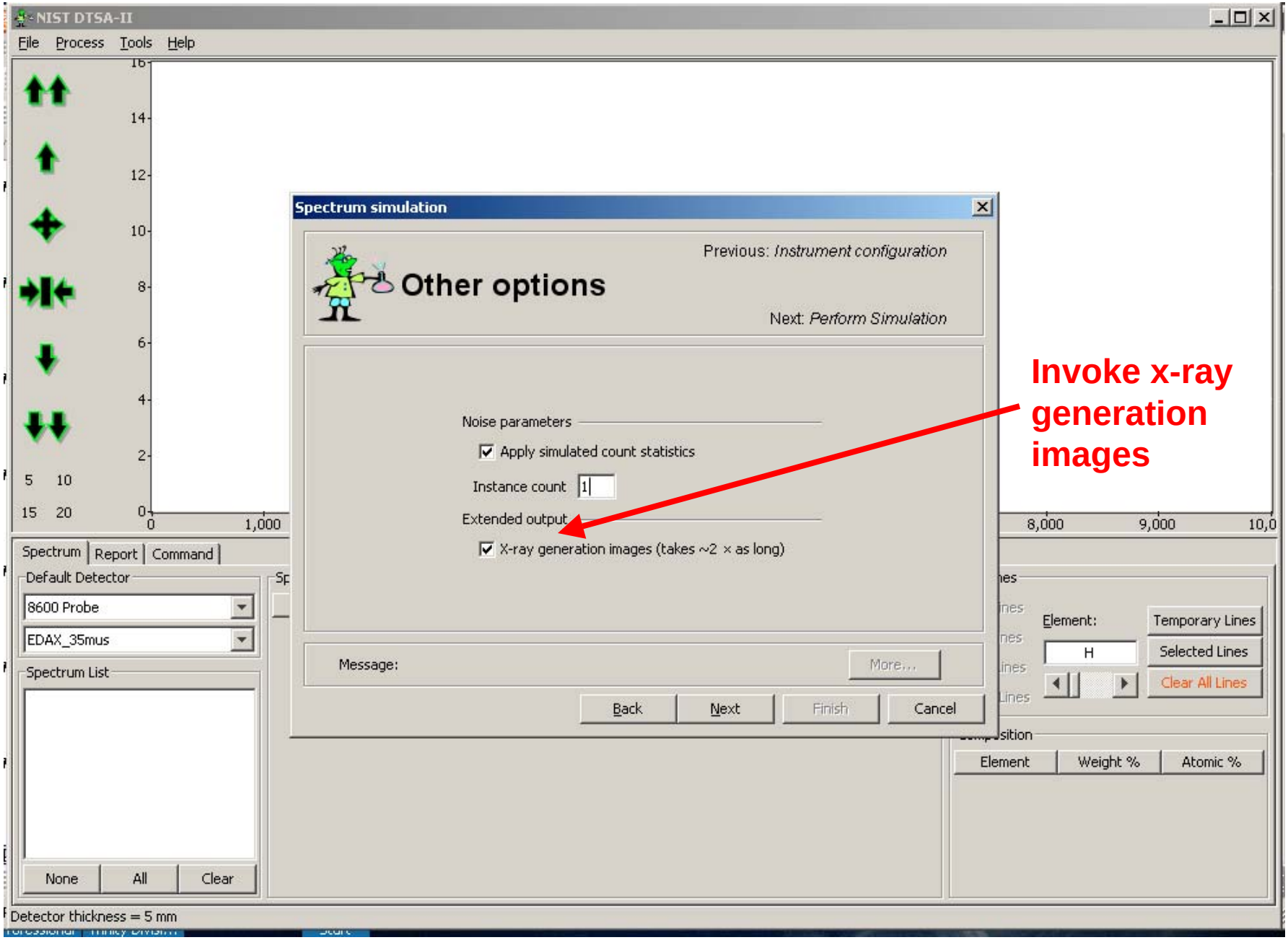
# Simulation Alien: Monte Carlo simulation of a 1 μm K411 glass sphere on a C substrate



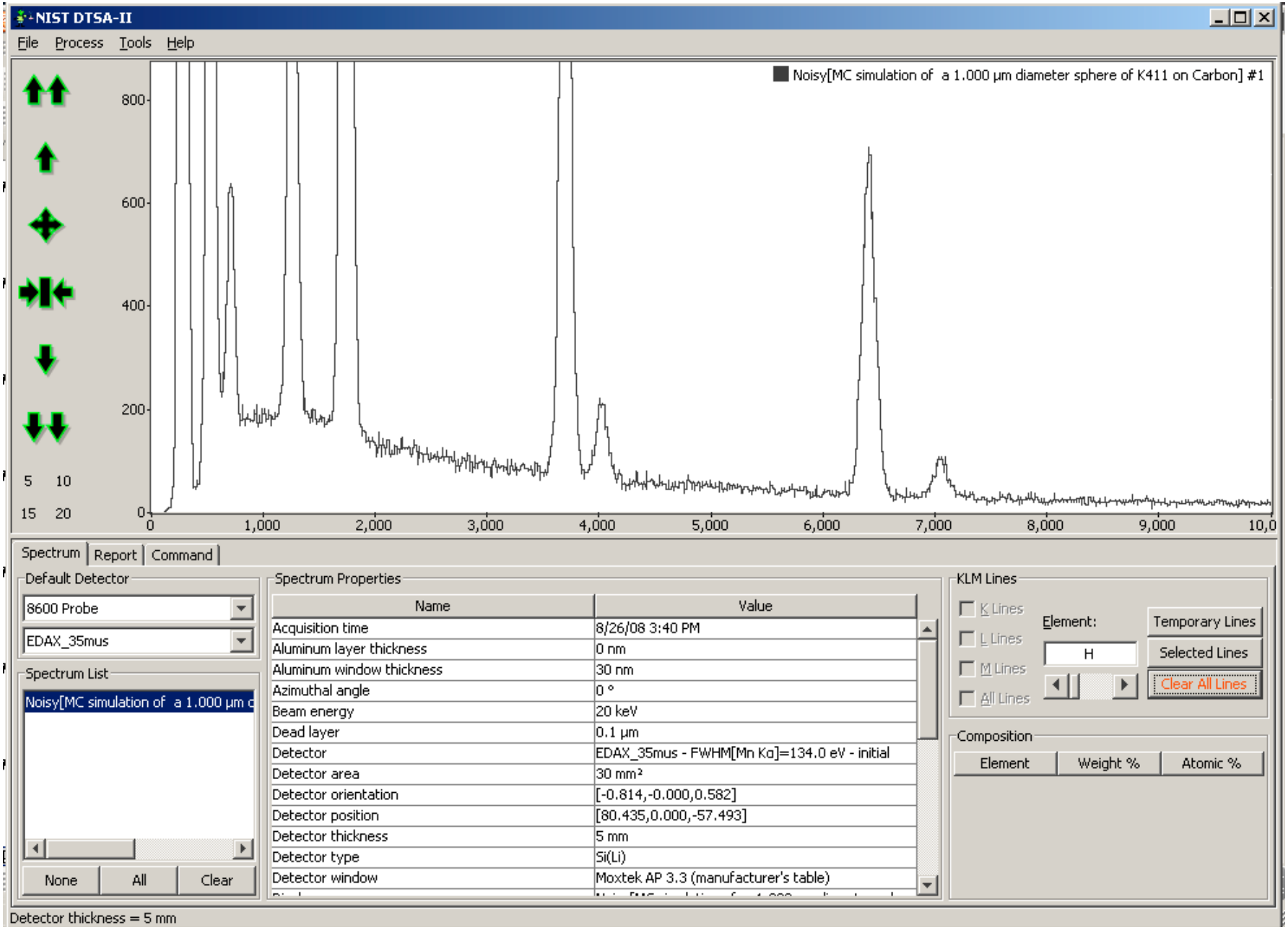
# Simulation Alien: Monte Carlo simulation of a 1 μm K411 glass sphere on a C substrate



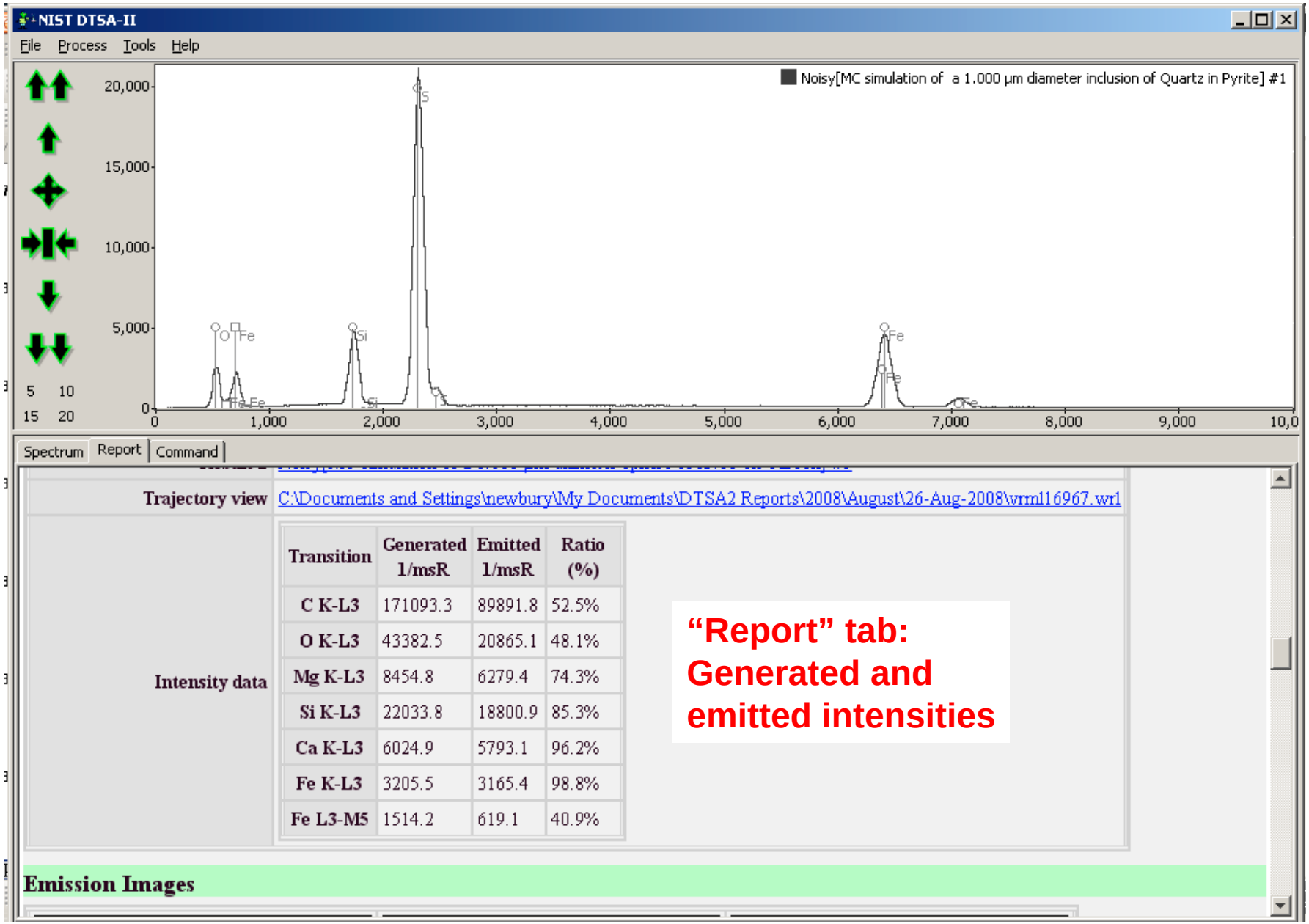
# Simulation Alien: Monte Carlo simulation of a 1 μm K411 glass sphere on a C substrate



# Simulation Alien: Monte Carlo simulation of a 1 μm K411 glass sphere on a C substrate

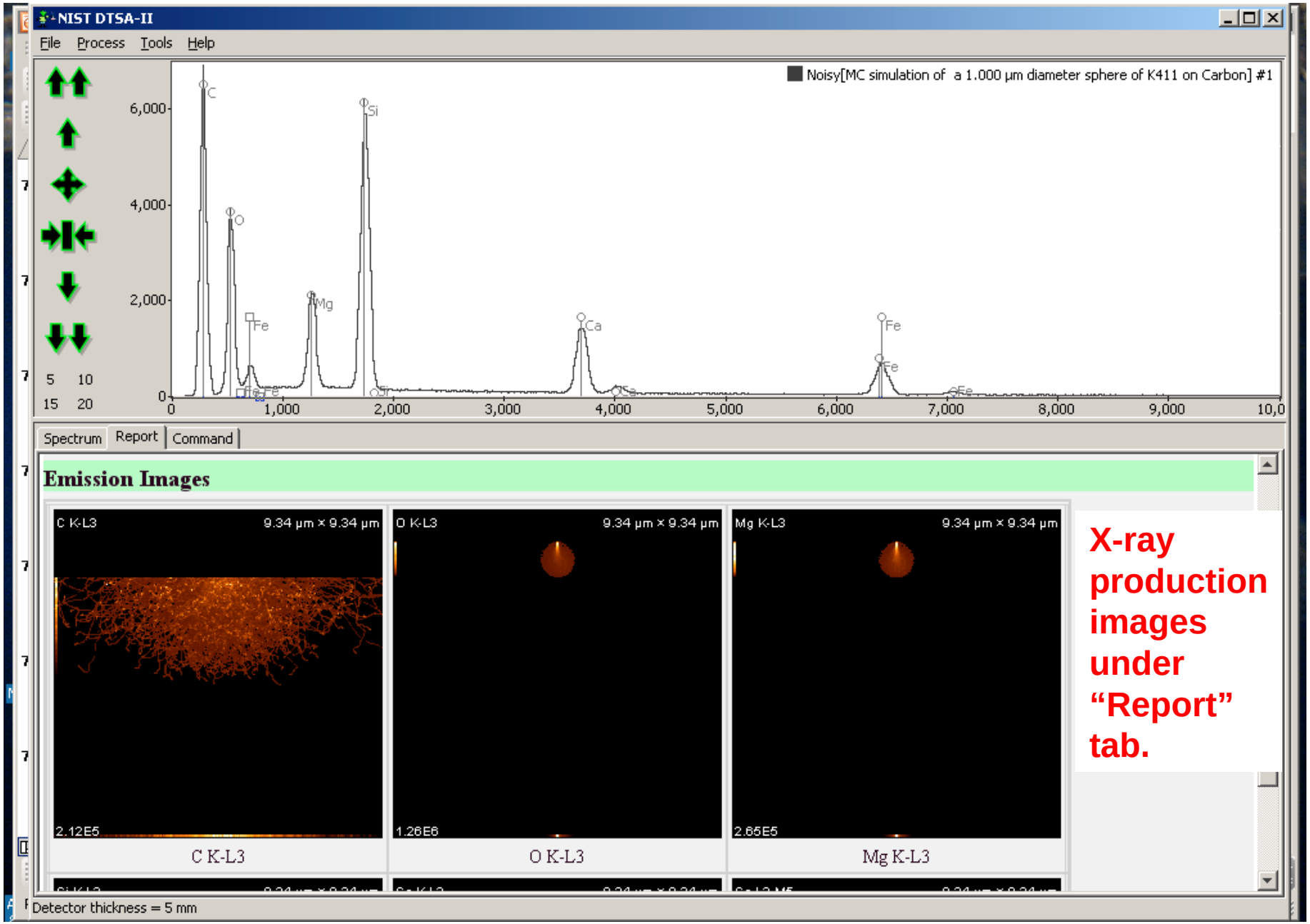


# Simulation Alien: Monte Carlo simulation of a 1 μm K411 glass sphere on a C substrate



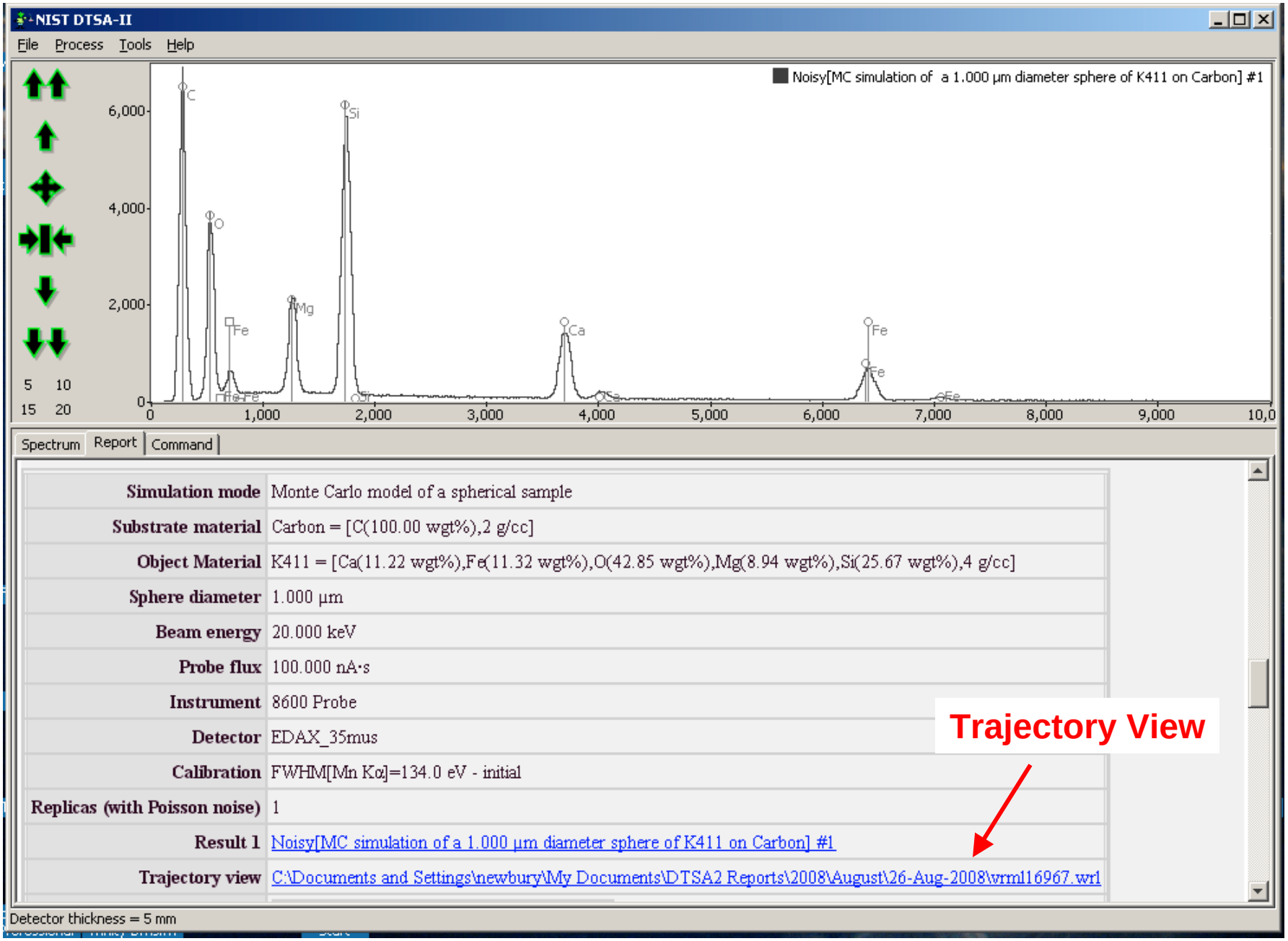

**"Report" tab: Generated and emitted intensities**

# Simulation Alien: Monte Carlo simulation of a 1 μm K411 glass sphere on a C substrate



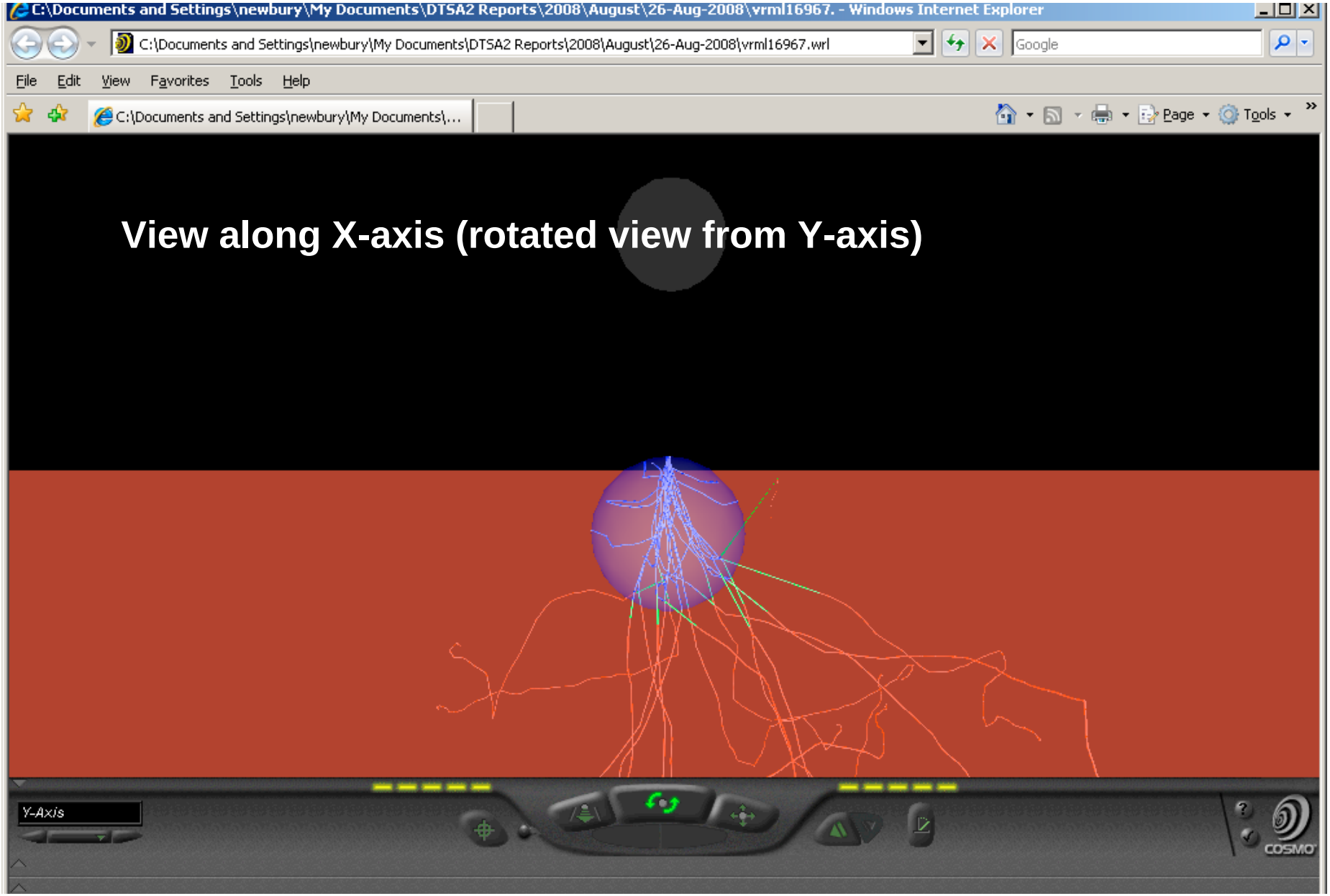

**X-ray production images under "Report" tab.**

# Simulation Alien: Monte Carlo simulation of a 1 μm K411 glass sphere on a C substrate

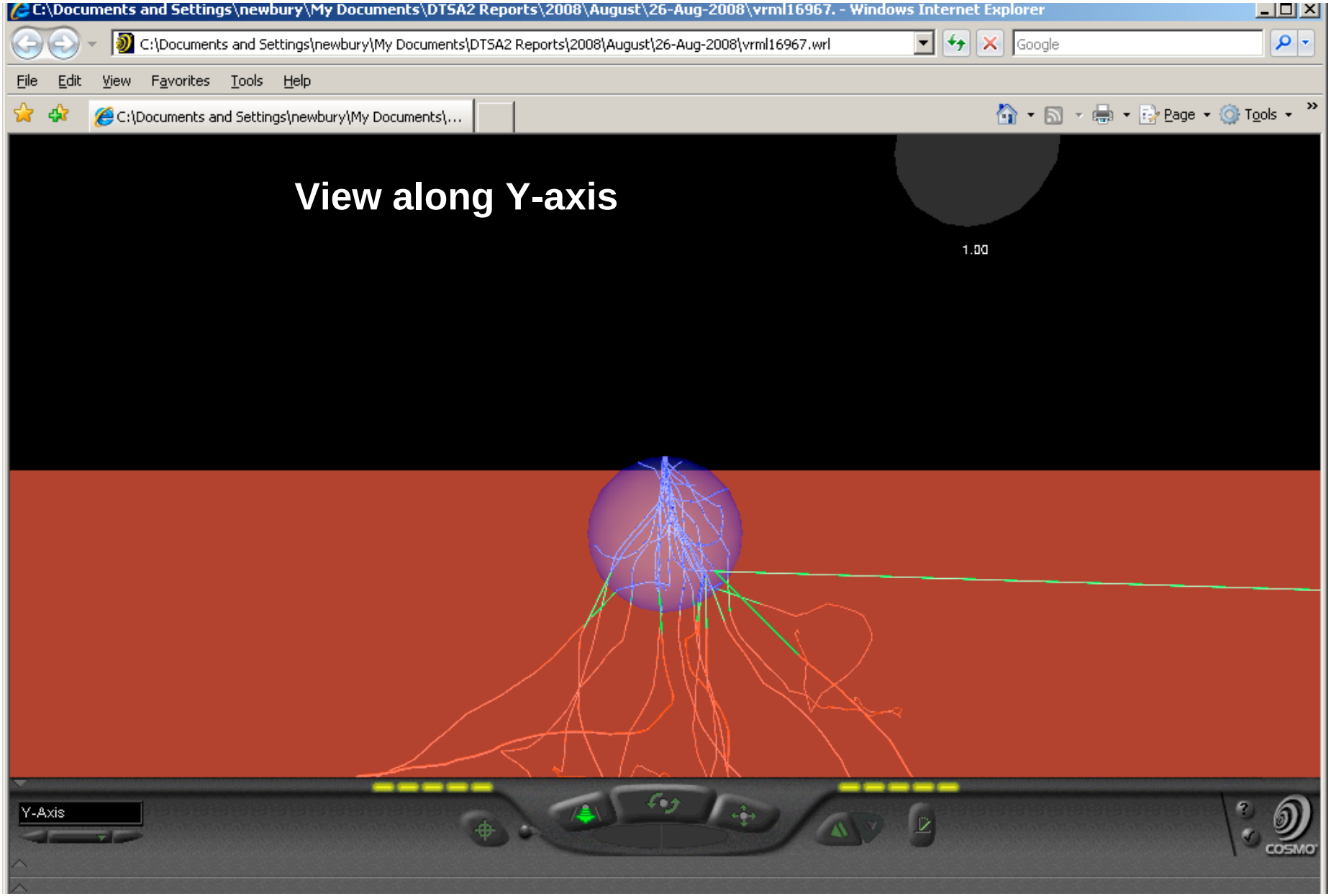


## Simulation Alien: Monte Carlo simulation trajectories can be viewed with Cosmo Player

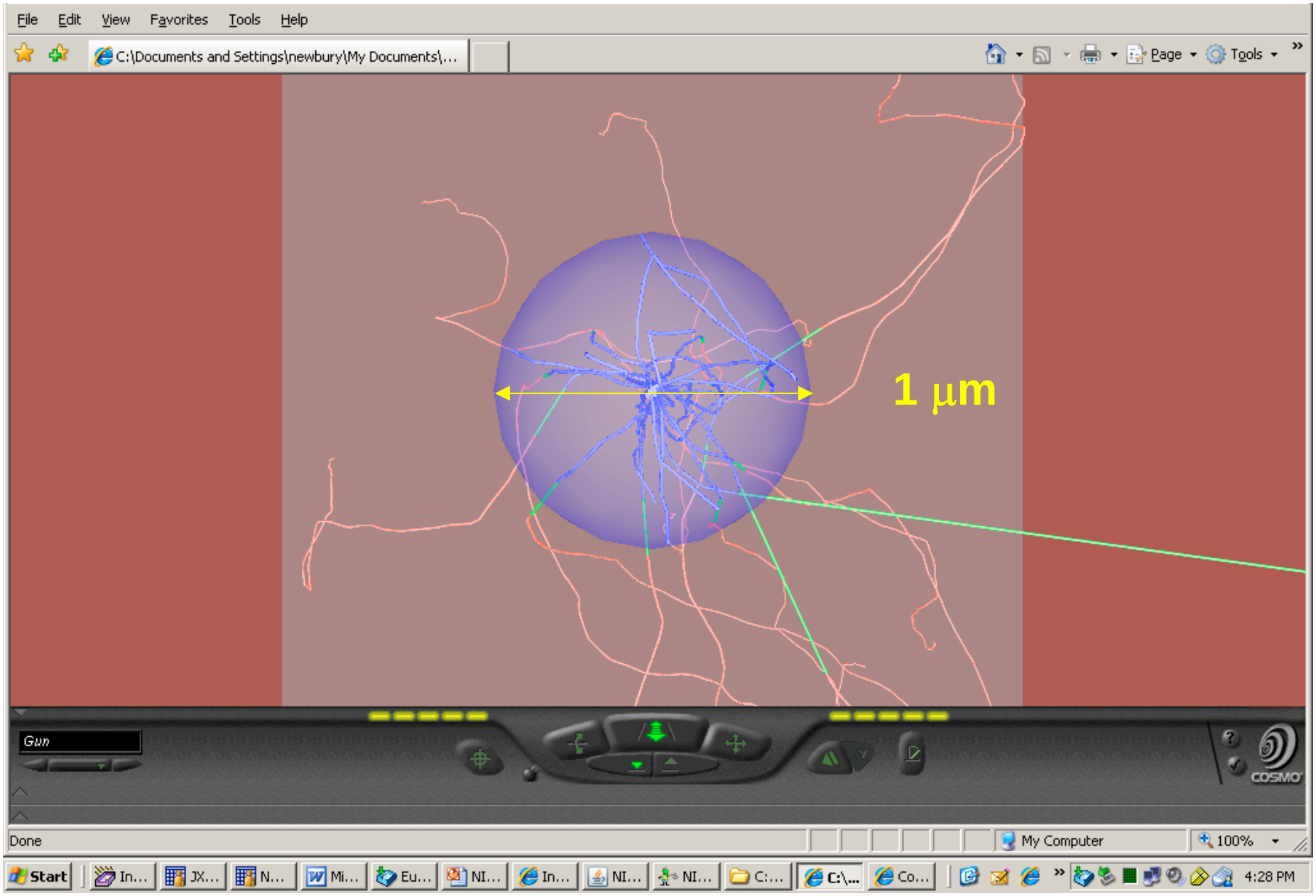
# Simulation Alien: Monte Carlo simulation of a 1 μm K411 glass sphere on a C substrate



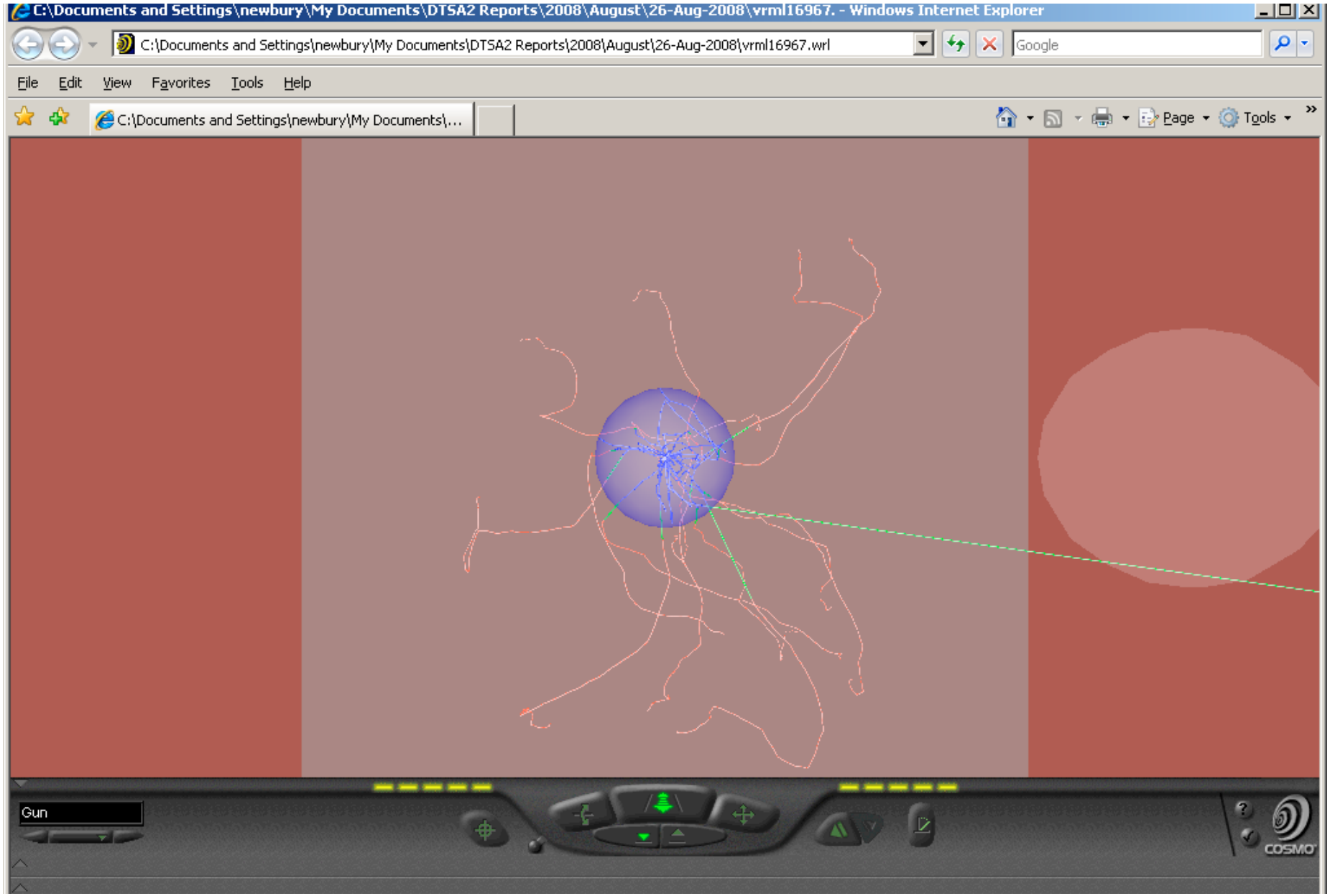
# Simulation Alien: Monte Carlo simulation of a 1 μm K411 glass sphere on a C substrate



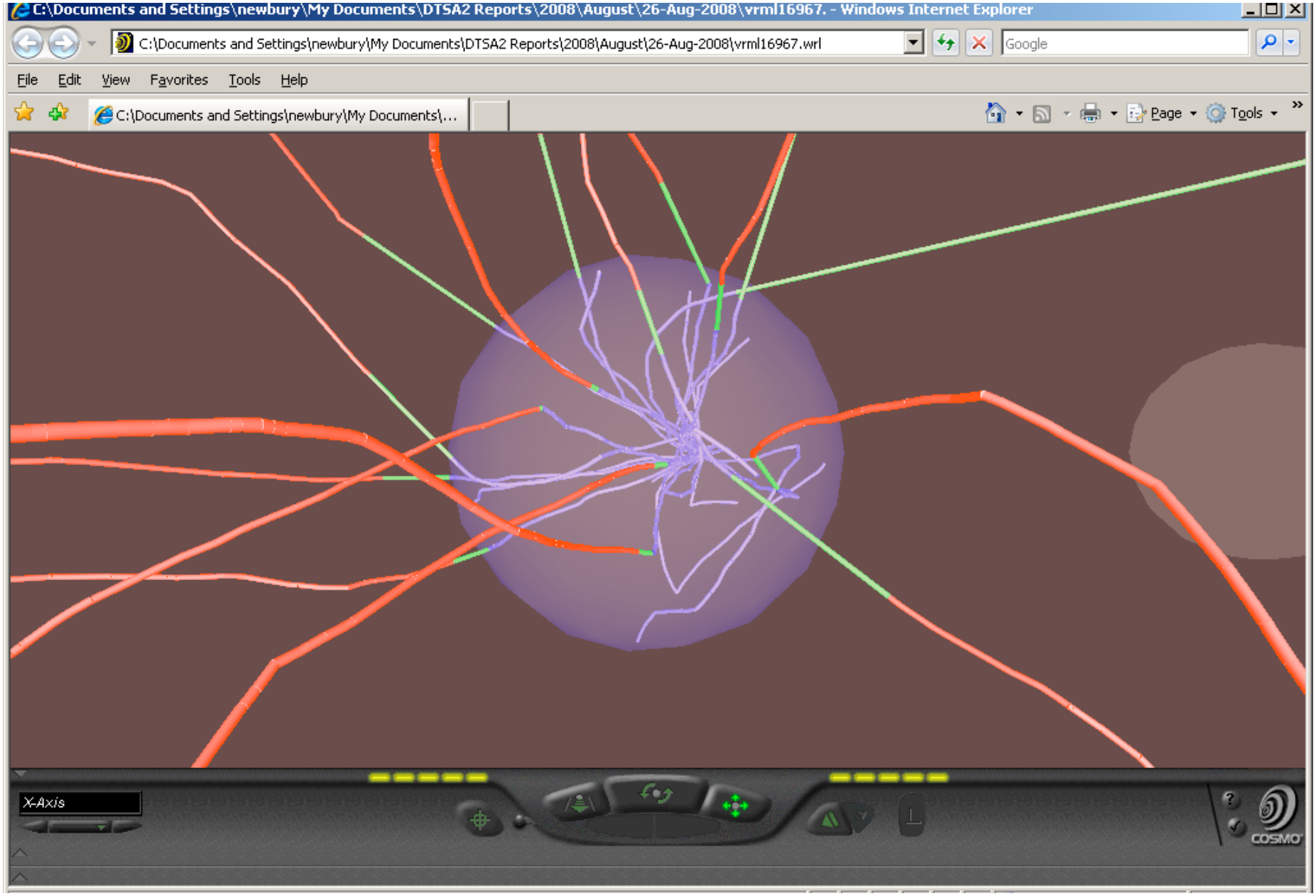
# View along the beam



# View along the beam



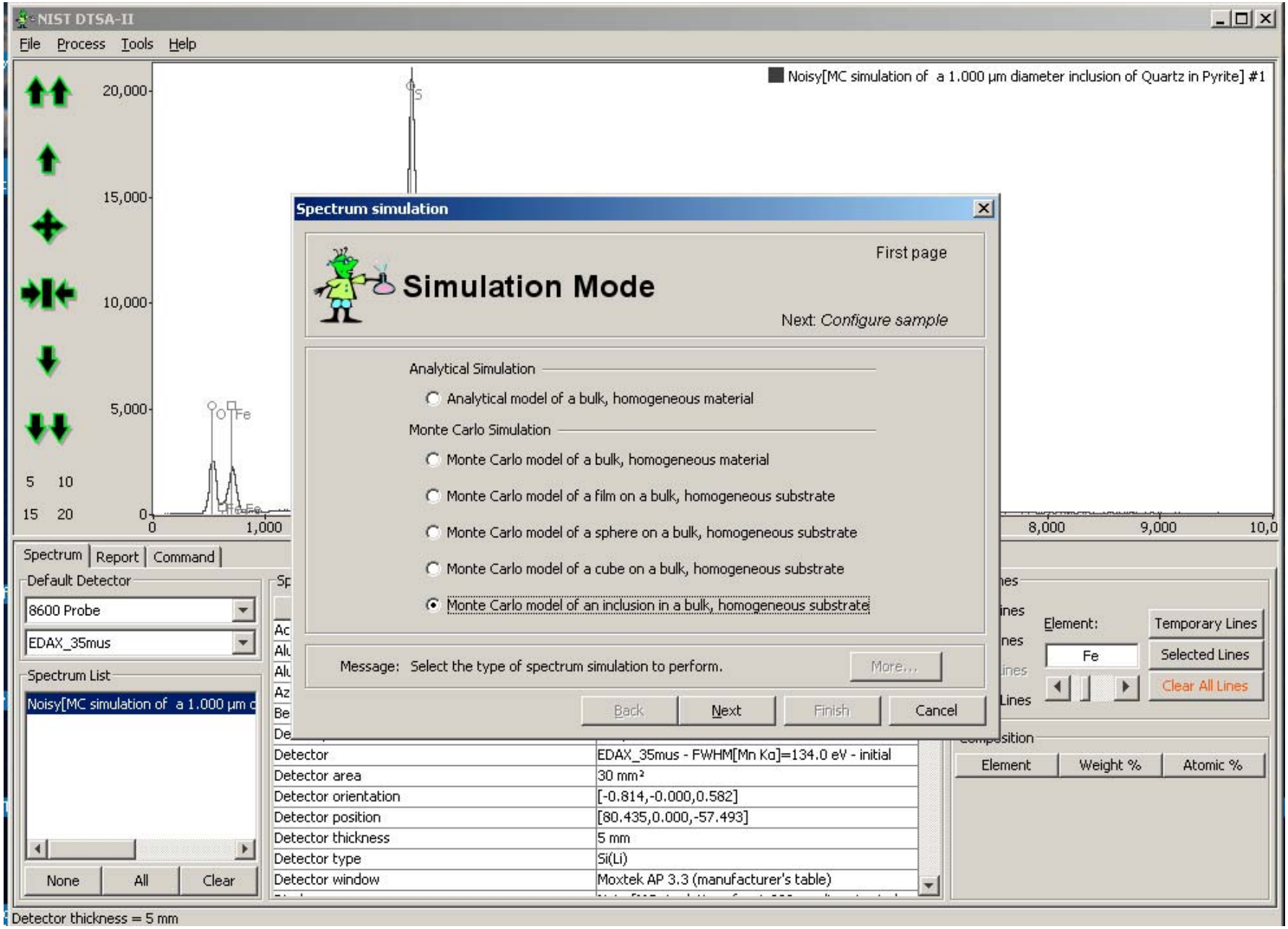
# View from bottom of particle



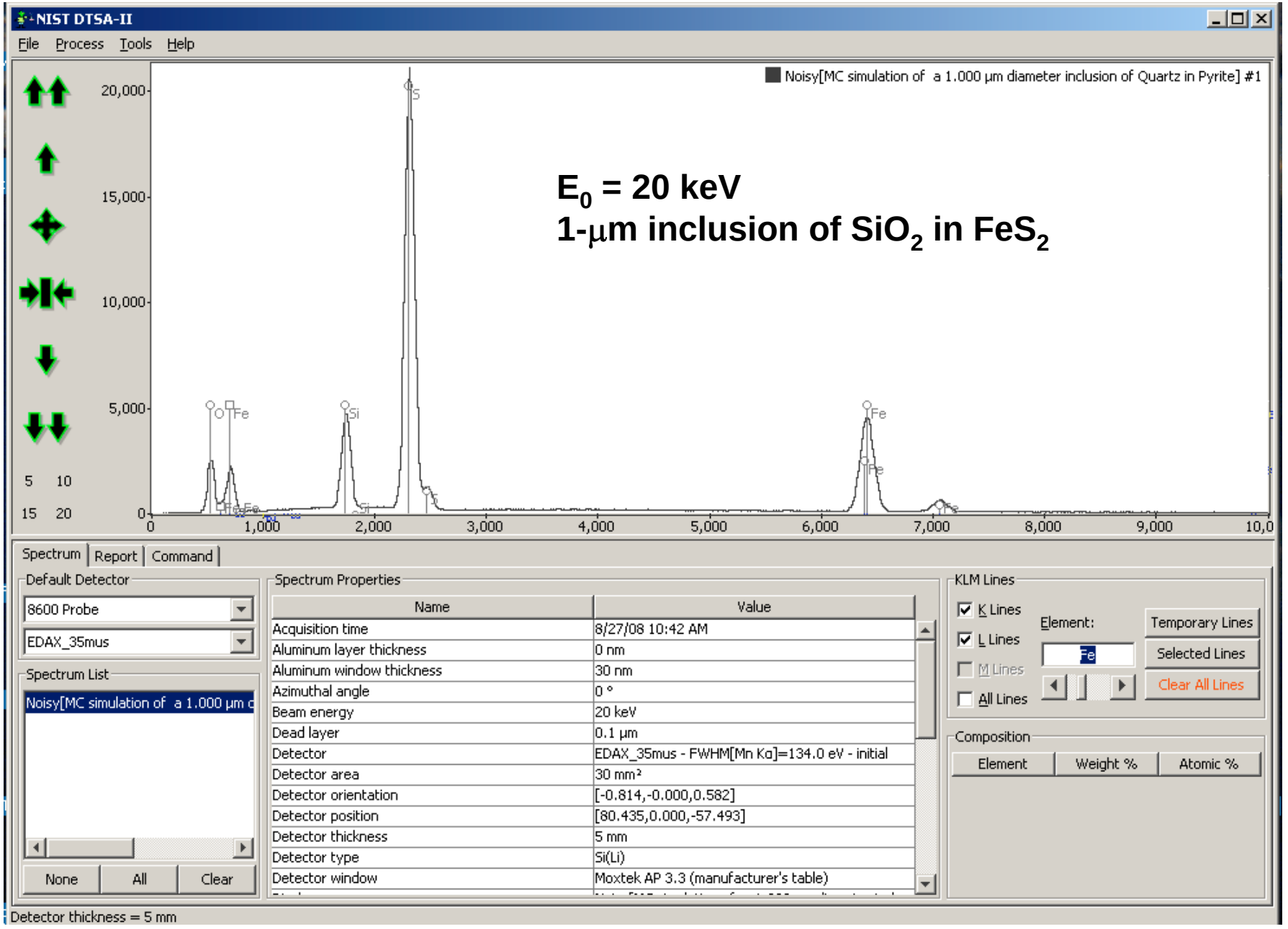
# DTSA-II Simulation Mode

- EDS spectra calculated from
  - 1. First principles, using best available cross sections and physical data (flat, bulk target only)
  - 2. Monte Carlo electron trajectory simulation for various specimen configurations:
    - 1. Flat, bulk
    - 2. Layer on bulk
    - **3. Inclusion (hemisphere) embedded in bulk**
    - 4. Spherical particle on substrate
    - 5. Cubic particle on substrate

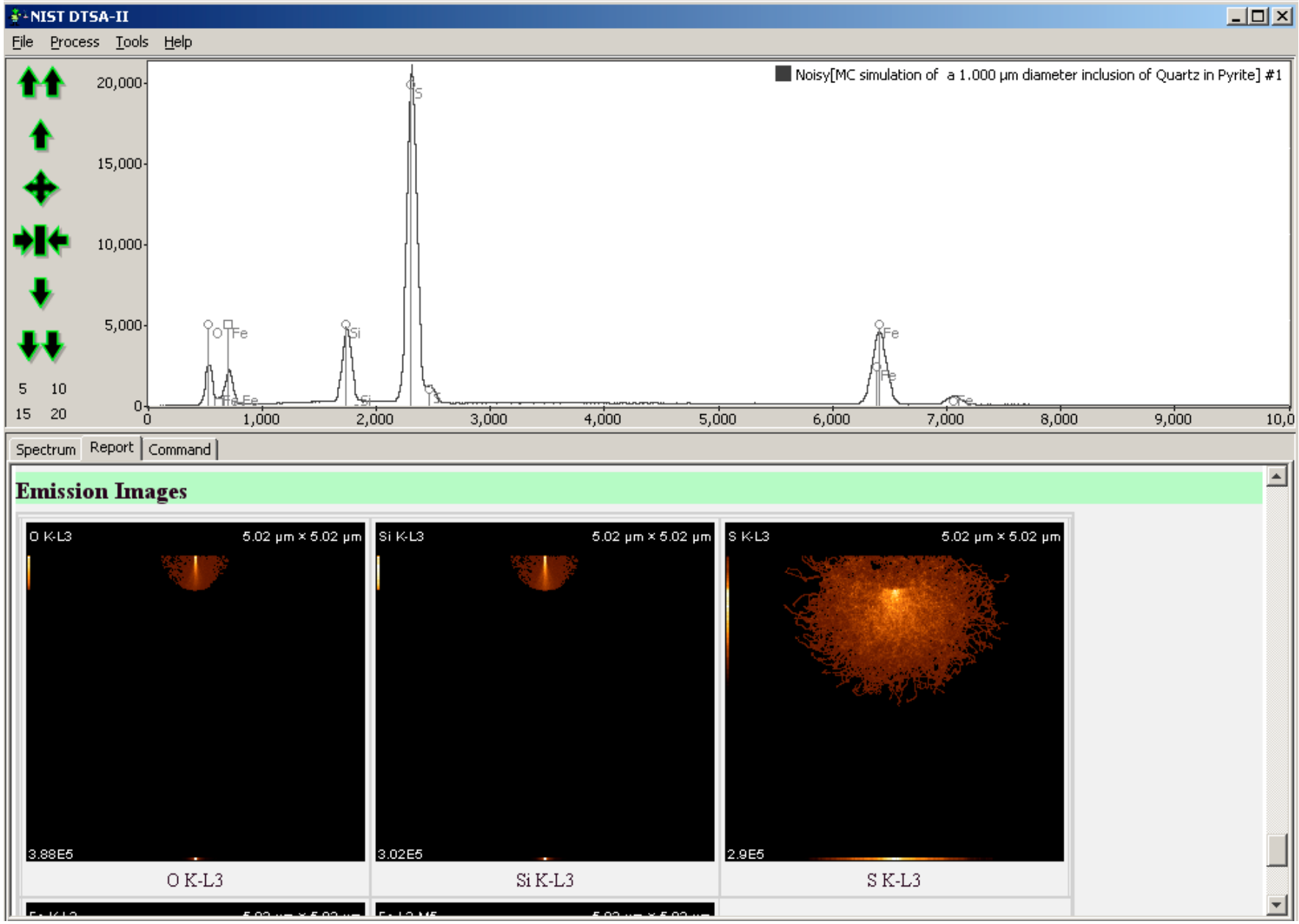
# Simulation Alien: Monte Carlo simulation of a 1 μm $SiO_2$ hemisphere in $FeS_2$



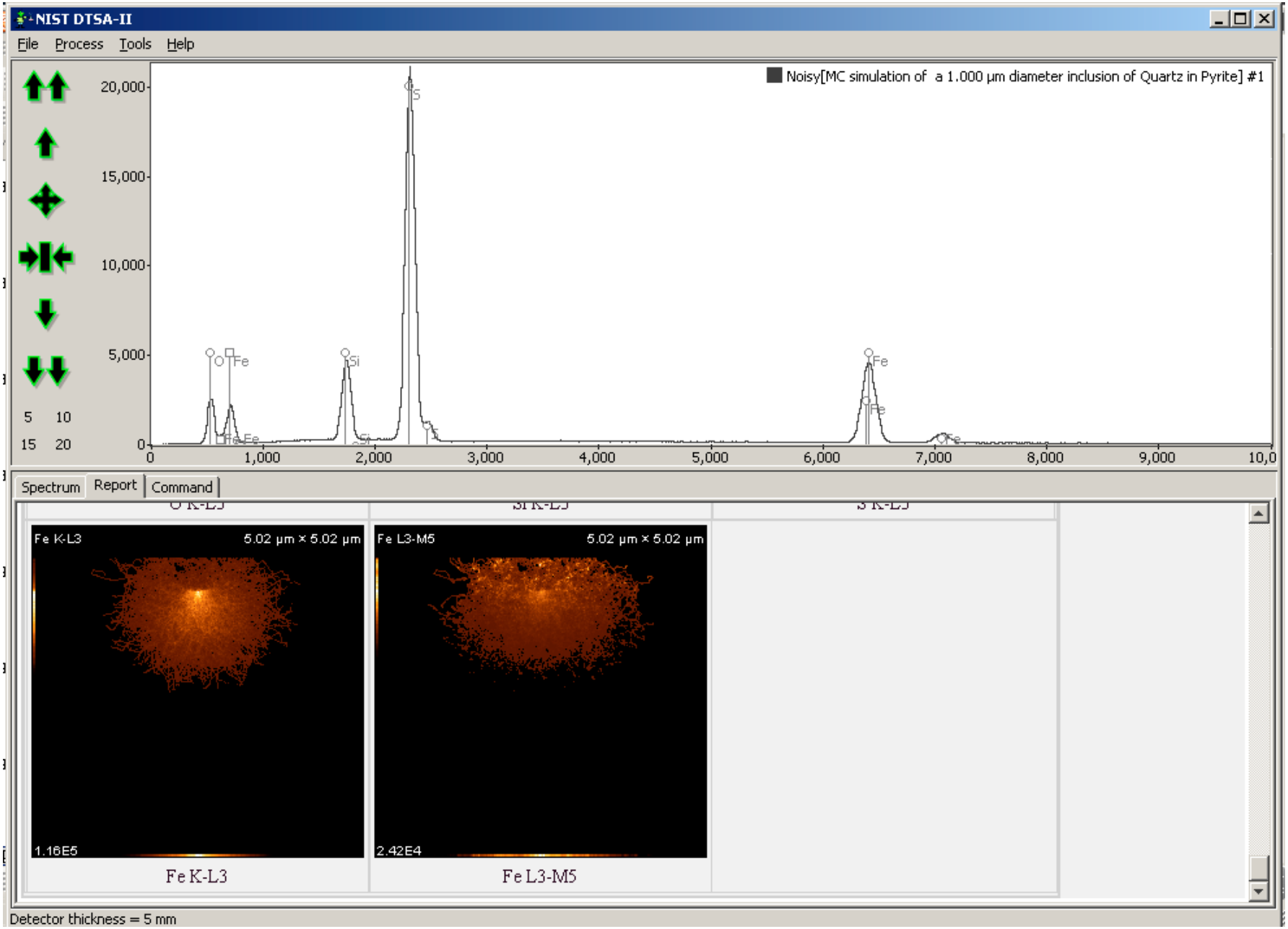
# Simulation Alien: Monte Carlo simulation of a 1 μm $SiO_2$ hemisphere in $FeS_2$



# Simulation Alien: Monte Carlo simulation of a 1 μm $SiO_2$ hemisphere in $FeS_2$

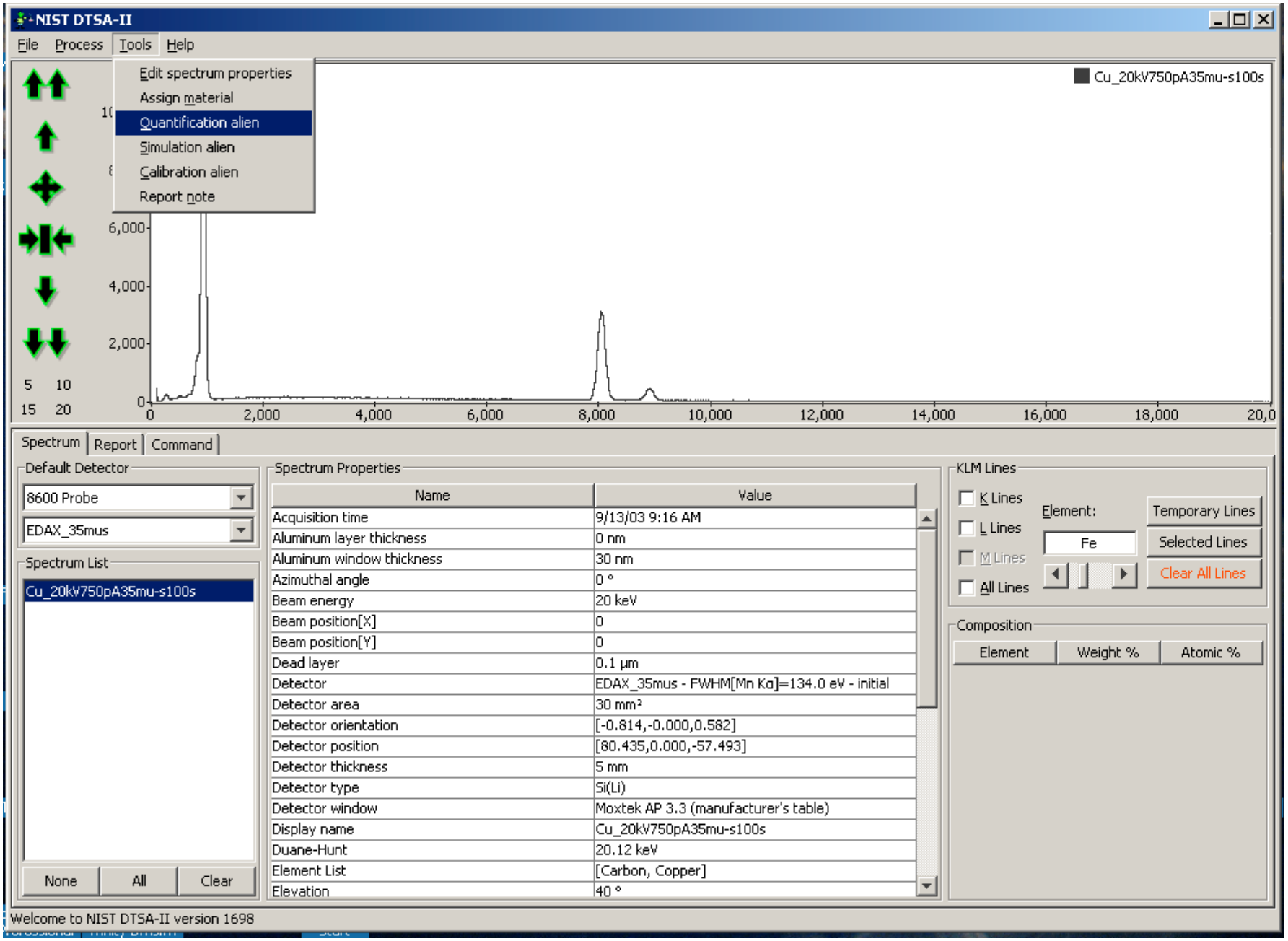


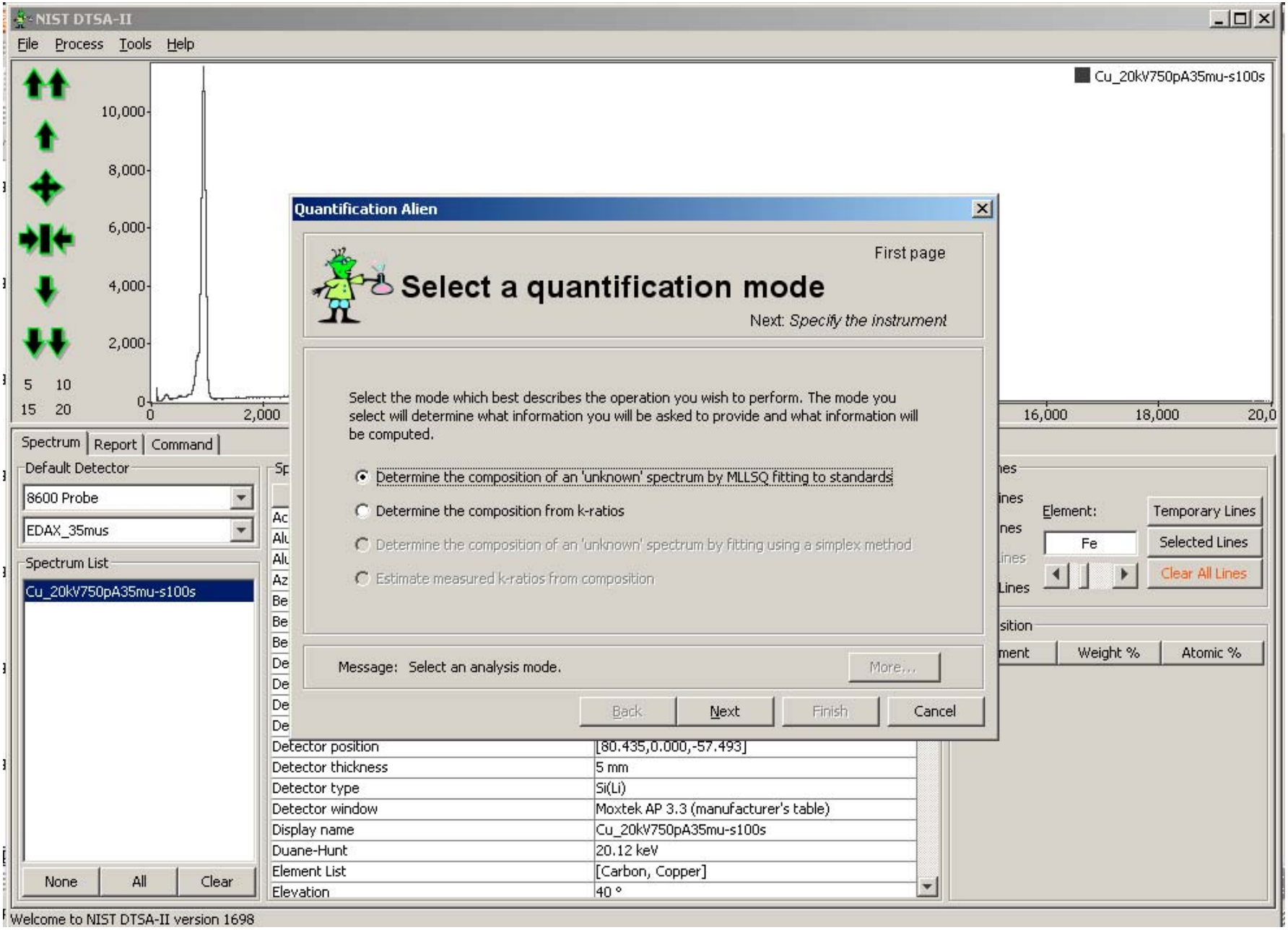
# Simulation Alien: Monte Carlo simulation of a 1 μm $SiO_2$ hemisphere in $FeS_2$

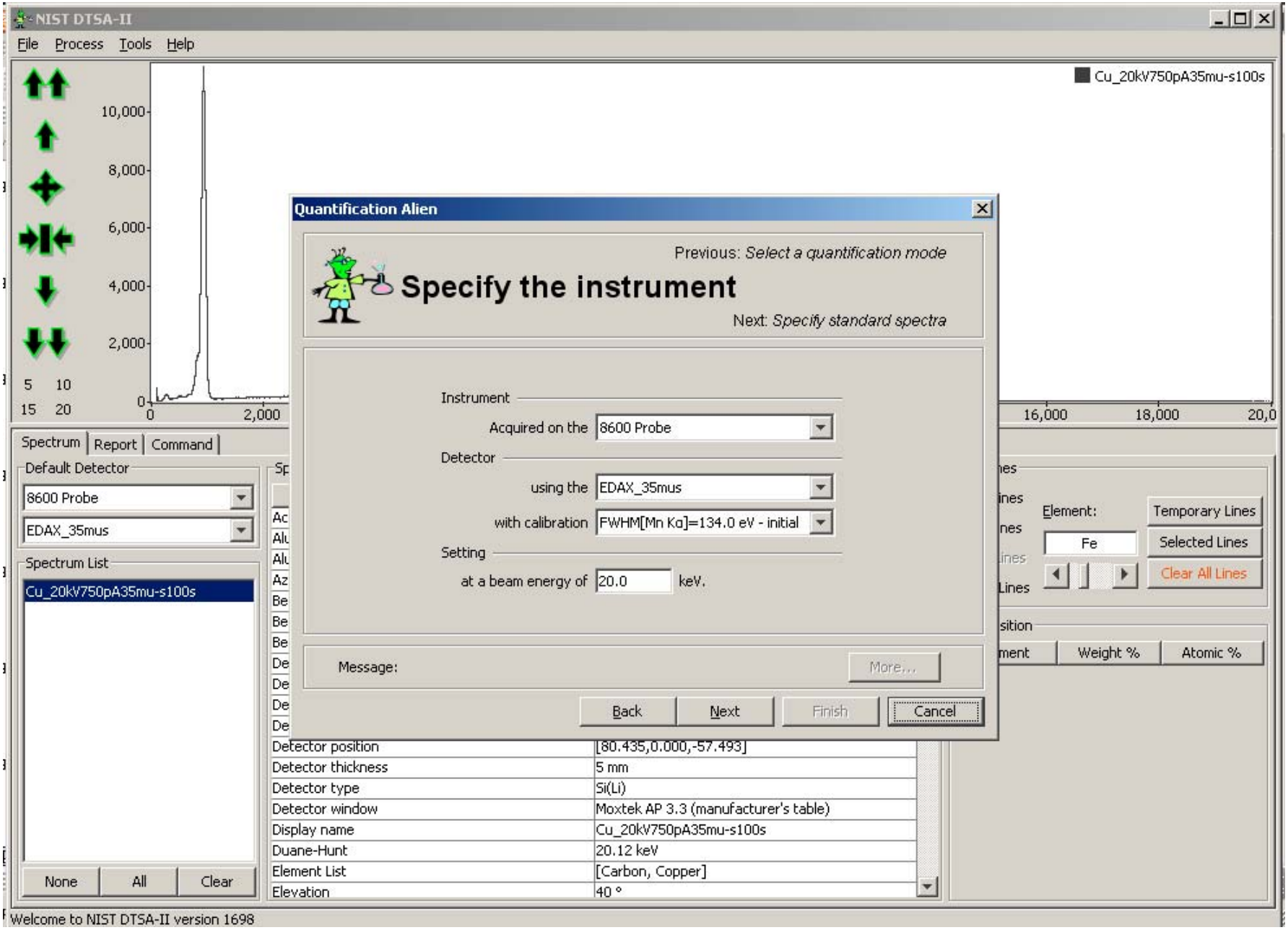


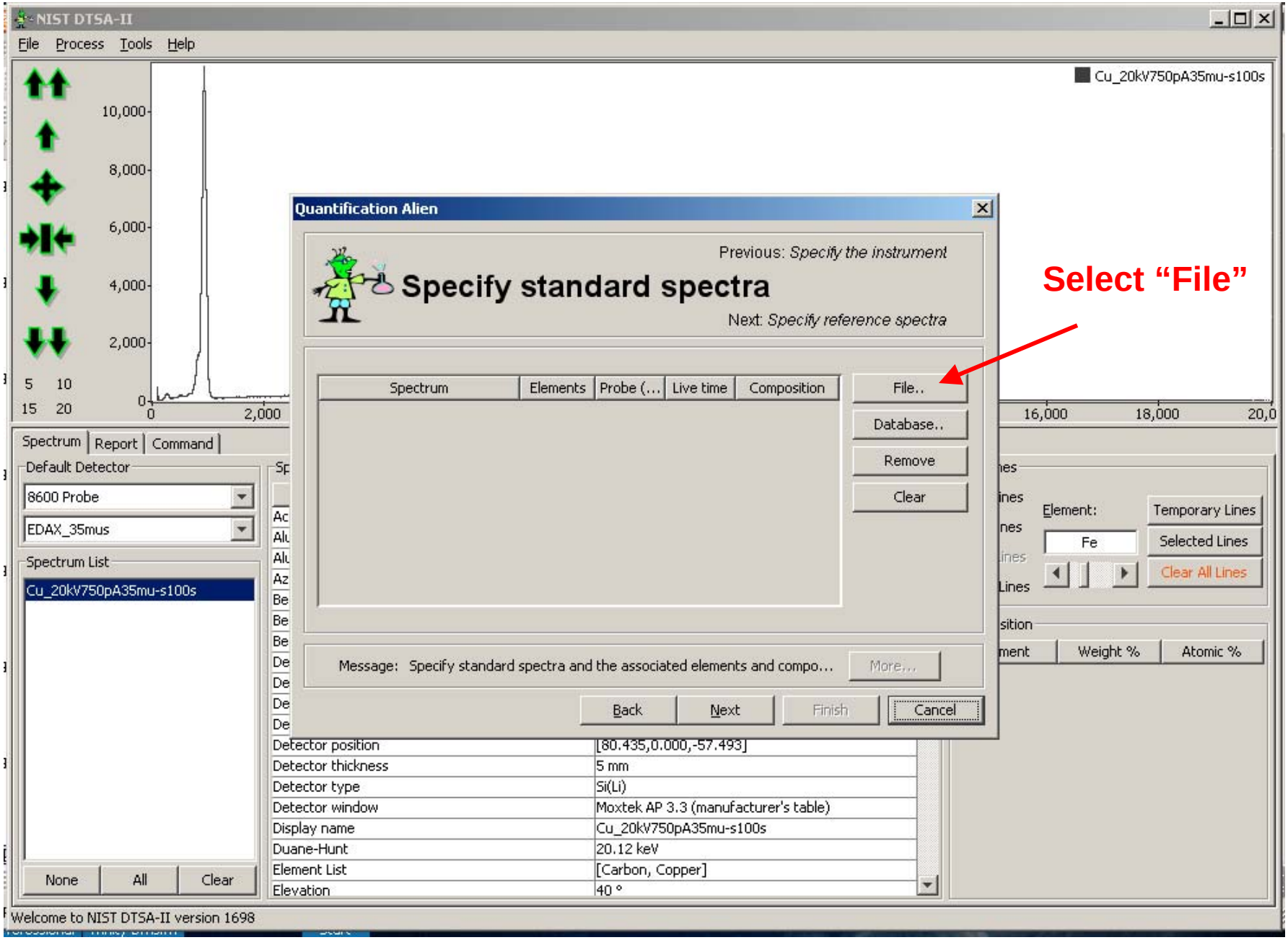
# DTSA-II: Quantitative Analysis

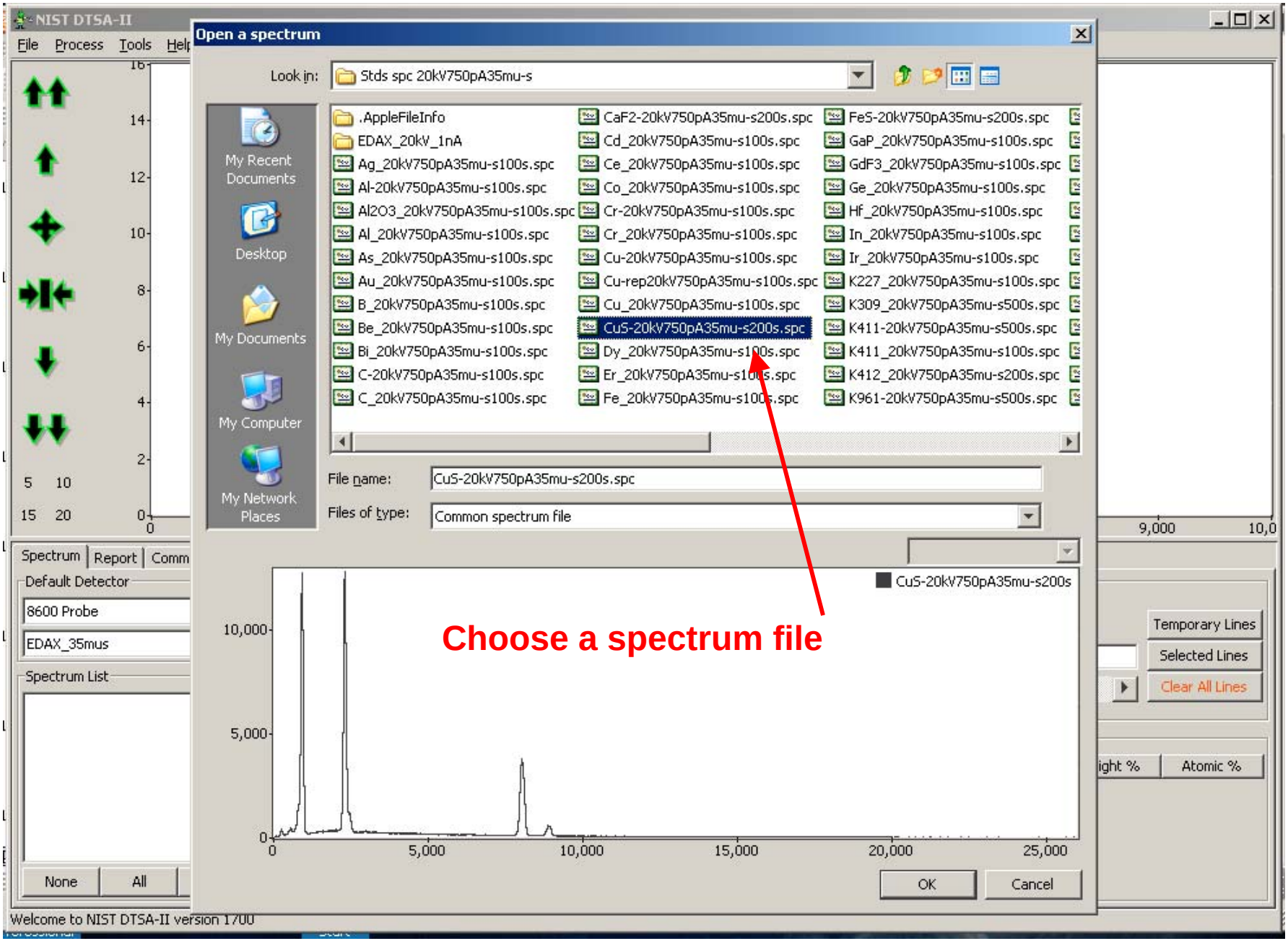
- ZAF analysis against standards
- Standards are used to extract needed peak references for MLLS fit.
- Report contains pertinent data (ZAF factors, weight%, atom%, normalized weight%; 1$\sigma$ statistics)

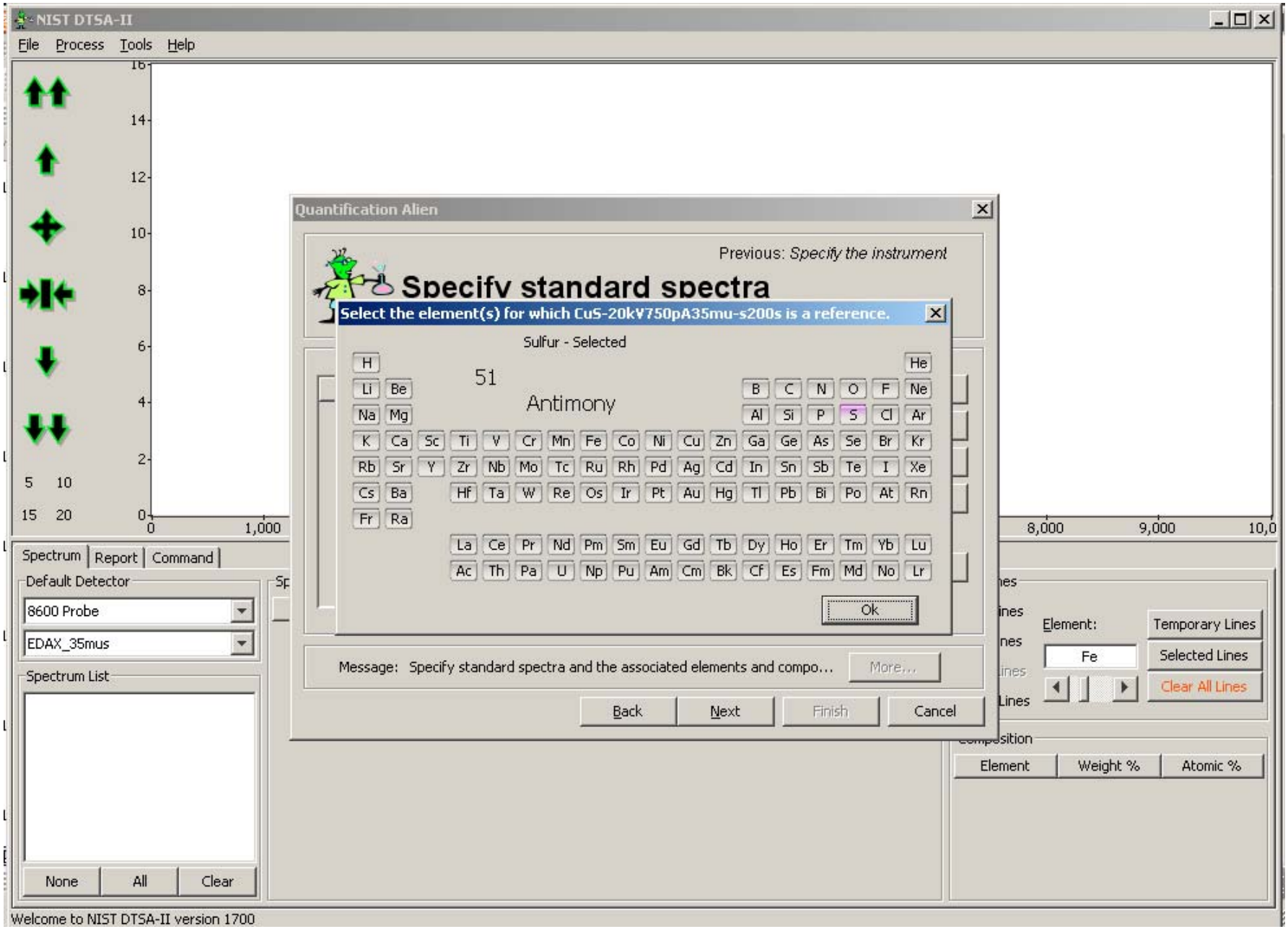

NIST DTSA-II
File
Process
Tools
Help
Edit spectrum properties
Assign material
Quantification alien
Simulation alien
Calibration alien
Report note
Cu_20kV750pA35mu-s100s
6,000
4,000
2,000
0
0
2,000
4,000
6,000
8,000
10,000
12,000
14,000
16,000
18,000
20,0
5
10
15
20
Spectrum
Report
Command
Default Detector
8600 Probe
EDAX_35mus
Spectrum List
Cu_20kV750pA35mu-s100s
None
All
Clear
Spectrum Properties
Name
Value
Acquisition time
9/13/03 9:16 AM
Aluminum layer thickness
0 nm
Aluminum window thickness
30 nm
Azimuthal angle
0 °
Beam energy
20 keV
Beam position[X]
0
Beam position[Y]
0
Dead layer
0.1 µm
Detector
EDAX_35mus - FWHM[Mn Kα]=134.0 eV - initial
Detector area
30 mm²
Detector orientation
[-0.814,-0.000,0.582]
Detector position
[80.435,0.000,-57.493]
Detector thickness
5 mm
Detector type
Si(Li)
Detector window
Moxtek AP 3.3 (manufacturer's table)
Display name
Cu_20kV750pA35mu-s100s
Duane-Hunt
20.12 keV
Element List
[Carbon, Copper]
Elevation
40 °
KLM Lines
K Lines
L Lines
M Lines
All Lines
Element:
Fe
Temporary Lines
Selected Lines
Clear All Lines
Composition
Element
Weight %
Atomic %
Welcome to NIST DTSA-II version 1698

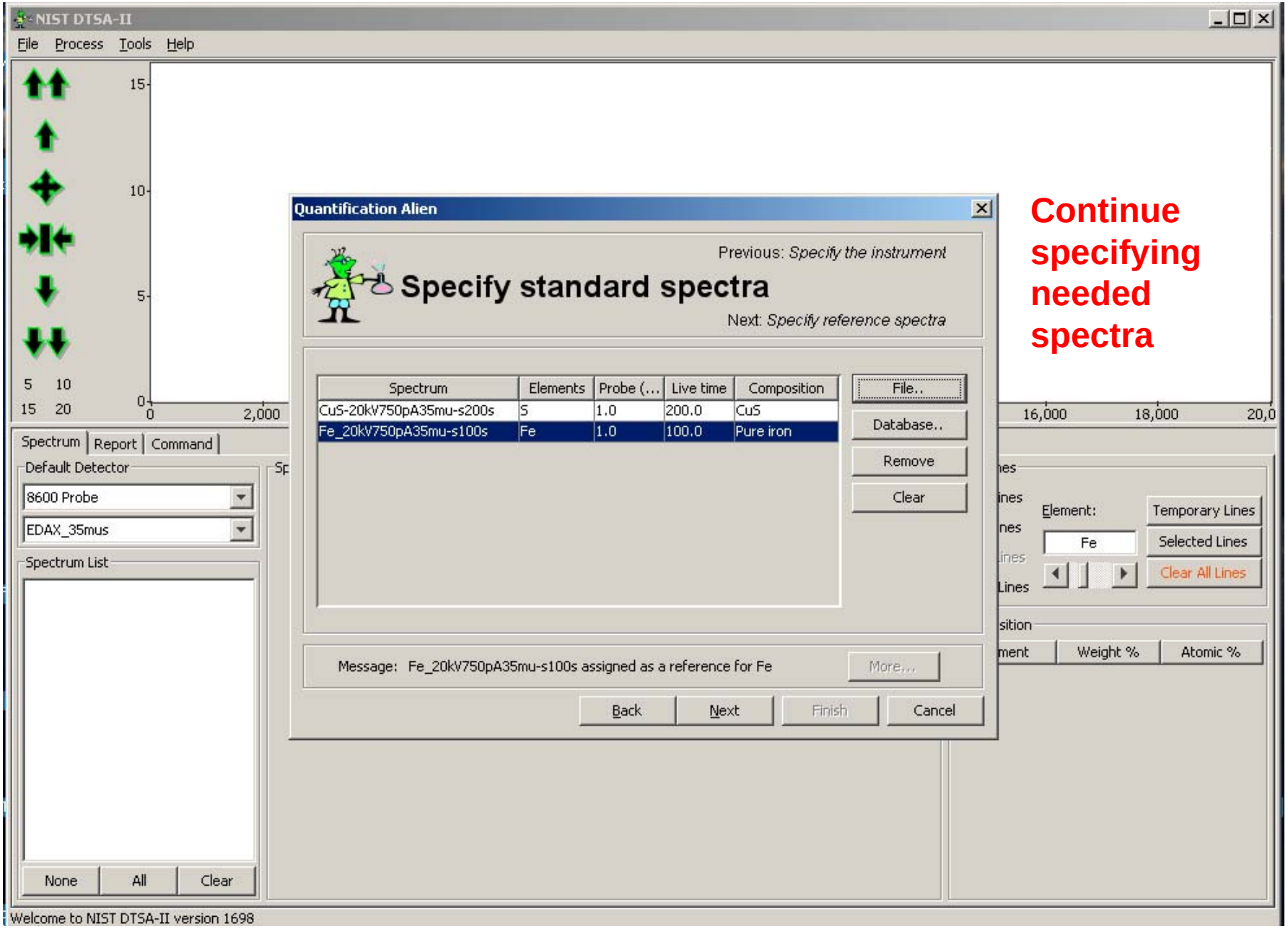

NIST DTSA-II
File Process Tools Help
Cu_20kV750pA35mu-s100s
Quantification Alien
First page
Select a quantification mode
Next: Specify the instrument
Select the mode which best describes the operation you wish to perform. The mode you select will determine what information you will be asked to provide and what information will be computed.
Determine the composition of an 'unknown' spectrum by MLLSQ fitting to standards
Determine the composition from k-ratios
Determine the composition of an 'unknown' spectrum by fitting using a simplex method
Estimate measured k-ratios from composition
Message: Select an analysis mode.
More...
Back
Next
Finish
Cancel
Spectrum
Report
Command
Default Detector
8600 Probe
EDAX_35mus
Spectrum List
Cu_20kV750pA35mu-s100s
None
All
Clear
Element:
Fe
Temporary Lines
Selected Lines
Clear All Lines
Weight %
Atomic %
Detector position [80.435,0.000,-57.493]
Detector thickness 5 mm
Detector type Si(Li)
Detector window Moxtek AP 3.3 (manufacturer's table)
Display name Cu_20kV750pA35mu-s100s
Duane-Hunt 20.12 keV
Element List [Carbon, Copper]
Elevation 40 °
Welcome to NIST DTSA-II version 1698

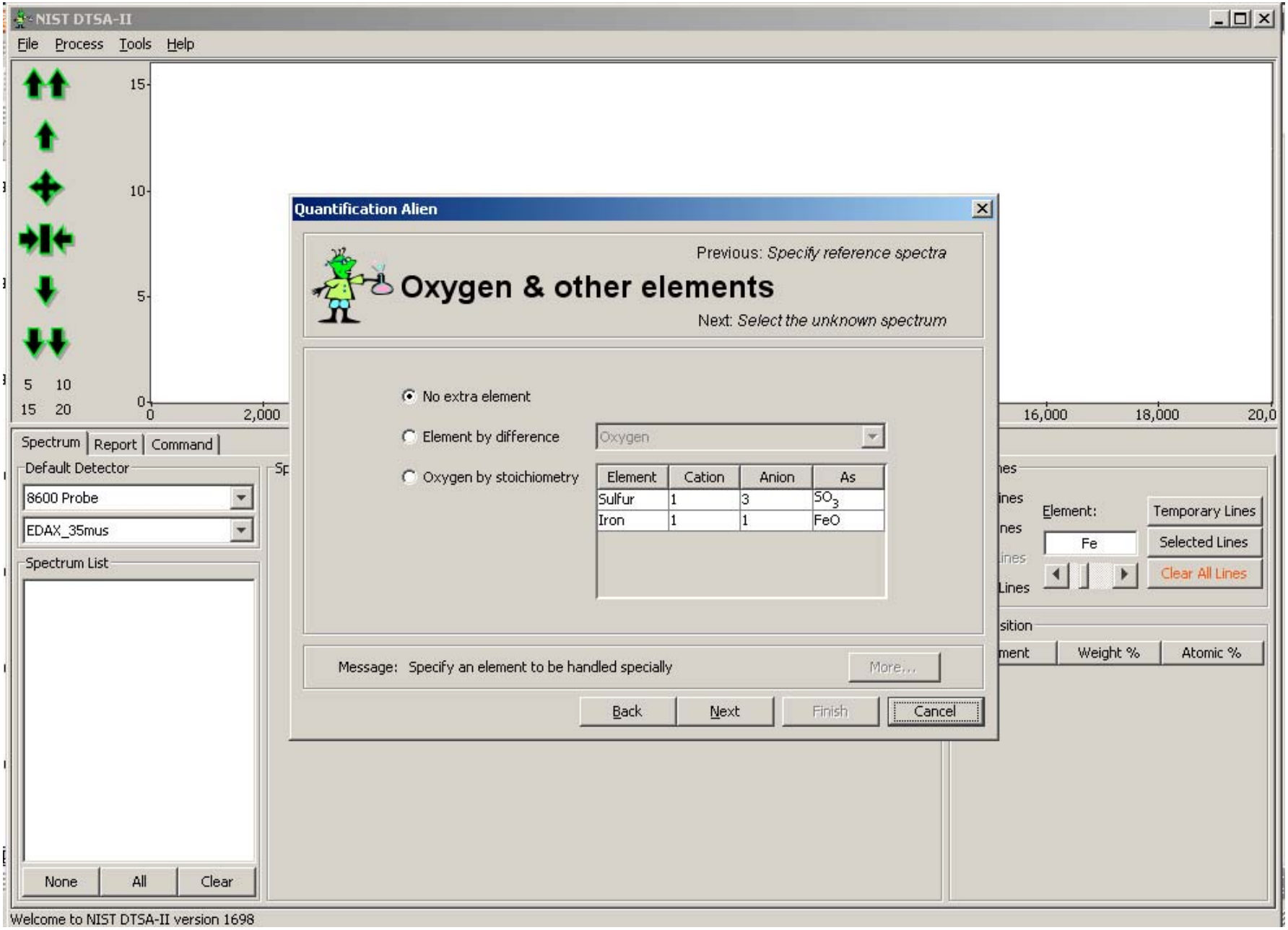

NIST DTSA-II
File Process Tools Help
Cu_20kV750pA35mu-s100s
Quantification Alien
Previous: Select a quantification mode
Specify the instrument
Next: Specify standard spectra
Instrument
Acquired on the 8600 Probe
Detector
using the EDAX_35mus
with calibration FWHM[Mn Kα]=134.0 eV - initial
Setting
at a beam energy of 20.0 keV.
Message:
More...
Back
Next
Finish
Cancel
Spectrum
Report
Command
Default Detector
8600 Probe
EDAX_35mus
Spectrum List
Cu_20kV750pA35mu-s100s
None
All
Clear
Element:
Fe
Temporary Lines
Selected Lines
Clear All Lines
Weight %
Atomic %
Detector position [80.435,0.000,-57.493]
Detector thickness 5 mm
Detector type Si(Li)
Detector window Moxtek AP 3.3 (manufacturer's table)
Display name Cu_20kV750pA35mu-s100s
Duane-Hunt 20.12 keV
Element List [Carbon, Copper]
Elevation 40 °
Welcome to NIST DTSA-II version 1698

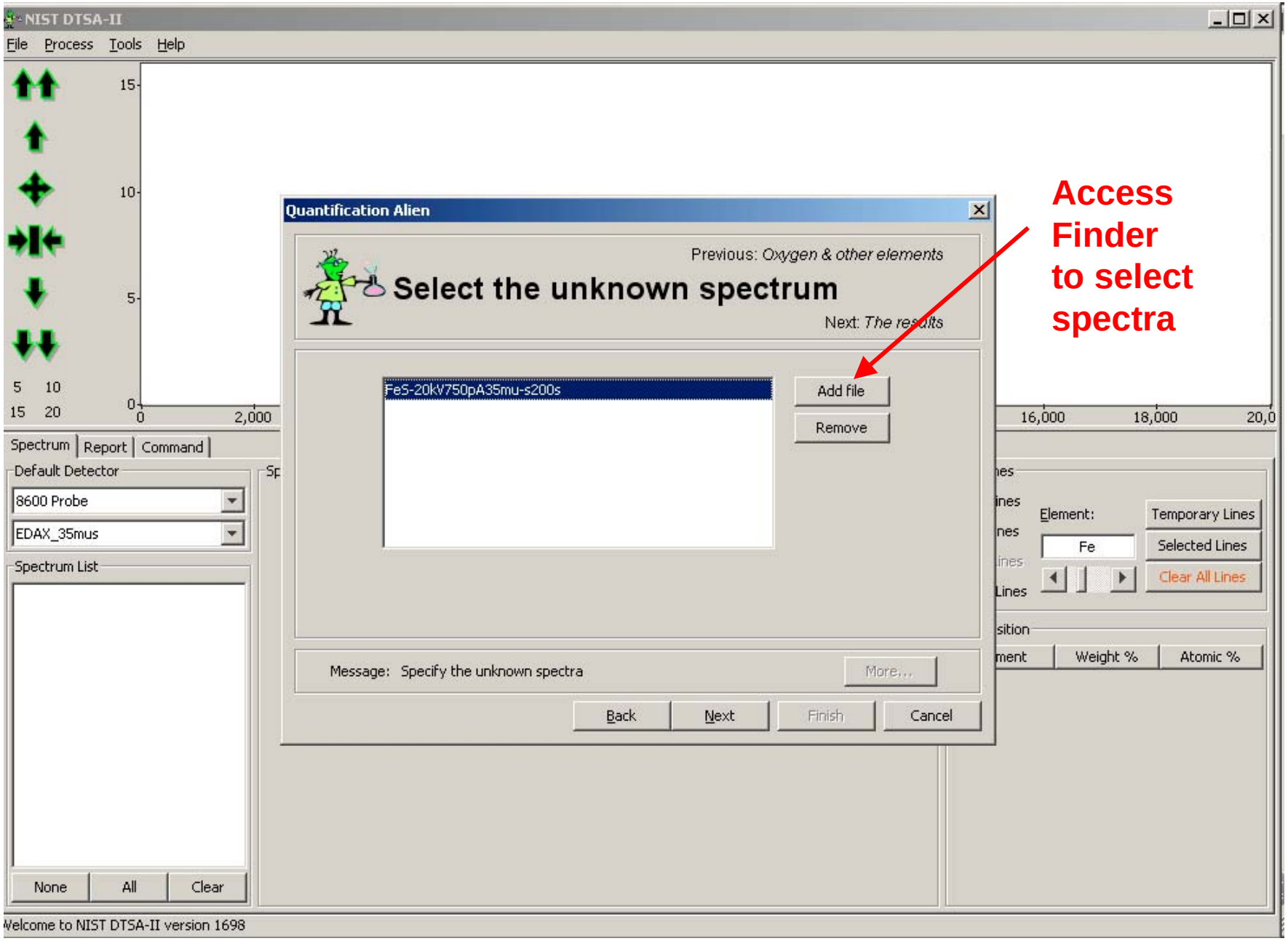

NIST DTSA-II
File Process Tools Help
Cu_20kV750pA35mu-s100s
Quantification Alien
Previous: Specify the instrument
Specify standard spectra
Next: Specify reference spectra
Spectrum Elements Probe (... Live time Composition
File..
Database..
Remove
Clear
Select “File”
Message: Specify standard spectra and the associated elements and compo...
More...
Back Next Finish Cancel
Spectrum Report Command
Default Detector
8600 Probe
EDAX_35mus
Spectrum List
Cu_20kV750pA35mu-s100s
None All Clear
Element:
Fe
Temporary Lines
Selected Lines
Clear All Lines
Weight %
Atomic %
Detector position [80.435,0.000,-57.493]
Detector thickness 5 mm
Detector type Si(Li)
Detector window Moxtek AP 3.3 (manufacturer's table)
Display name Cu_20kV750pA35mu-s100s
Duane-Hunt 20.12 keV
Element List [Carbon, Copper]
Elevation 40 °
Welcome to NIST DTSA-II version 1698

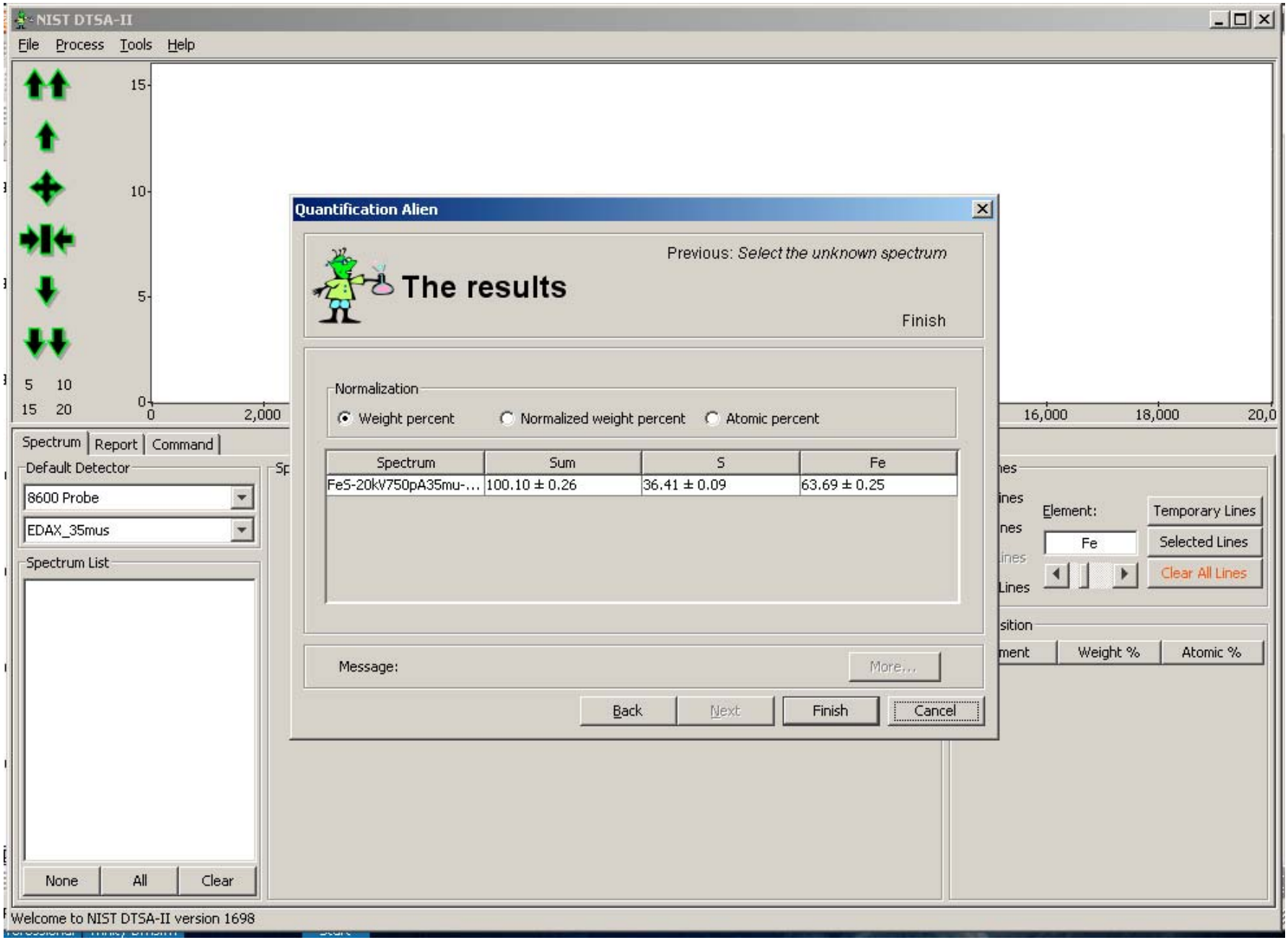

NIST DTSA-II
File Process Tools Help
Open a spectrum
Look in: Stds spc 20kV750pA35mu-s
.AppleFileInfo
EDAX_20kV_1nA
Ag_20kV750pA35mu-s100s.spc
Al-20kV750pA35mu-s100s.spc
Al2O3_20kV750pA35mu-s100s.spc
Al_20kV750pA35mu-s100s.spc
As_20kV750pA35mu-s100s.spc
Au_20kV750pA35mu-s100s.spc
B_20kV750pA35mu-s100s.spc
Be_20kV750pA35mu-s100s.spc
Bi_20kV750pA35mu-s100s.spc
C-20kV750pA35mu-s100s.spc
C_20kV750pA35mu-s100s.spc
CaF2-20kV750pA35mu-s200s.spc
Cd_20kV750pA35mu-s100s.spc
Ce_20kV750pA35mu-s100s.spc
Co_20kV750pA35mu-s100s.spc
Cr-20kV750pA35mu-s100s.spc
Cr_20kV750pA35mu-s100s.spc
Cu-20kV750pA35mu-s100s.spc
Cu-rep20kV750pA35mu-s100s.spc
Cu_20kV750pA35mu-s100s.spc
CuS-20kV750pA35mu-s200s.spc
Dy_20kV750pA35mu-s100s.spc
Er_20kV750pA35mu-s100s.spc
Fe_20kV750pA35mu-s100s.spc
FeS-20kV750pA35mu-s200s.spc
GaP_20kV750pA35mu-s100s.spc
GdF3_20kV750pA35mu-s100s.spc
Ge_20kV750pA35mu-s100s.spc
Hf_20kV750pA35mu-s100s.spc
In_20kV750pA35mu-s100s.spc
Ir_20kV750pA35mu-s100s.spc
K227_20kV750pA35mu-s100s.spc
K309_20kV750pA35mu-s500s.spc
K411-20kV750pA35mu-s500s.spc
K411_20kV750pA35mu-s100s.spc
K412_20kV750pA35mu-s200s.spc
K961-20kV750pA35mu-s500s.spc
My Recent Documents
Desktop
My Documents
My Computer
My Network Places
File name: CuS-20kV750pA35mu-s200s.spc
Files of type: Common spectrum file
CuS-20kV750pA35mu-s200s
Choose a spectrum file
OK
Cancel
Spectrum Report Comm
Default Detector
8600 Probe
EDAX_35mus
Spectrum List
None All
Temporary Lines
Selected Lines
Clear All Lines
Atomic %
Welcome to NIST DTSA-II version 1700

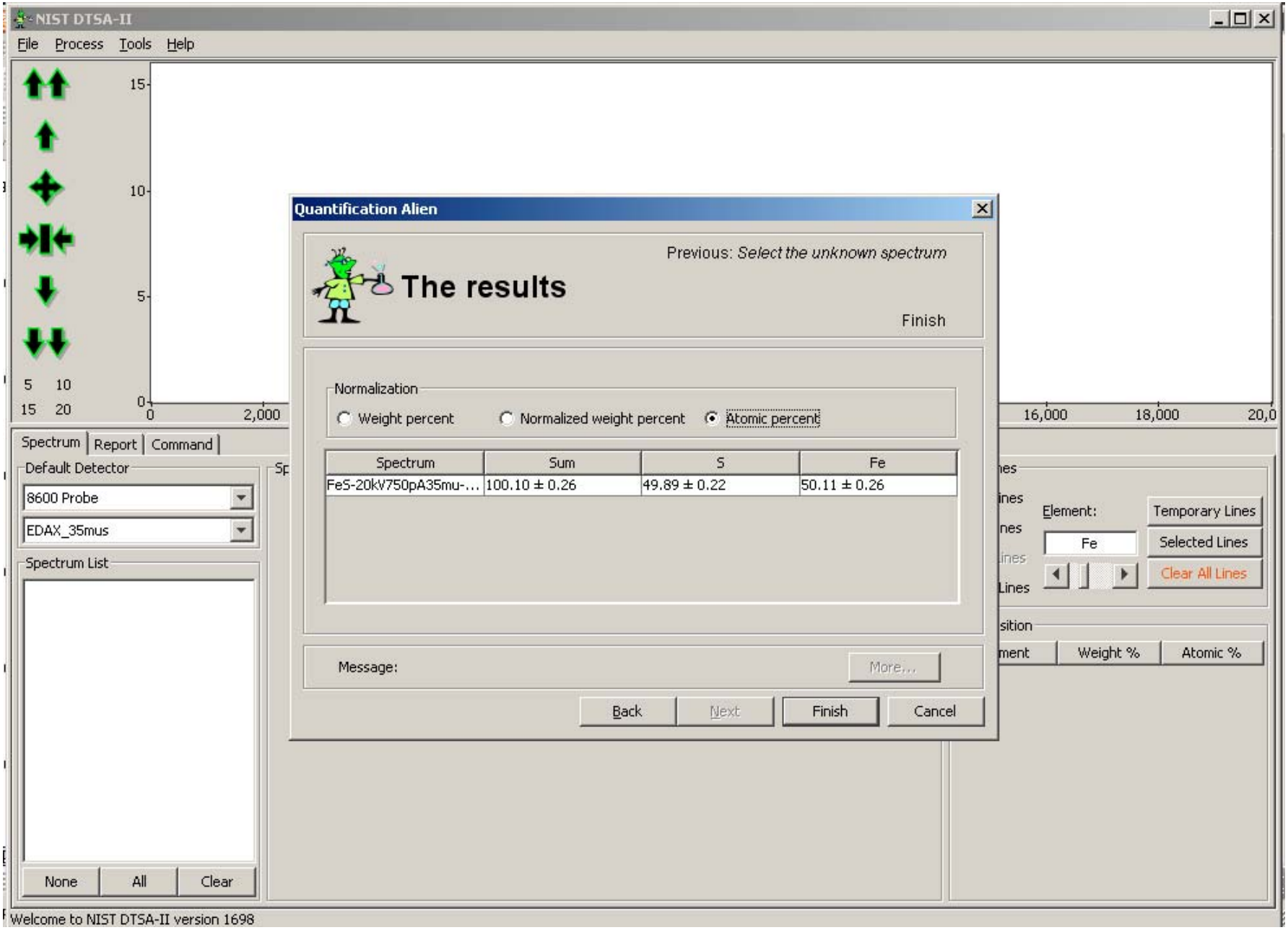

NIST DTSA-II
File Process Tools Help
Quantification Alien
Previous: Specify the instrument
Specify standard spectra
Select the element(s) for which CuS-20kV750pA35mu-s200s is a reference.
Sulfur - Selected
51
Antimony
Ok
Message: Specify standard spectra and the associated elements and compo...
More...
Back
Next
Finish
Cancel
Spectrum
Report
Command
Default Detector
8600 Probe
EDAX_35mus
Spectrum List
None
All
Clear
Element:
Fe
Temporary Lines
Selected Lines
Clear All Lines
Element
Weight %
Atomic %
Welcome to NIST DTSA-II version 1700


NIST DTSA-II
File Process Tools Help
Quantification Alien
Previous: Specify the instrument
Specify standard spectra
Next: Specify reference spectra
Spectrum Elements Probe (... Live time Composition
CuS-20kV750pA35mu-s200s S 1.0 200.0 CuS
Fe_20kV750pA35mu-s100s Fe 1.0 100.0 Pure iron
File..
Database..
Remove
Clear
Message: Fe_20kV750pA35mu-s100s assigned as a reference for Fe
More...
Back
Next
Finish
Cancel
Continue specifying needed spectra
Spectrum Report Command
Default Detector
8600 Probe
EDAX_35mus
Spectrum List
None
All
Clear
Element:
Fe
Temporary Lines
Selected Lines
Clear All Lines
Weight %
Atomic %
Welcome to NIST DTSA-II version 1698


NIST DTSA-II
File Process Tools Help
Quantification Alien
Previous: Specify reference spectra
Oxygen & other elements
Next: Select the unknown spectrum
No extra element
Element by difference
Oxygen
Oxygen by stoichiometry
Element Cation Anion As
Sulfur 1 3 SO3
Iron 1 1 FeO
Message: Specify an element to be handled specially
More...
Back Next Finish Cancel
Spectrum Report Command
Default Detector
8600 Probe
EDAX_35mus
Spectrum List
None All Clear
Element:
Fe
Temporary Lines
Selected Lines
Clear All Lines
Weight %
Atomic %
Welcome to NIST DTSA-II version 1698

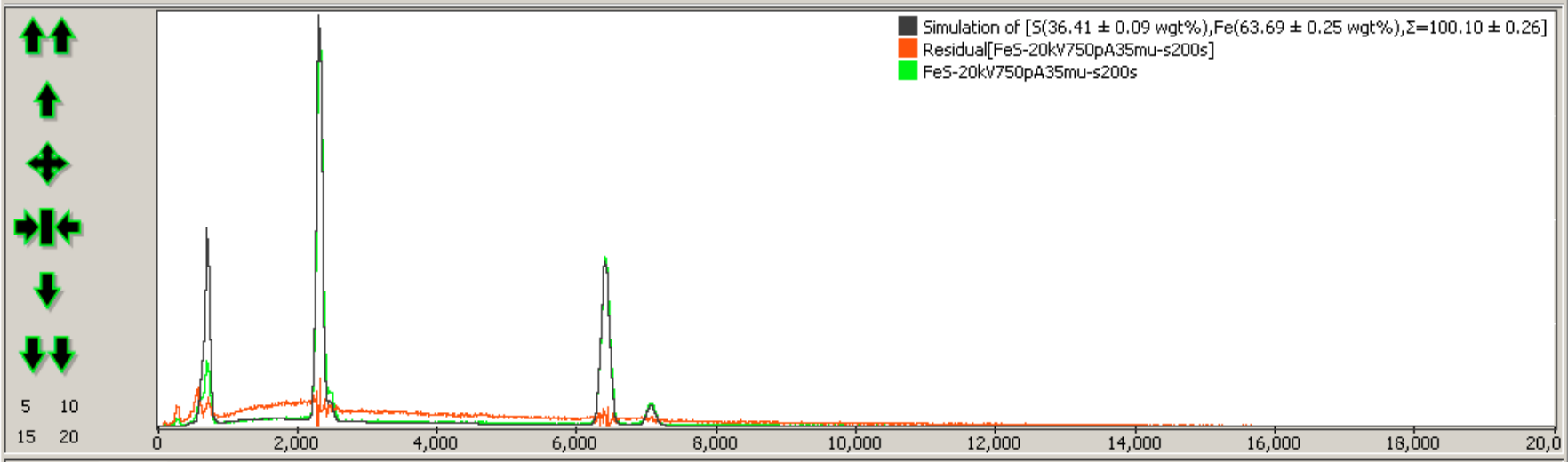

NIST DTSA-II
File Process Tools Help
Quantification Alien
Previous: Oxygen & other elements
Select the unknown spectrum
Next: The results
FeS-20kV750pA35mu-s200s
Add file
Remove
Message: Specify the unknown spectra
More...
Back
Next
Finish
Cancel
Access Finder to select spectra
Spectrum
Report
Command
Default Detector
8600 Probe
EDAX_35mus
Spectrum List
None
All
Clear
Element:
Fe
Temporary Lines
Selected Lines
Clear All Lines
Weight %
Atomic %
Welcome to NIST DTSA-II version 1698


NIST DTSA-II
File Process Tools Help
Quantification Alien
Previous: Select the unknown spectrum
The results
Finish
Normalization
Weight percent
Normalized weight percent
Atomic percent
Spectrum | Sum | S | Fe
FeS-20kV750pA35mu-... | 100.10 ± 0.26 | 36.41 ± 0.09 | 63.69 ± 0.25
Message:
More...
Back
Next
Finish
Cancel
Spectrum
Report
Command
Default Detector
8600 Probe
EDAX_35mus
Spectrum List
None
All
Clear
Element:
Fe
Temporary Lines
Selected Lines
Clear All Lines
Weight %
Atomic %
Welcome to NIST DTSA-II version 1698


NIST DTSA-II
File Process Tools Help
Quantification Alien
Previous: Select the unknown spectrum
The results
Finish
Normalization
Weight percent
Normalized weight percent
Atomic percent
Spectrum
Sum
S
Fe
FeS-20kV750pA35mu-...
100.10 ± 0.26
49.89 ± 0.22
50.11 ± 0.26
Message:
More...
Back
Next
Finish
Cancel
Spectrum
Report
Command
Default Detector
8600 Probe
EDAX_35mus
Spectrum List
None
All
Clear
Element:
Fe
Temporary Lines
Selected Lines
Clear All Lines
Weight %
Atomic %
Welcome to NIST DTSA-II version 1698

NIST DTSA-II

File Process Tools Help




Spectrum | Report | Command

| | | | | | |
|---|---|---|---|---|---|
| S | CuS = [S(33.54 wgt%),Cu (66.46 wgt%),4.6 g/cc] | C:\Documents and Settings\newbury\My Documents\EDAX\Standards EDAX JEOL\20 keV 750pA 35mu-s\Stds spc 20kV750pA35mu-s\CuS-20kV750pA35mu-s200s.spc | Yes | 1.000 | 200.0 |
| Fe | Pure iron = [Fe(100.00 wgt%),7.9 g/cc] | C:\Documents and Settings\newbury\My Documents\EDAX\Standards EDAX JEOL\20 keV 750pA 35mu-s\Stds spc 20kV750pA35mu-s\Fe_20kV750pA35mu-s100s.spc | Yes | 1.000 | 100.0 |

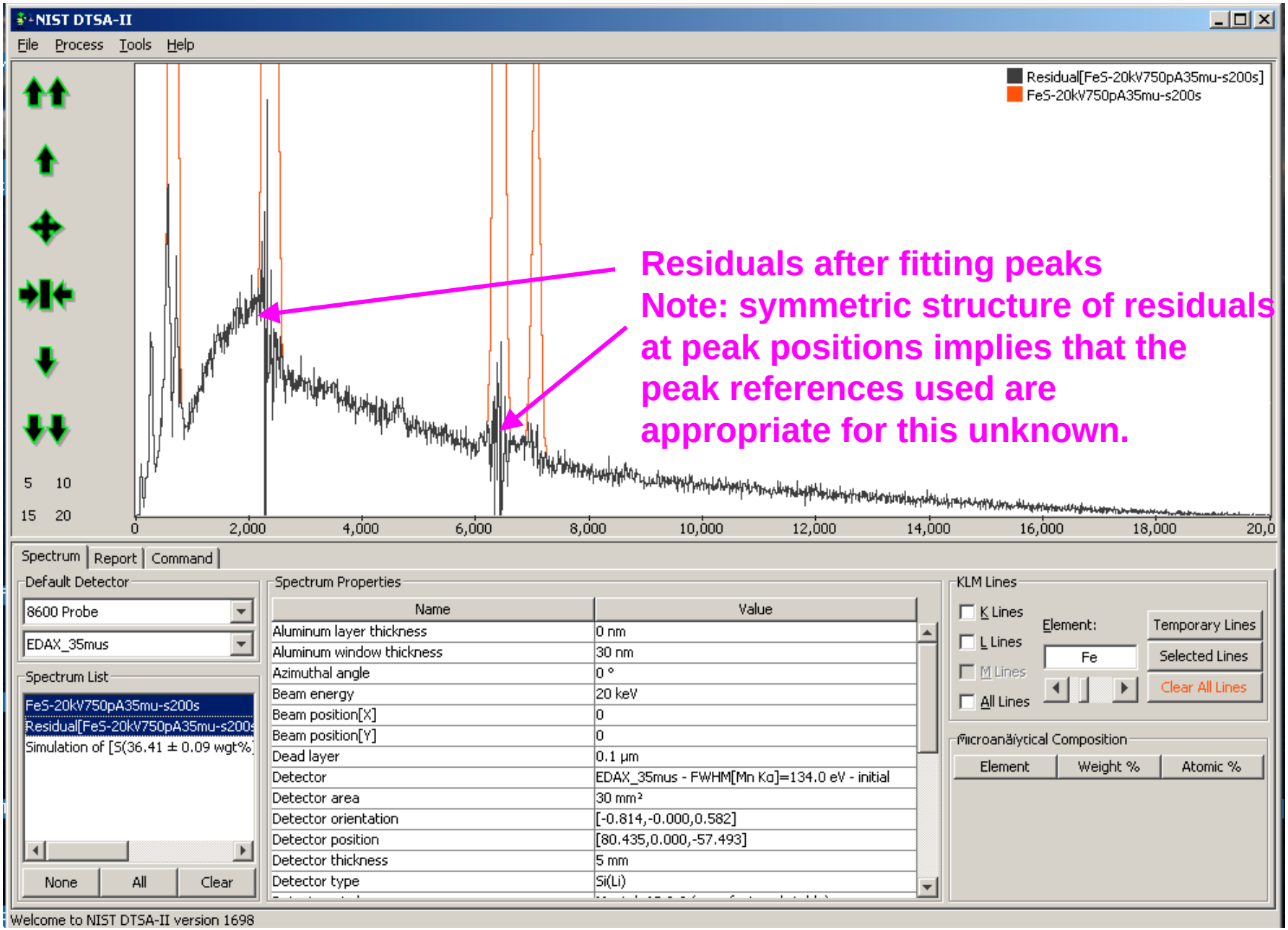
**Results**

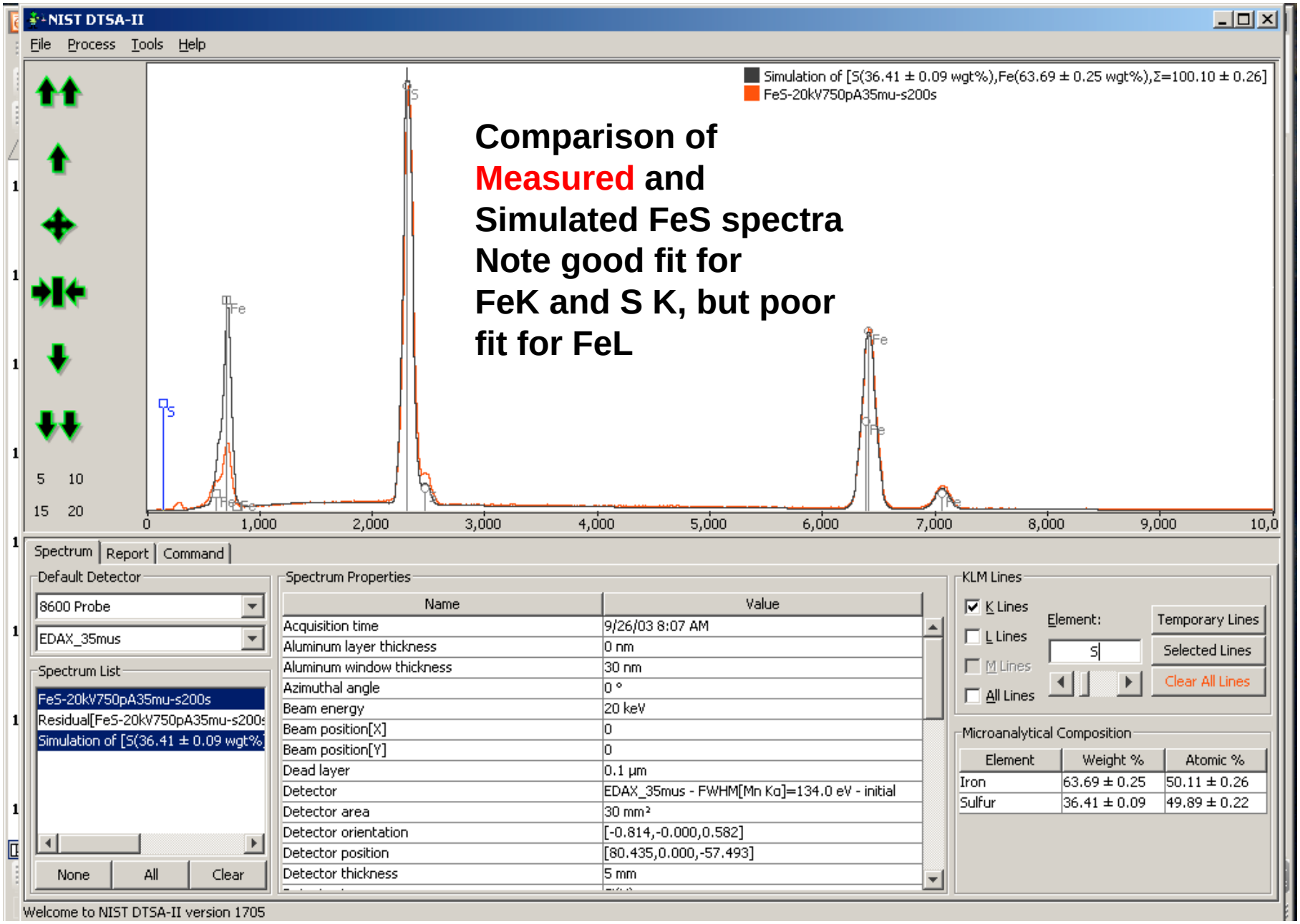
| Spectrum | Quantity | S | | | Fe | | | Sum |
|---|---|---|---|---|---|---|---|---|
| | Line | S K-family | | | Fe Kα | | | |
| FeS-20kV750pA35mu-s200s | Z·A·F | 0.98 | 1.12 | 1.00 | 0.95 | 0.98 | 1.00 | |
| | k-ratios | 1.1897 | ± | 0.0029 | 0.5956 | ± | 0.0023 | |
| | weight % | **36.41** | ± | 0.09 | **63.69** | ± | 0.25 | 100.10 |
| I = 1.000 nA | norm(wgt %) | 36.38 | ± | 0.09 | 63.62 | ± | 0.25 | - |
| LT = 200.0 s | atomic % | 49.89 | | | 50.11 | | | |

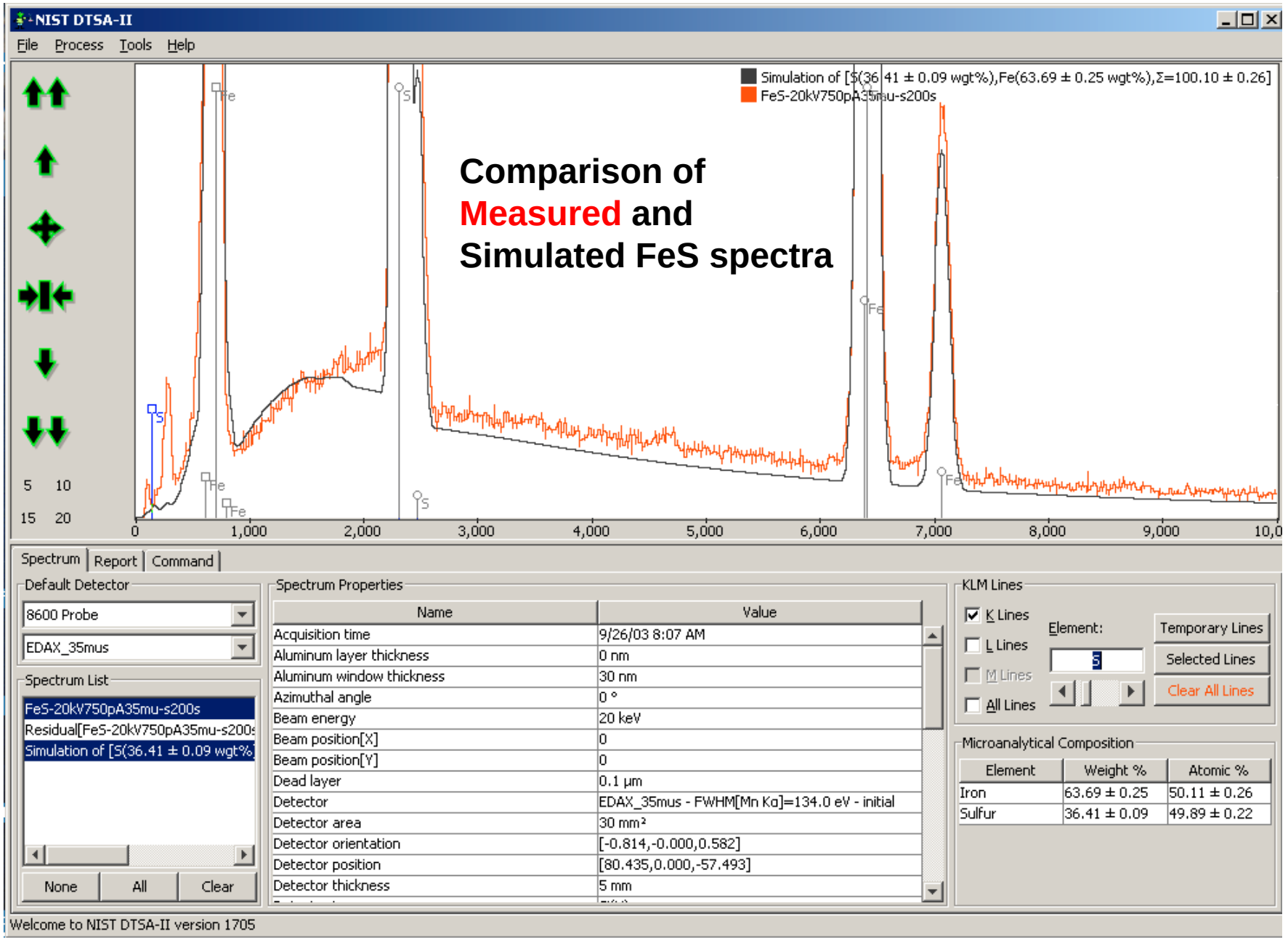
**Table:** Quantiative results (uncertainties are statistical-only, 1 σ)

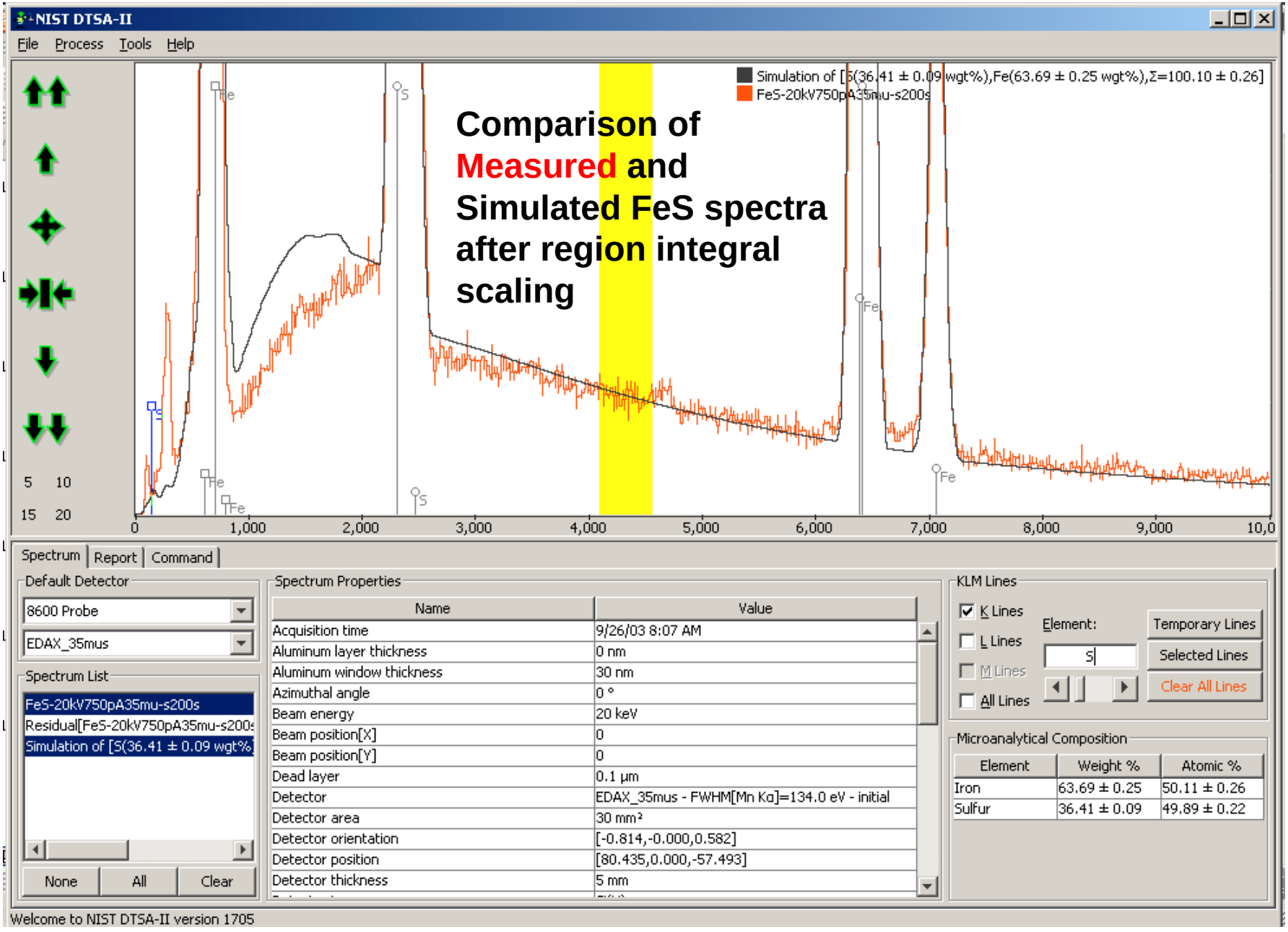
**Report contains ZAF details**

Welcome to NIST DTSA-II version 1705

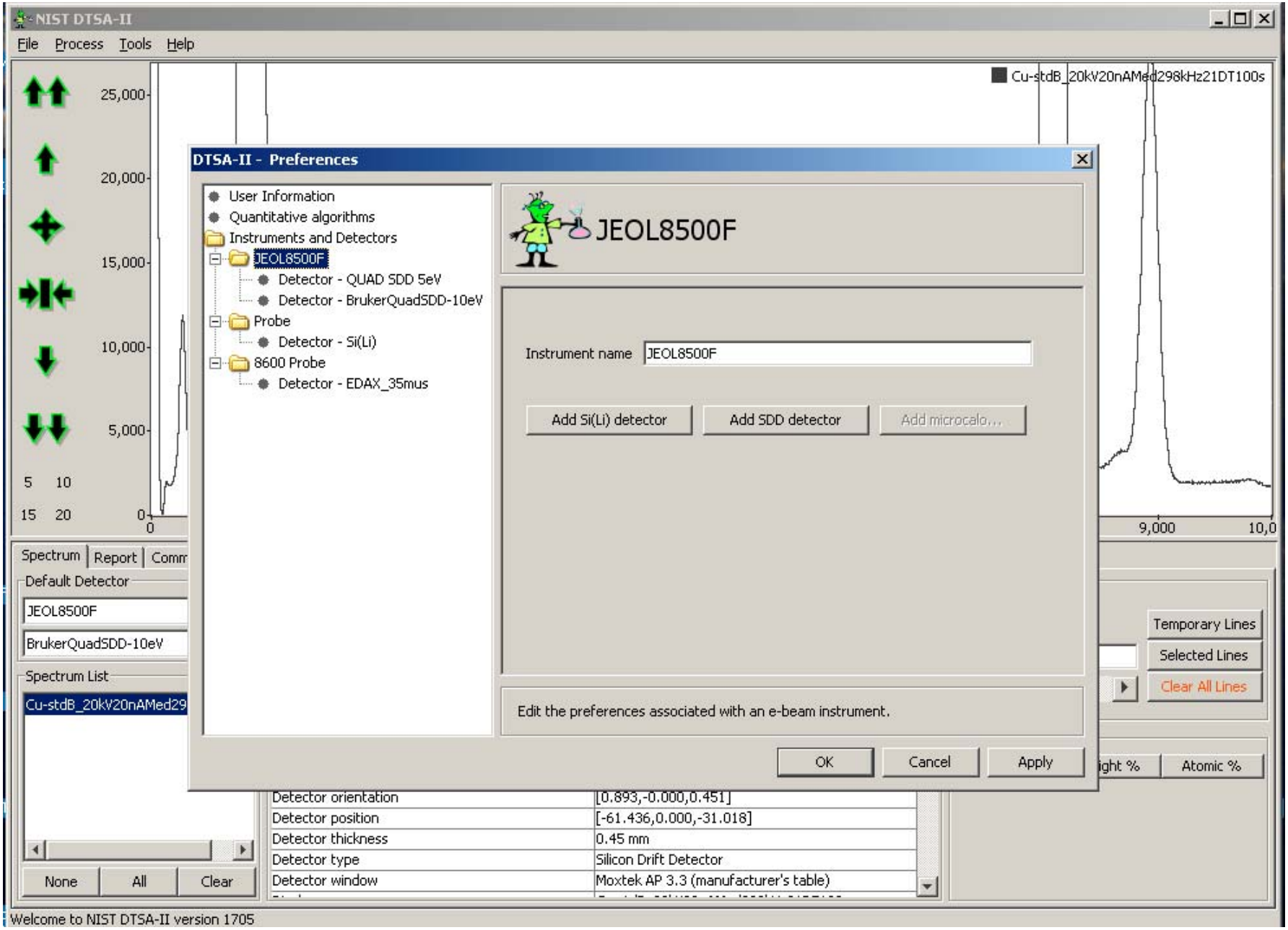

NIST DTSA-II
File Process Tools Help
Residual[FeS-20kV750pA35mu-s200s]
FeS-20kV750pA35mu-s200s
Residuals after fitting peaks
Note: symmetric structure of residuals at peak positions implies that the peak references used are appropriate for this unknown.
0 2,000 4,000 6,000 8,000 10,000 12,000 14,000 16,000 18,000 20,0
Spectrum Report Command
Default Detector
8600 Probe
EDAX_35mus
Spectrum List
FeS-20kV750pA35mu-s200s
Residual[FeS-20kV750pA35mu-s200s
Simulation of [S(36.41 ± 0.09 wgt%
None All Clear
Spectrum Properties
Name Value
Aluminum layer thickness 0 nm
Aluminum window thickness 30 nm
Azimuthal angle 0 °
Beam energy 20 keV
Beam position[X] 0
Beam position[Y] 0
Dead layer 0.1 µm
Detector EDAX_35mus - FWHM[Mn Kα]=134.0 eV - initial
Detector area 30 mm²
Detector orientation [-0.814,-0.000,0.582]
Detector position [80.435,0.000,-57.493]
Detector thickness 5 mm
Detector type Si(Li)
KLM Lines
K Lines
L Lines
M Lines
All Lines
Element:
Fe
Temporary Lines
Selected Lines
Clear All Lines
Microanalytical Composition
Element Weight % Atomic %
Welcome to NIST DTSA-II version 1698


NIST DTSA-II
File Process Tools Help
Simulation of [S(36.41 ± 0.09 wgt%),Fe(63.69 ± 0.25 wgt%),Σ=100.10 ± 0.26]
FeS-20kV750pA35mu-s200s
Comparison of
Measured and
Simulated FeS spectra
Note good fit for
FeK and S K, but poor
fit for FeL
0 1,000 2,000 3,000 4,000 5,000 6,000 7,000 8,000 9,000 10,0
Spectrum Report Command
Default Detector
8600 Probe
EDAX_35mus
Spectrum List
FeS-20kV750pA35mu-s200s
Residual[FeS-20kV750pA35mu-s200s
Simulation of [S(36.41 ± 0.09 wgt%
None All Clear
Spectrum Properties
Name Value
Acquisition time 9/26/03 8:07 AM
Aluminum layer thickness 0 nm
Aluminum window thickness 30 nm
Azimuthal angle 0 °
Beam energy 20 keV
Beam position[X] 0
Beam position[Y] 0
Dead layer 0.1 µm
Detector EDAX_35mus - FWHM[Mn Kα]=134.0 eV - initial
Detector area 30 mm²
Detector orientation [-0.814,-0.000,0.582]
Detector position [80.435,0.000,-57.493]
Detector thickness 5 mm
KLM Lines
K Lines
L Lines
M Lines
All Lines
Element:
S
Temporary Lines
Selected Lines
Clear All Lines
Microanalytical Composition
Element Weight % Atomic %
Iron 63.69 ± 0.25 50.11 ± 0.26
Sulfur 36.41 ± 0.09 49.89 ± 0.22
Welcome to NIST DTSA-II version 1705

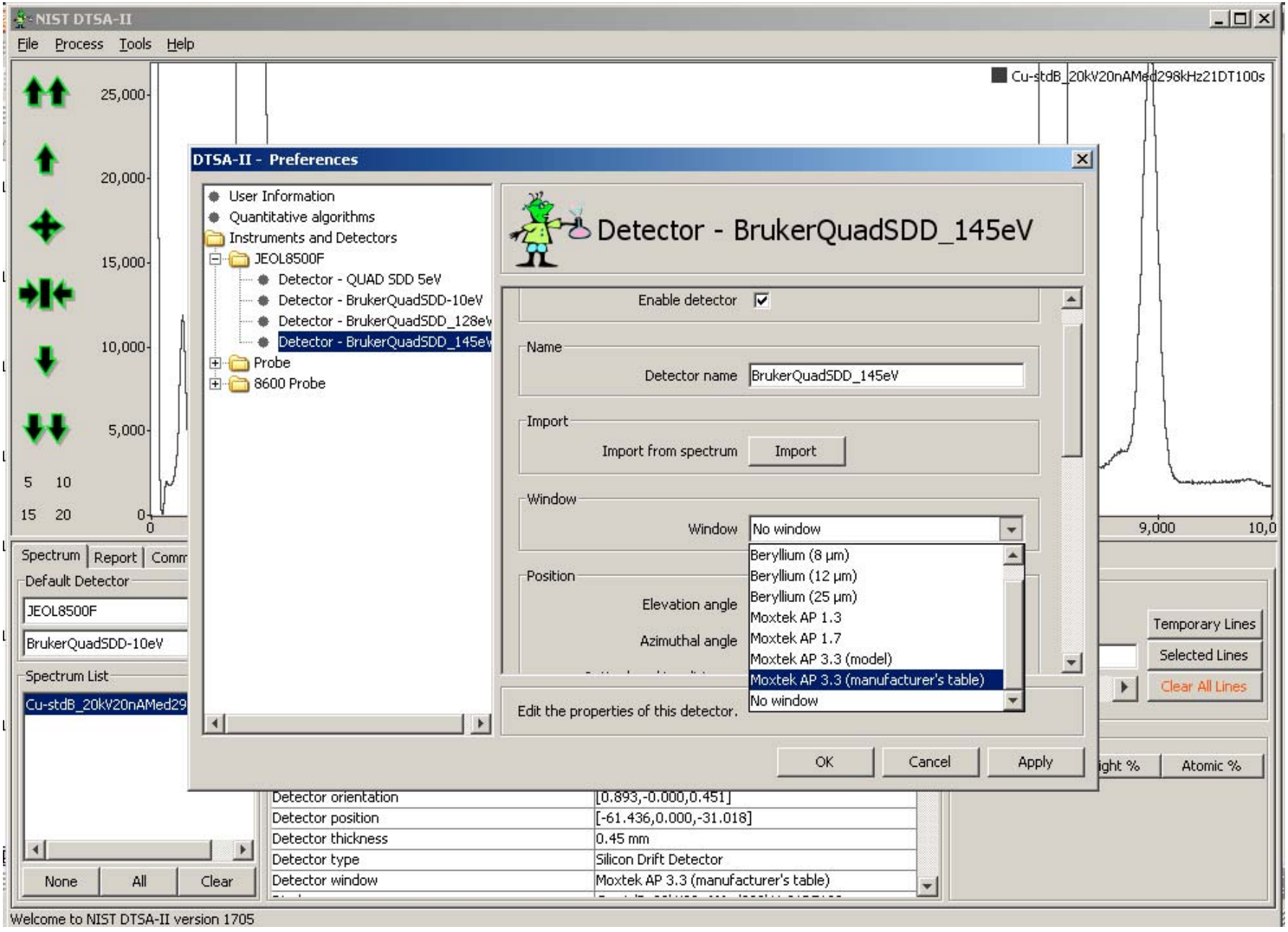

NIST DTSA-II
File Process Tools Help
Simulation of [S(36.41 ± 0.09 wgt%),Fe(63.69 ± 0.25 wgt%),Σ=100.10 ± 0.26]
FeS-20kV750pA35mu-s200s
Comparison of
Measured and
Simulated FeS spectra
0 1,000 2,000 3,000 4,000 5,000 6,000 7,000 8,000 9,000 10,0
Spectrum Report Command
Default Detector
8600 Probe
EDAX_35mus
Spectrum List
FeS-20kV750pA35mu-s200s
Residual[FeS-20kV750pA35mu-s200s
Simulation of [S(36.41 ± 0.09 wgt%)
None All Clear
Spectrum Properties
Name Value
Acquisition time 9/26/03 8:07 AM
Aluminum layer thickness 0 nm
Aluminum window thickness 30 nm
Azimuthal angle 0 °
Beam energy 20 keV
Beam position[X] 0
Beam position[Y] 0
Dead layer 0.1 µm
Detector EDAX_35mus - FWHM[Mn Kα]=134.0 eV - initial
Detector area 30 mm²
Detector orientation [-0.814,-0.000,0.582]
Detector position [80.435,0.000,-57.493]
Detector thickness 5 mm
KLM Lines
K Lines
L Lines
M Lines
All Lines
Element:
Temporary Lines
Selected Lines
Clear All Lines
Microanalytical Composition
Element Weight % Atomic %
Iron 63.69 ± 0.25 50.11 ± 0.26
Sulfur 36.41 ± 0.09 49.89 ± 0.22
Welcome to NIST DTSA-II version 1705


NIST DTSA-II
File Process Tools Help
Simulation of [S(36.41 ± 0.09 wgt%),Fe(63.69 ± 0.25 wgt%),Σ=100.10 ± 0.26]
FeS-20kV750pA35mu-s200s
Comparison of
Measured and
Simulated FeS spectra
after region integral
scaling
Fe
S
0
1,000
2,000
3,000
4,000
5,000
6,000
7,000
8,000
9,000
10,0
Spectrum
Report
Command
Default Detector
8600 Probe
EDAX_35mus
Spectrum List
FeS-20kV750pA35mu-s200s
Residual[FeS-20kV750pA35mu-s200s
Simulation of [S(36.41 ± 0.09 wgt%
None
All
Clear
Spectrum Properties
Name
Value
Acquisition time
9/26/03 8:07 AM
Aluminum layer thickness
0 nm
Aluminum window thickness
30 nm
Azimuthal angle
0 °
Beam energy
20 keV
Beam position[X]
0
Beam position[Y]
0
Dead layer
0.1 µm
Detector
EDAX_35mus - FWHM[Mn Kα]=134.0 eV - initial
Detector area
30 mm²
Detector orientation
[-0.814,-0.000,0.582]
Detector position
[80.435,0.000,-57.493]
Detector thickness
5 mm
KLM Lines
K Lines
L Lines
M Lines
All Lines
Element:
S
Temporary Lines
Selected Lines
Clear All Lines
Microanalytical Composition
Element
Weight %
Atomic %
Iron
63.69 ± 0.25
50.11 ± 0.26
Sulfur
36.41 ± 0.09
49.89 ± 0.22
Welcome to NIST DTSA-II version 1705

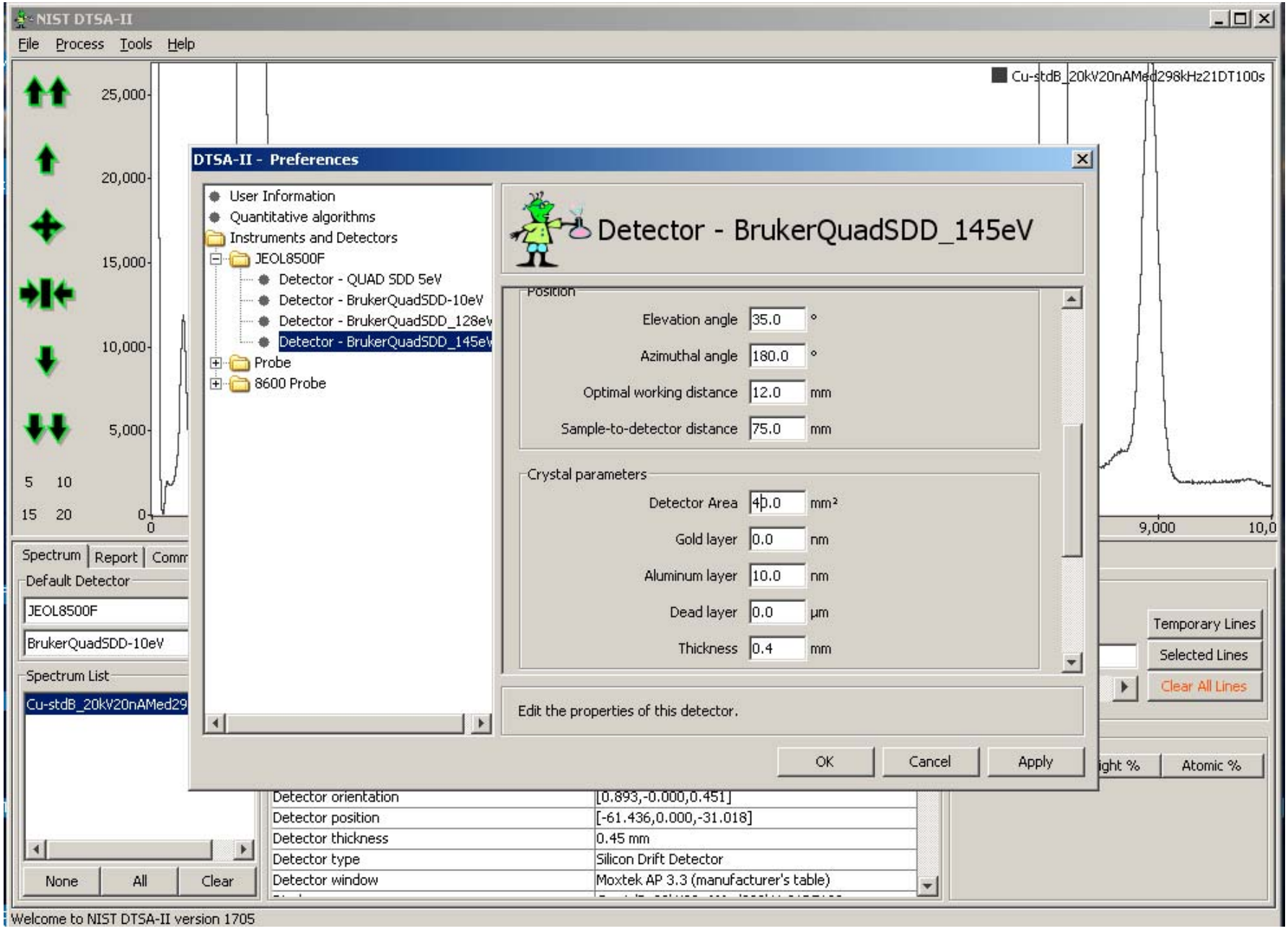
# Adding a new detector to the list under “Preferences”



# Adding a new detector to the list under “Preferences”



# Adding a new detector to the list under “Preferences”



# Adding a new detector to the list under “Preferences”