

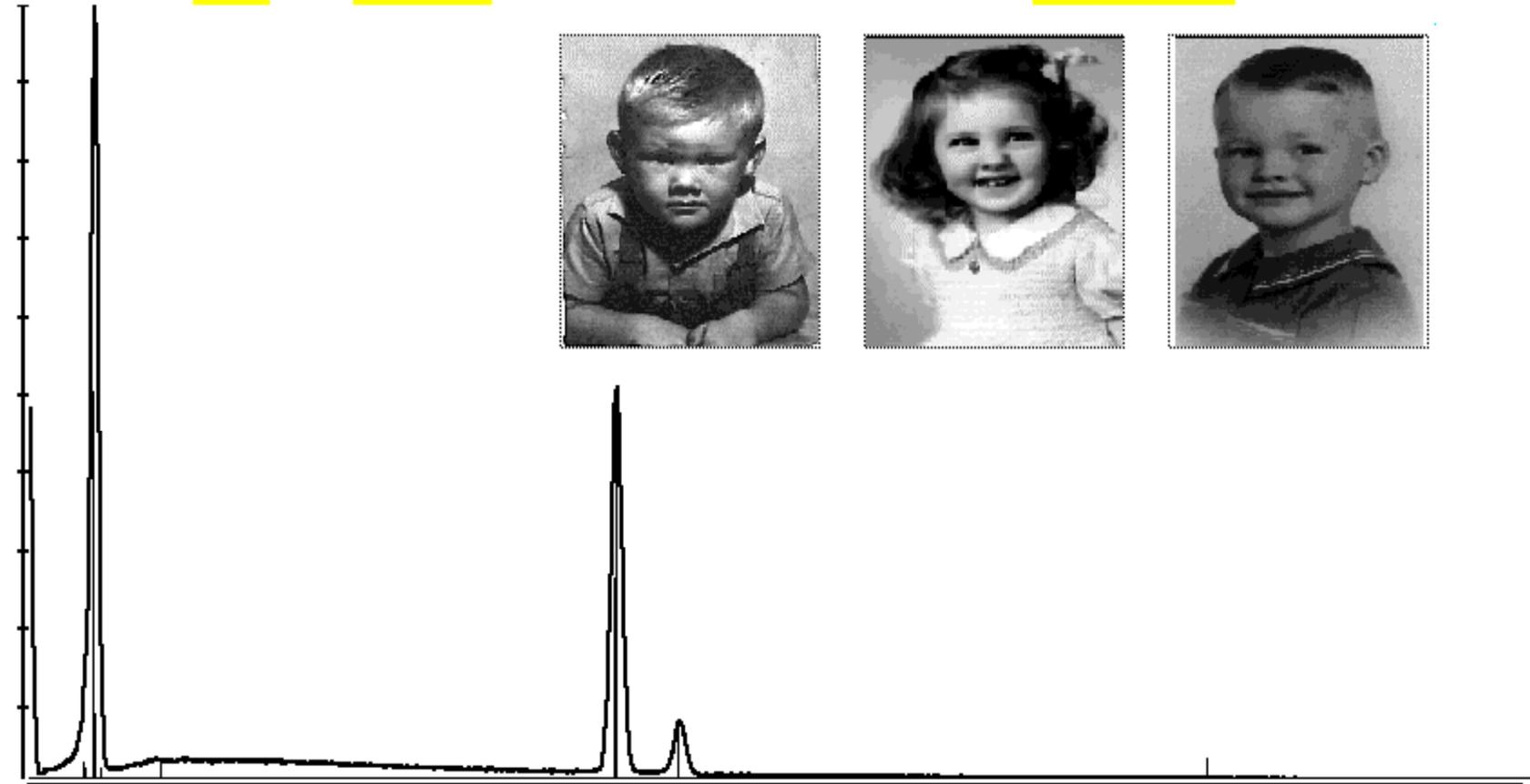
# **NIST DTSA-II (“Son of DTSA”): Step-by-Step**

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

# NIST-NIH Desktop Spectrum Analyzer (DTSA)

24283 Ch#: 695 Ch kV: 6.9500 Work: 253 Results: 0 Marker: Cu 29

9:58 AM DTSA 3.0.2

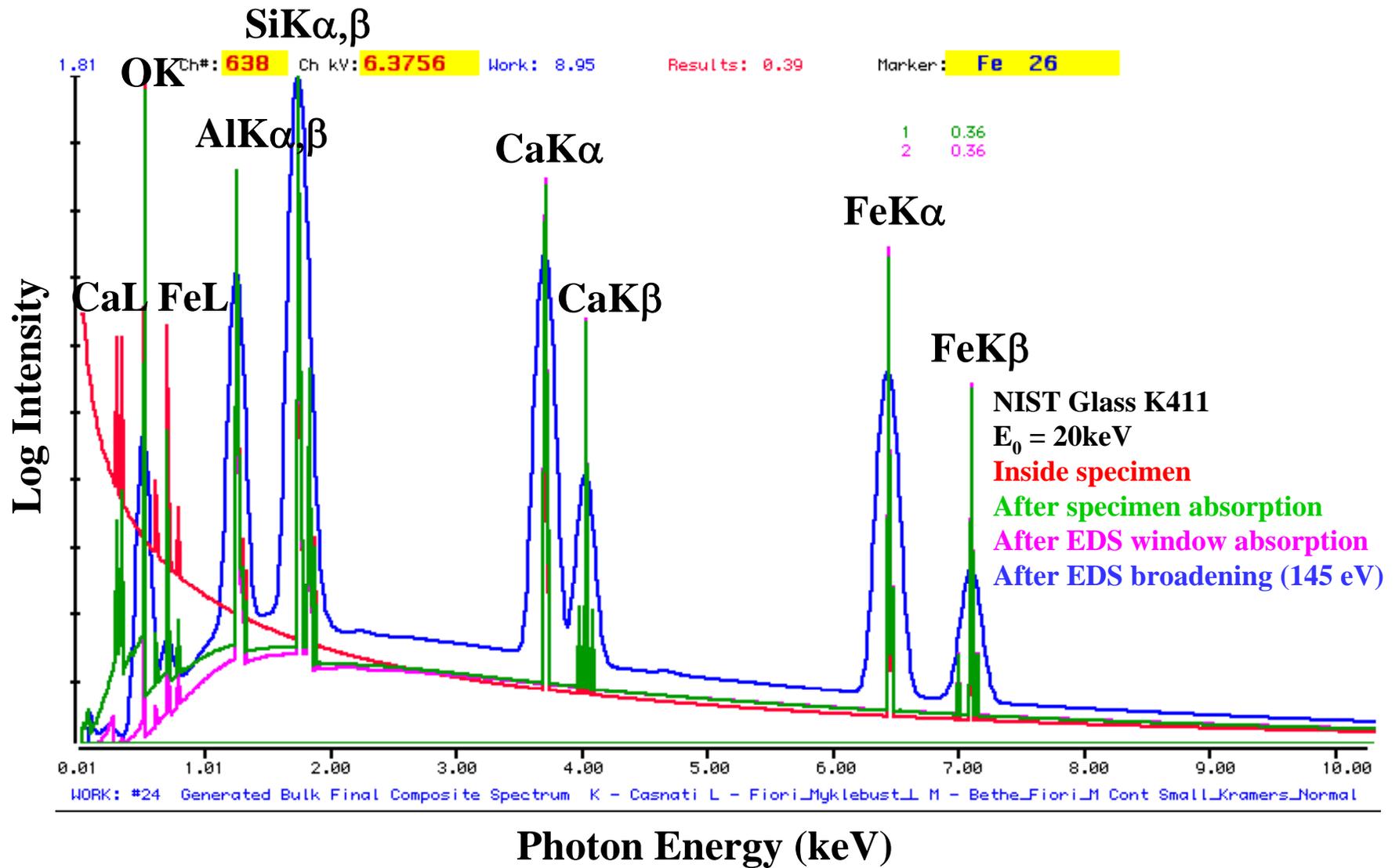


0.00 2.00 4.00 6.00 8.00 10.00 12.00 14.00 16.00 18.00 20.00

WORK: #1 Cu std 20 keV/0.5 nA/32%DT/20kX 9-28-94

ROI	Calibrate	Real 0 s	Click at Point in Spectrum to:	Pks+Escs+Dbles	Scale	● Linear ○ Log ○ Sqr Root □ Bipolar ☑ Auto Scale	
MLLSQ	Peak ID	Live 0 s		◀▶ KLM KLM			Off
Simplex	Calculator	Dead 0 %		Select Spectrum:			◀▶
Do a Fit	Copy Work		Expand Horiz		.5K 1K 2K 4K 8K	9//93 ResEdit	
Add Fit	Copy Rslt		Contract Horiz			9//93 Trash	
See Fit	Save Work	Input Output	Expand Vert				
			Contract Vert				
			Swap Wk & Rslt				
			Scan File				

# 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](mailto: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

Google The Ne... APOD: ... NIST Wi... MST Inside ... NIST D... NIST D... NIS... x

Chemical Science and Technology Laboratory  
Surface and Microanalysis Science Division

NIST  
National Institute of  
Standards and Technology

DTSA-II Son of DeskTop Spectrum Analyzer



**INTRODUCTION**

Geeky scientist in lab coat

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 techniques. 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.

[Introduction](#)  
[Installation](#)  
[Getting Started](#)  
[Simulation](#)  
[Quantification](#)  
[Scripting](#)  
[Why Java?](#)  
[3rd Party Licenses](#)  
[Contact Us](#)

[NIST Home Page](#)      [CSTL Home Page](#)      [SMSD Home Page](#)      [NISTMonte Home Page](#)

DISCLAIMER: *Any mention of commercial products is for information only; it does not imply recommendation or endorsement by NIST nor does it imply that the products mentioned are necessarily the best available for the purpose.*

Done Local intranet 100%

Start E... I... N... J... S... M... N... A... M... li... I... C... M... 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

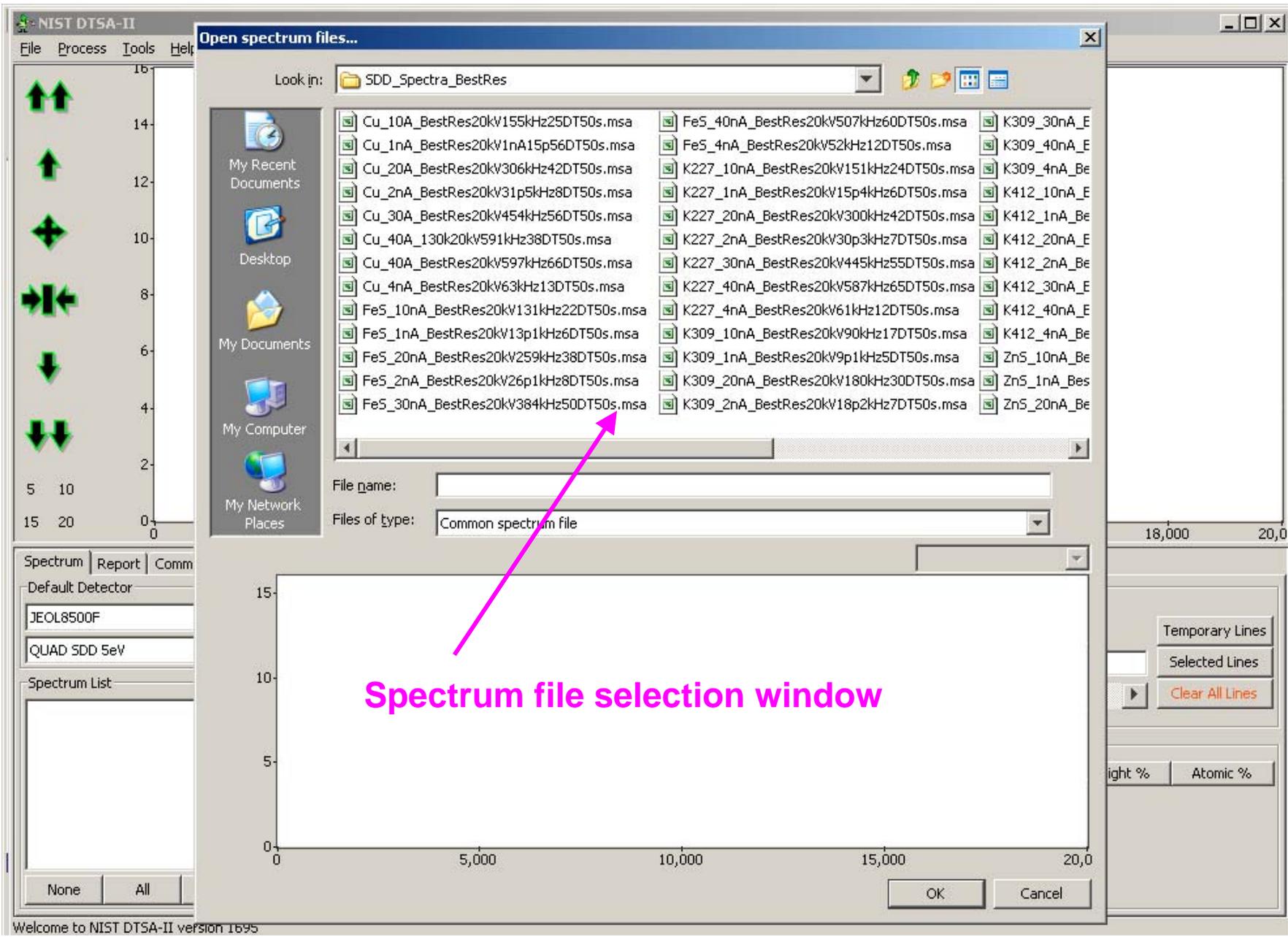
# Display and overlay spectra with various scaling options on linear/log/sqrt axes

The screenshot displays the NIST DTSA-II software interface. The main window features a plot area with a vertical axis ranging from 0 to 16 and a horizontal axis ranging from 0 to 20,000. A vertical toolbar on the left side of the plot area contains several green icons for zooming and panning: two upward arrows, one upward arrow, a four-way arrow, two inward-pointing arrows, one downward arrow, and two downward arrows. Below these icons are numerical values: 5, 10, 15, and 20. The plot area is currently empty, with the text "Basic DTSA-II display window" overlaid in pink.

The control panel at the bottom of the window includes the following sections:

- Spectrum Properties:** Contains dropdown menus for "Default Detector" (set to JEOL8500F) and "QUAD SDD 5eV".
- Spectrum List:** A list box with "None", "All", and "Clear" buttons below it.
- KLM Lines:** Includes checkboxes for "K Lines", "L Lines", "M Lines", and "All Lines". It also features an "Element:" field with "He" selected, and buttons for "Temporary Lines", "Selected Lines", and "Clear All Lines".
- Composition:** A table with columns for "Element", "Weight %", and "Atomic %".

At the bottom left of the window, a status bar reads: "Welcome to NIST DTSA-II version 1695".



Open spectrum files...

Look in: SDD\_Spectra\_BestRes

- My Recent Documents
  - Desktop
  - My Documents
  - My Computer
  - My Network Places
- |   |  |   |
|---|--|---|
| <input checked="" type="checkbox"/> Cu_10A_BestRes20kV155kHz25DT50s.msa   | <input checked="" type="checkbox"/> Fe5_40nA_BestRes20kV507kHz60DT50s.msa  | <input checked="" type="checkbox"/> K309_30nA_E |
| <input checked="" type="checkbox"/> Cu_1nA_BestRes20kV1nA15p56DT50s.msa   | <input checked="" type="checkbox"/> Fe5_4nA_BestRes20kV52kHz12DT50s.msa    | <input checked="" type="checkbox"/> K309_40nA_E |
| <input checked="" type="checkbox"/> Cu_20A_BestRes20kV306kHz42DT50s.msa   | <input checked="" type="checkbox"/> K227_10nA_BestRes20kV151kHz24DT50s.msa | <input checked="" type="checkbox"/> K309_4nA_Be |
| <input checked="" type="checkbox"/> Cu_2nA_BestRes20kV31p5kHz8DT50s.msa   | <input checked="" type="checkbox"/> K227_1nA_BestRes20kV15p4kHz6DT50s.msa  | <input checked="" type="checkbox"/> K412_10nA_E |
| <input checked="" type="checkbox"/> Cu_30A_BestRes20kV454kHz56DT50s.msa   | <input checked="" type="checkbox"/> K227_20nA_BestRes20kV300kHz42DT50s.msa | <input checked="" type="checkbox"/> K412_1nA_Be |
| <input checked="" type="checkbox"/> Cu_40A_130k20kV591kHz38DT50s.msa      | <input checked="" type="checkbox"/> K227_2nA_BestRes20kV30p3kHz7DT50s.msa  | <input checked="" type="checkbox"/> K412_20nA_E |
| <input checked="" type="checkbox"/> Cu_40A_BestRes20kV597kHz66DT50s.msa   | <input checked="" type="checkbox"/> K227_30nA_BestRes20kV445kHz55DT50s.msa | <input checked="" type="checkbox"/> K412_2nA_Be |
| <input checked="" type="checkbox"/> Cu_4nA_BestRes20kV63kHz13DT50s.msa    | <input checked="" type="checkbox"/> K227_40nA_BestRes20kV587kHz65DT50s.msa | <input checked="" type="checkbox"/> K412_30nA_E |
| <input checked="" type="checkbox"/> Fe5_10nA_BestRes20kV131kHz22DT50s.msa | <input checked="" type="checkbox"/> K227_4nA_BestRes20kV61kHz12DT50s.msa   | <input checked="" type="checkbox"/> K412_40nA_E |
| <input checked="" type="checkbox"/> Fe5_1nA_BestRes20kV13p1kHz6DT50s.msa  | <input checked="" type="checkbox"/> K309_10nA_BestRes20kV90kHz17DT50s.msa  | <input checked="" type="checkbox"/> K412_4nA_Be |
| <input checked="" type="checkbox"/> Fe5_20nA_BestRes20kV259kHz38DT50s.msa | <input checked="" type="checkbox"/> K309_1nA_BestRes20kV9p1kHz5DT50s.msa   | <input checked="" type="checkbox"/> Zn5_10nA_Be |
| <input checked="" type="checkbox"/> Fe5_2nA_BestRes20kV26p1kHz8DT50s.msa  | <input checked="" type="checkbox"/> K309_20nA_BestRes20kV180kHz30DT50s.msa | <input checked="" type="checkbox"/> Zn5_1nA_Bes |
| <input checked="" type="checkbox"/> Fe5_30nA_BestRes20kV384kHz50DT50s.msa | <input checked="" type="checkbox"/> K309_2nA_BestRes20kV18p2kHz7DT50s.msa  | <input checked="" type="checkbox"/> Zn5_20nA_Be |

File name:   
Files of type: Common spectrum file

Spectrum file selection window

Spectrum | Report | Comm

Default Detector

JEOL8500F

QUAD SDD 5eV

Spectrum List

None | All



Temporary Lines

Selected Lines

Clear All Lines

Light % | Atomic %

OK | Cancel

NIST DTSA-II

File Process Tools Help

16  
14  
12  
10  
8  
6  
4  
2  
0

5 10  
15 20

Spectrum Report Comm

Default Detector

JEOL8500F

QUAD SDD 5eV

Spectrum List

None All

18,000 20,0

Light % Atomic %

OK Cancel

Temporary Lines  
Selected Lines  
Clear All Lines

Open spectrum files...

Look in: SDD\_Spectra\_BestRes

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  
Fe5\_10nA\_BestRes20kV131kHz22DT50s.msa  
Fe5\_1nA\_BestRes20kV13p1kHz6DT50s.msa  
Fe5\_20nA\_BestRes20kV259kHz38DT50s.msa  
Fe5\_2nA\_BestRes20kV26p1kHz8DT50s.msa  
Fe5\_30nA\_BestRes20kV384kHz50DT50s.msa  
Fe5\_40nA\_BestRes20kV507kHz60DT50s.msa  
Fe5\_4nA\_BestRes20kV52kHz12DT50s.msa  
K227\_10nA\_BestRes20kV151kHz24DT50s.msa  
K227\_1nA\_BestRes20kV15p4kHz6DT50s.msa  
K227\_20nA\_BestRes20kV300kHz42DT50s.msa  
K227\_2nA\_BestRes20kV30p3kHz7DT50s.msa  
K227\_30nA\_BestRes20kV445kHz55DT50s.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\_4nA\_Be  
K412\_4nA\_E  
Zn5\_10nA\_Be  
Zn5\_1nA\_Bes  
Zn5\_20nA\_Be

File name: Cu\_20A\_BestRes20kV306kHz42DT50s.msa

Files of type: Common spectrum file

400,000  
200,000  
0

0 5,000 10,000 15,000 20,0

Cu\_20A\_BestRes20kV306kHz42DT50s

A single spectrum is selected.  
Spectrum preview opens in this window.

Welcome to NIST DTSA-II version 1695

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

The screenshot shows the NIST DTSA-II software interface. The main window displays a spectrum plot with the following characteristics:

- Y-axis:** Intensity (x-ray counts), ranging from 0 to 400,000.
- X-axis:** Energy scale in eV, ranging from 0 to 20,000.
- Plot:** A single spectrum showing a sharp peak at approximately 8,000 eV and a smaller peak at approximately 9,000 eV.
- Annotations:** Green arrows on the left indicate zoom and pan controls. A pink arrow points to the y-axis label "Intensity (x-ray counts)". Another pink arrow points to the x-axis label "Energy scale in eV".

Below the plot, the "Spectrum Properties" table is visible:

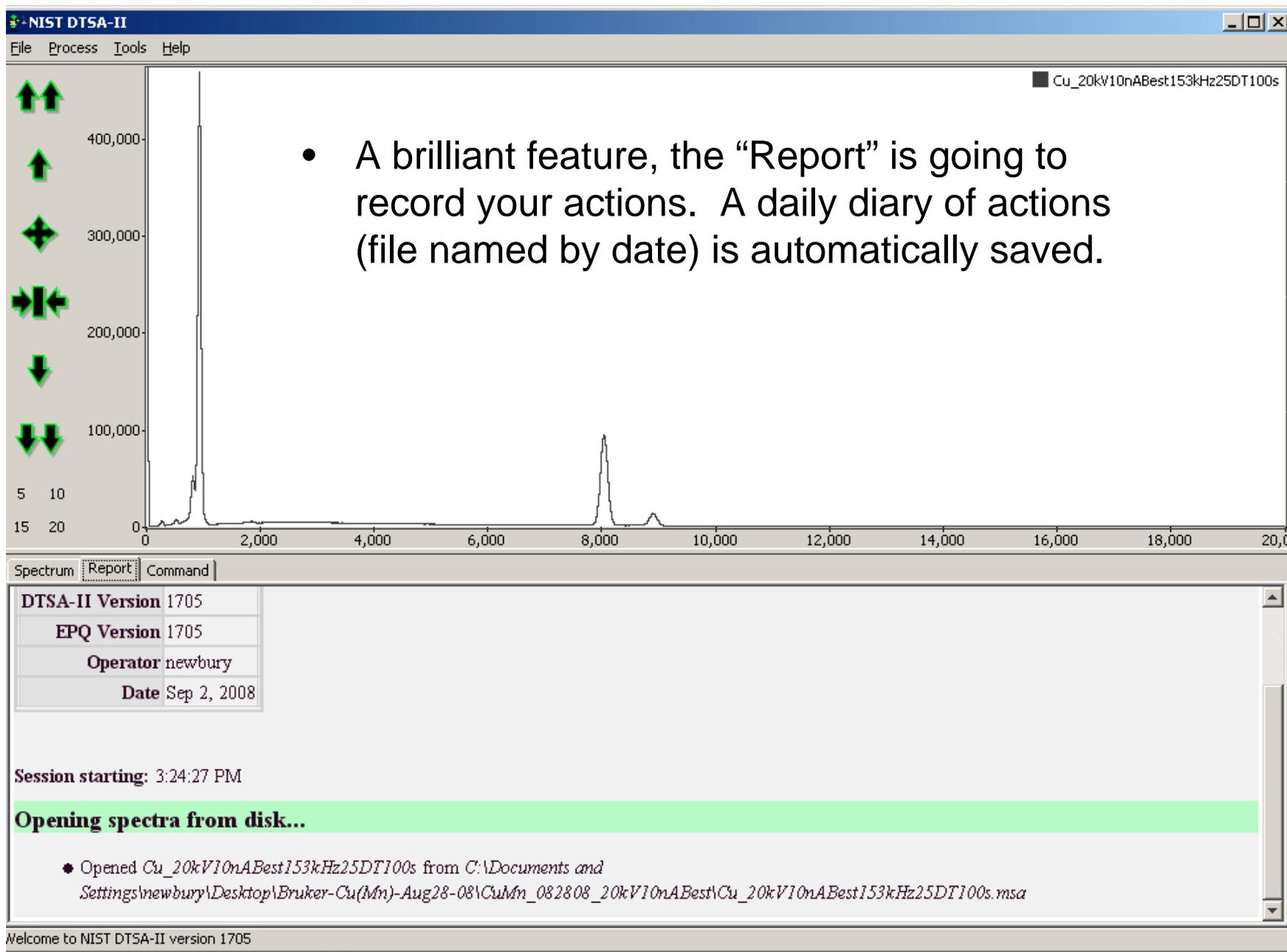
Name	Value
Acquisition time	8/18/08 1:30 PM
Aluminum layer thickness	10 nm
Aluminum window thickness	30 nm
Azimuthal angle	180 °
Beam energy	20 keV
Dead layer	0 μm
Detector	QUAD SDD 5eV - FWHM[Mn Kα]=125.0 eV - Aug...
Detector area	40 mm <sup>2</sup>
Detector orientation	[0.893,-0.000,0.451]
Detector 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)

Other interface elements include:

- Spectrum List:** A list of spectra with "Cu\_20A\_BestRes20kV306kHz42DT50" selected. A pink annotation says "Opened spectra are listed here".
- KLM Lines:** A section for selecting characteristic lines, currently showing "He" as the element.
- Composition:** A section for displaying the composition of the sample.

At the bottom left, the text "Welcome to NIST DTSA-II version 1695" is visible.

# But wait!



The screenshot displays the NIST DTSA-II software interface. The main window shows a spectrum plot with a y-axis ranging from 0 to 400,000 and an x-axis from 0 to 20,000. A prominent peak is visible at approximately 8,000. The plot is titled "Cu\_20kV10nABest153kHz25DT100s".

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

The interface includes a menu bar (File, Process, Tools, Help) and a toolbar with various navigation icons. Below the plot, there are tabs for "Spectrum", "Report", and "Command". The "Report" tab is active, displaying the following information:

DTSA-II Version	1705
EPQ Version	1705
Operator	newbury
Date	Sep 2, 2008

Session starting: 3:24:27 PM

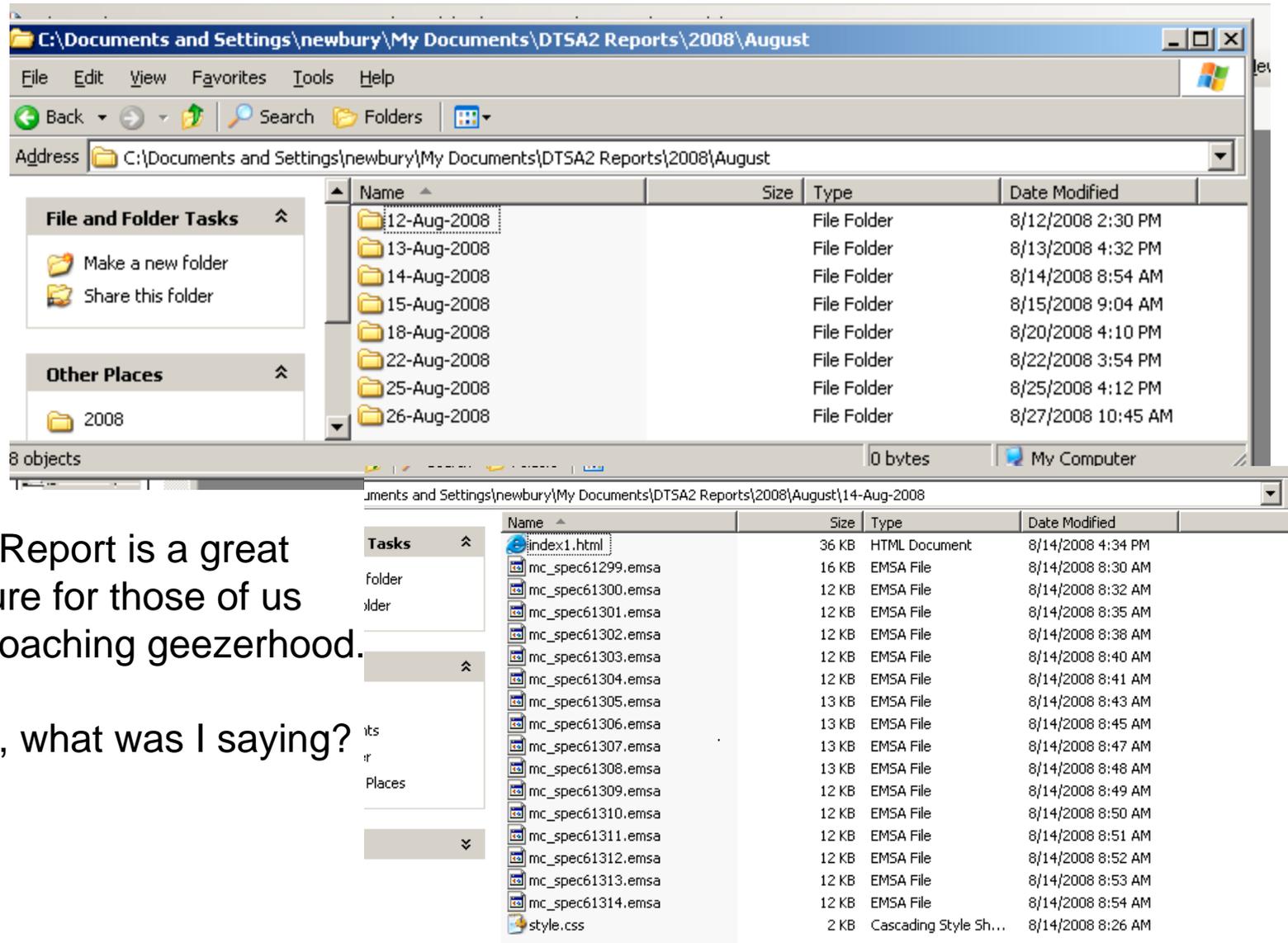
**Opening spectra from disk...**

- Opened Cu\_20kV10nABest153kHz25DT100s from C:\Documents and Settings\newbury\Desktop\Bruker-Cu(Mn)-Aug28-08\CuMn\_082808\_20kV10nABest\Cu\_20kV10nABest153kHz25DT100s.msa

Welcome to NIST DTSA-II version 1705

# 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

16  
14  
12  
10  
8  
6  
4  
2  
0

5 10  
15 20

Spectrum Report Comm

Default Detector

JEOL8500F

QUAD SDD 5eV

Spectrum List

None All

Open spectrum files...

Look in: SDD\_Spectra\_BestRes

My Recent Documents  
Desktop  
My Documents  
My Computer  
My Network Places

<input type="checkbox"/> Cu_10A_BestRes20kV155kHz25DT50s.msa	<input type="checkbox"/> Fe5_40nA_BestRes20kV507kHz60DT50s.msa	<input type="checkbox"/> K309_30nA_E
<input type="checkbox"/> Cu_1nA_BestRes20kV1nA15p56DT50s.msa	<input type="checkbox"/> Fe5_4nA_BestRes20kV52kHz12DT50s.msa	<input type="checkbox"/> K309_40nA_E
<input type="checkbox"/> Cu_20A_BestRes20kV306kHz42DT50s.msa	<input type="checkbox"/> K227_10nA_BestRes20kV151kHz24DT50s.msa	<input type="checkbox"/> K309_4nA_Be
<input type="checkbox"/> Cu_2nA_BestRes20kV31p5kHz8DT50s.msa	<input type="checkbox"/> K227_1nA_BestRes20kV15p4kHz6DT50s.msa	<input type="checkbox"/> K412_10nA_E
<input type="checkbox"/> Cu_30A_BestRes20kV454kHz56DT50s.msa	<input type="checkbox"/> K227_20nA_BestRes20kV300kHz42DT50s.msa	<input type="checkbox"/> K412_1nA_Be
<input type="checkbox"/> Cu_40A_130k20kV591kHz38DT50s.msa	<input type="checkbox"/> K227_2nA_BestRes20kV30p3kHz7DT50s.msa	<input type="checkbox"/> K412_20nA_E
<input type="checkbox"/> Cu_40A_BestRes20kV597kHz66DT50s.msa	<input type="checkbox"/> K227_30nA_BestRes20kV445kHz55DT50s.msa	<input type="checkbox"/> K412_2nA_Be
<input type="checkbox"/> Cu_4nA_BestRes20kV63kHz13DT50s.msa	<input type="checkbox"/> K227_40nA_BestRes20kV587kHz65DT50s.msa	<input type="checkbox"/> K412_30nA_E
<input type="checkbox"/> Fe5_10nA_BestRes20kV131kHz22DT50s.msa	<input type="checkbox"/> K227_4nA_BestRes20kV61kHz12DT50s.msa	<input type="checkbox"/> K412_40nA_E
<input type="checkbox"/> Fe5_1nA_BestRes20kV13p1kHz6DT50s.msa	<input type="checkbox"/> K309_10nA_BestRes20kV90kHz17DT50s.msa	<input type="checkbox"/> K412_4nA_Be
<input type="checkbox"/> Fe5_20nA_BestRes20kV259kHz38DT50s.msa	<input type="checkbox"/> K309_1nA_BestRes20kV9p1kHz5DT50s.msa	<input type="checkbox"/> Zn5_10nA_Be
<input type="checkbox"/> Fe5_2nA_BestRes20kV26p1kHz8DT50s.msa	<input type="checkbox"/> K309_20nA_BestRes20kV180kHz30DT50s.msa	<input type="checkbox"/> Zn5_1nA_Bes
<input type="checkbox"/> Fe5_30nA_BestRes20kV384kHz50DT50s.msa	<input type="checkbox"/> K309_2nA_BestRes20kV18p2kHz7DT50s.msa	<input type="checkbox"/> Zn5_20nA_Be

File name: sa "Fe5\_1nA\_BestRes20kV13p1kHz6DT50s.msa" "Fe5\_20nA\_BestRes20kV259kHz38DT50s.msa"

Files of type: Common spectrum file

Fe5\_10nA\_BestRes20kV131kHz22DT50s  
 Fe5\_1nA\_BestRes20kV13p1kHz6DT50s  
 Fe5\_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

Welcome to NIST DTSA-II version 1695

**NIST DTSA-II**

File Process Tools Help

16  
14  
12  
10  
8  
6  
4  
2  
0

5 10  
15 20

Spectrum Report Comm

Default Detector

JEOL8500F

QUAD SDD 5eV

Spectrum List

None All

Welcome to NIST DTSA-II version 1695

**Open spectrum files...**

Look in: SDD\_Spectra\_BestRes

My Recent Documents  
Desktop  
My Documents  
My Computer  
My Network Places

<input checked="" type="checkbox"/> Cu_10A_BestRes20kV155kHz25DT50s.msa	<input checked="" type="checkbox"/> FeS_40nA_BestRes20kV507kHz60DT50s.msa	<input checked="" type="checkbox"/> K309_30nA_E
<input checked="" type="checkbox"/> Cu_1nA_BestRes20kV1nA15p56DT50s.msa	<input checked="" type="checkbox"/> FeS_4nA_BestRes20kV52kHz12DT50s.msa	<input checked="" type="checkbox"/> K309_40nA_E
<input checked="" type="checkbox"/> Cu_20A_BestRes20kV306kHz42DT50s.msa	<input checked="" type="checkbox"/> K227_10nA_BestRes20kV151kHz24DT50s.msa	<input checked="" type="checkbox"/> K309_4nA_Be
<input checked="" type="checkbox"/> Cu_2nA_BestRes20kV31p5kHz8DT50s.msa	<input checked="" type="checkbox"/> K227_1nA_BestRes20kV15p4kHz6DT50s.msa	<input checked="" type="checkbox"/> K412_10nA_E
<input checked="" type="checkbox"/> Cu_30A_BestRes20kV454kHz56DT50s.msa	<input checked="" type="checkbox"/> K227_20nA_BestRes20kV300kHz42DT50s.msa	<input checked="" type="checkbox"/> K412_1nA_Be
<input checked="" type="checkbox"/> Cu_40A_130k20kV591kHz38DT50s.msa	<input checked="" type="checkbox"/> K227_2nA_BestRes20kV30p3kHz7DT50s.msa	<input checked="" type="checkbox"/> K412_20nA_E
<input checked="" type="checkbox"/> Cu_40A_BestRes20kV597kHz66DT50s.msa	<input checked="" type="checkbox"/> K227_30nA_BestRes20kV445kHz55DT50s.msa	<input checked="" type="checkbox"/> K412_2nA_Be
<input checked="" type="checkbox"/> Cu_4nA_BestRes20kV63kHz13DT50s.msa	<input checked="" type="checkbox"/> K227_40nA_BestRes20kV587kHz65DT50s.msa	<input checked="" type="checkbox"/> K412_30nA_E
<input checked="" type="checkbox"/> FeS_10nA_BestRes20kV131kHz22DT50s.msa	<input checked="" type="checkbox"/> K227_4nA_BestRes20kV61kHz12DT50s.msa	<input checked="" type="checkbox"/> K412_40nA_E
<input checked="" type="checkbox"/> FeS_1nA_BestRes20kV13p1kHz6DT50s.msa	<input checked="" type="checkbox"/> K309_10nA_BestRes20kV90kHz17DT50s.msa	<input checked="" type="checkbox"/> K412_4nA_Be
<input checked="" type="checkbox"/> FeS_20nA_BestRes20kV259kHz38DT50s.msa	<input checked="" type="checkbox"/> K309_1nA_BestRes20kV9p1kHz5DT50s.msa	<input checked="" type="checkbox"/> ZnS_10nA_Be
<input checked="" type="checkbox"/> FeS_2nA_BestRes20kV26p1kHz8DT50s.msa	<input checked="" type="checkbox"/> K309_20nA_BestRes20kV180kHz30DT50s.msa	<input checked="" type="checkbox"/> ZnS_1nA_Bes
<input checked="" type="checkbox"/> FeS_30nA_BestRes20kV384kHz50DT50s.msa	<input checked="" type="checkbox"/> K309_2nA_BestRes20kV18p2kHz7DT50s.msa	<input checked="" type="checkbox"/> ZnS_20nA_Be

File name: a" "FeS\_20nA\_BestRes20kV259kHz38DT50s.msa" "FeS\_30nA\_BestRes20kV384kHz50DT50s.msa"

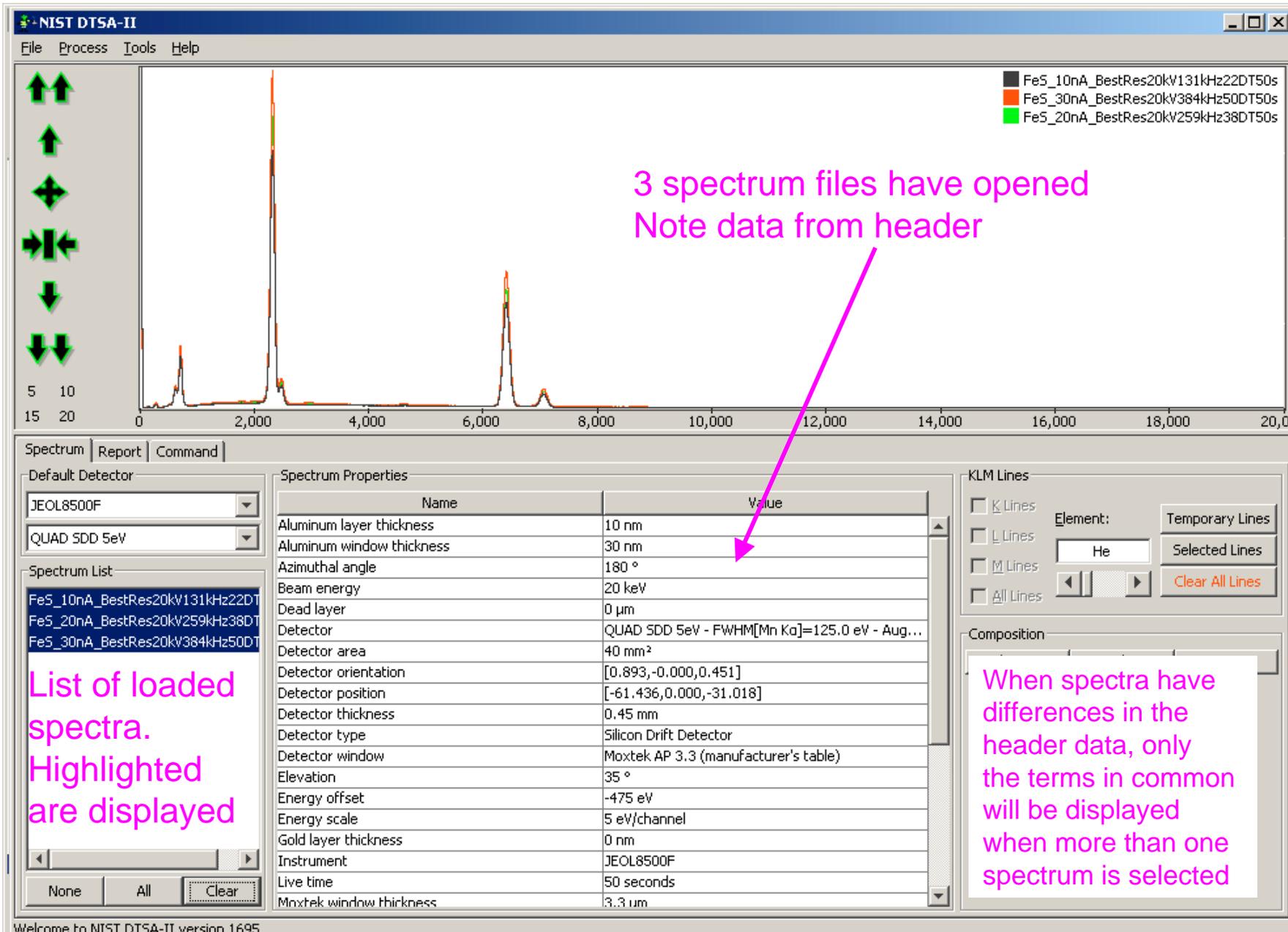
Files of type: Common spectrum file

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



# Basic operations

- Opening and manipulating spectral files
- Display of spectra

# Basic display of single spectrum

The screenshot shows the NIST DTSA-II software interface. The main window displays a spectrum plot for the file 'Cu\_10A\_BestRes20kV155kHz25DT50s'. The y-axis represents intensity, ranging from 0 to 5,000. The x-axis represents energy in eV, ranging from 0 to 20,000. The spectrum shows a broad peak around 2,000 eV and several sharp peaks at higher energies. On the left side of the plot, there are several green arrow icons for zooming: two up arrows, one up arrow, a four-way arrow, two left arrows, one down arrow, and two down arrows. Below these icons are numerical fields for zooming: '5 10' and '15 20'. Two pink arrows point from text annotations to the zoom controls. The bottom of the window contains a control panel with tabs for 'Spectrum', 'Report', and 'Command'. The 'Spectrum' tab is active, showing 'Default Detector' (JEOL8500F), 'Spectrum List' (Cu\_10A\_BestRes20kV155kHz25DT50s), and 'Spectrum Properties' table. The 'KLM Lines' section has checkboxes for K, L, M, and All Lines, with 'Element' set to 'He'. The 'Composition' section has columns for Element, Weight %, and Atomic %.

Changing the vertical axis scale:  
Method 1: Use arrows: x2 or x5 /2 or /5  
This arrow button restores full spectrum display  
Method 2: Mouse in y-axis number field; click and drag up or down

Name	Value
Acquisition time	8/18/08 11:17 AM
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 Ka]=125.0 eV - Aug...
Detector area	40 mm <sup>2</sup>
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)

Welcome to NIST DTSA-II version 1695

# Basic display of single spectrum

Changing the vertical axis scale:  
Method 3  
Right click in spectrum display brings up this Window; choose zoom in or zoom out; this operation can be repeated.  
Note: "Zoom to all" restores full spectrum

Default Detector: JEOL8500F  
QUAD SDD 5eV

Spectrum List:  
Cu\_10A\_BestRes20kV155kHz25DT50s

Spectrum Properties

Name	Value
Acquisition time	8/18/08 11:17 AM
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 mm <sup>2</sup>
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)

KLM Lines

K Lines  
 L Lines  
 M Lines  
 All Lines

Element: He  
Temporary Lines  
Selected Lines  
Clear All Lines

Composition

Element	Weight %	Atomic %
---------	----------	----------

Welcome to NIST DTSA-II version 1695

# Basic display of single spectrum

Changing the vertical axis scale from linear to log  
1. Right click in spectrum window.  
2. Select "Ordinate scale"  
3. Select "Log"

Copy  
Save  
Print  
Zoom to all  
Zoom in by 2  
Zoom in by 5  
Zoom out by 2  
Zoom out by 5  
Ordinate Scale  
Spectrum Comparison  
KLM Labels  
Create an ROI...

Linear  
Log  
Square root

Default Detector: JEOL8500F  
QUAD SDD 5eV

Spectrum List: Cu\_10A\_BestRes20kv155kHz25DT50

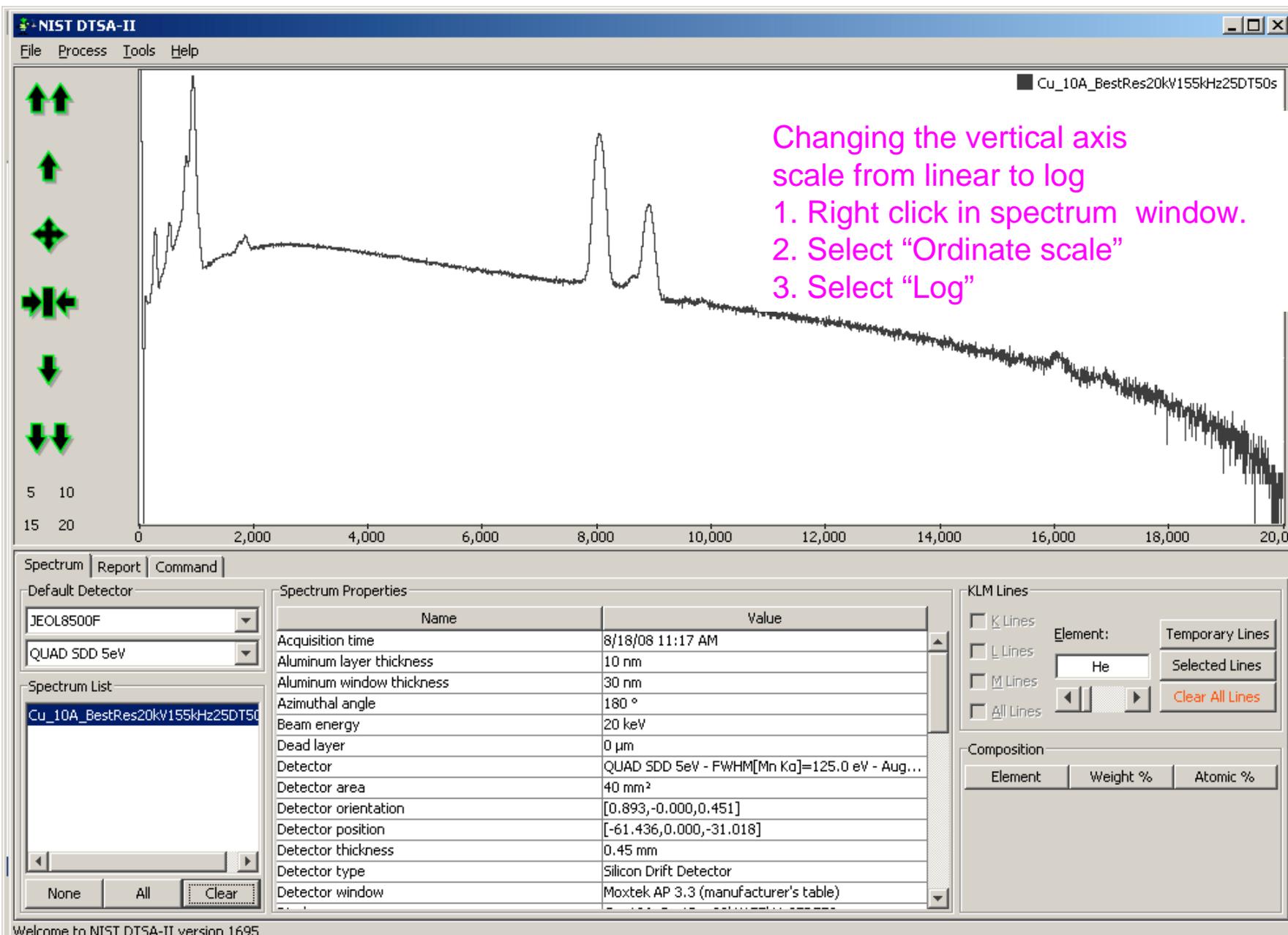
Name	Value
Acquisition time	8/18/08 11:17 AM
Aluminum layer thickness	10 nm
Aluminum window thickness	30 nm
Azimuthal angle	180 °
Beam energy	20 keV
Dead layer	0 µm
Detector	QUAD SDD 5eV - FWHM[Mn Kα]=125.0 eV - Aug...
Detector area	40 mm <sup>2</sup>
Detector orientation	[0.893,-0.000,0.451]
Detector 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)

KLM Lines  
Element: He  
Temporary Lines  
Selected Lines  
Clear All Lines

Composition  
Element Weight % Atomic %

Welcome to NIST DTSA-II version 1695

## Basic display of single spectrum



# Basic display of single spectrum

Changing the vertical axis scale from linear to square root

1. Right click in spectrum window.
2. Select "Ordinate scale"
3. Select "Square root"

**Spectrum Properties**

Name	Value
Acquisition time	8/18/08 10:42 AM
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 mm <sup>2</sup>
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)

**KLM Lines**

K Lines  
 L Lines  
 M Lines  
 All Lines

Element: He  
Temporary Lines  
Selected Lines  
Clear All Lines

**Composition**

Element	Weight %	Atomic %
---------	----------	----------

Welcome to NIST DTSA-II version 1695

# Basic display of single spectrum

The screenshot shows the NIST DTSA-II software interface. The main window displays a spectrum plot with a vertical axis ranging from 0 to 120,000 and a horizontal axis ranging from 0 to 20,000. A pink arrow points to the horizontal axis scale controls, which are labeled with values 5, 10, 15, and 20. The plot shows several peaks, with the most prominent one at approximately 2,000 eV. The software title bar indicates the file name: K309\_20nA\_BestRes20kV180kHz30DT50s.

Changing the horizontal axis scale: Method 1  
1. Click a preset to show 0-5, 0-10, 0-15, or 0-20 keV

Default Detector: JEOL8500F  
QUAD SDD 5eV

Spectrum List:  
Cu\_10A\_BestRes20kV155kHz25DT50  
K309\_1nA\_BestRes20kV9p1kHz5DT5  
K309\_20nA\_BestRes20kV180kHz30DT50

Spectrum Properties:

Name	Value
Acquisition time	8/18/08 1:23 PM
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 mm <sup>2</sup>
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)

KLM Lines:  
 K Lines  
 L Lines  
 M Lines  
 All Lines

Element: He  
Temporary Lines  
Selected Lines  
Clear All Lines

Composition:  
Element Weight % Atomic %

Welcome to NIST DTSA-II version 1695

# Basic display of single spectrum

The screenshot shows the NIST DTSA-II software interface. The main window displays a spectrum plot with a vertical axis ranging from 0 to 120,000 and a horizontal axis ranging from 0 to 5,000. A pink arrow points to the horizontal axis scale controls on the left side of the plot, which are labeled with the values 5, 10, 15, and 20. The plot shows several peaks, with the most prominent ones between 1,000 and 2,000 keV.

Changing the horizontal axis scale: Method 1

- Click a preset to show 0-5, 0-10, 0-15, or 0-20 keV
- **0 – 5 keV is shown**

The software interface includes a menu bar (File, Process, Tools, Help) and a title bar (NIST DTSA-II). The bottom panel contains several sections:

- Default Detector:** JEOL8500F, QUAD SDD 5eV
- Spectrum List:** Cu\_10A\_BestRes20kV155kHz25DT5C, K309\_1nA\_BestRes20kV9p1kHz5DTE, K309\_20nA\_BestRes20kV180kHz30DT50s
- Spectrum Properties:**

Name	Value
Acquisition time	8/18/08 1:23 PM
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 mm <sup>2</sup>
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)

- KLM Lines:** K Lines, L Lines, M Lines, All Lines (Element: H, Temporary Lines, Selected Lines, Clear All Lines)
- Composition:** Element, Weight %, Atomic %

Welcome to NIST DTSA-II version 1695

# Basic display of single spectrum

Changing the horizontal axis scale: method 2

- Right click in spectrum field
- Choose "create an ROI"

Default Detector: JEOL8500F  
QUAD SDD 5eV

Spectrum List:  
Cu\_10A\_BestRes20kV155kHz25DT5C  
K309\_1nA\_BestRes20kV9p1kHz5DT5C  
K309\_20nA\_BestRes20kV180kHz30DT50s

Spectrum Properties

Name	Value
Acquisition time	8/18/08 1:23 PM
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 mm <sup>2</sup>
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)

KLM Lines

Element: H  
Temporary Lines  
Selected Lines  
Clear All Lines

Composition

Element	Weight %	Atomic %
---------	----------	----------

Welcome to NIST DTSA-II version 1695

# Basic display of single spectrum

**Create an ROI**

Minimum energy  keV

Maximum energy  keV

Limits = [-1.0 keV, 21.0 keV]

Ok Cancel

Changing the horizontal axis scale: Method 2

1. Right click in spectrum field
2. Choose "create an ROI"
3. Define start and end energies

Spectrum | Report | Command

Default Detector: JEOL8500F  
QUAD SDD 5eV

Spectrum List:  
Cu\_10A\_BestRes20kV155kHz25DT50  
K309\_1nA\_BestRes20kV9p1kHz5DT50  
K309\_20nA\_BestRes20kV180kHz30DT50s

Spectrum Properties

Name	Value
Acquisition time	8/18/08 1:23 PM
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 mm <sup>2</sup>
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)

KLM Lines

K Lines  
 L Lines  
 M Lines  
 All Lines

Element: He  
Temporary Lines  
Selected Lines  
Clear All Lines

Composition

Element	Weight %	Atomic %
---------	----------	----------

Welcome to NIST DTSA-II version 1695

# Basic display of single spectrum

Changing the horizontal axis scale: Method 2

1. Right click in spectrum field
2. Choose "create an ROI"
3. Define start and end energies
4. "OK" This action creates yellow ROI
5. Click this icon to fully expand this ROI or
6. Click within ROI and select "Zoom to region"

Default Detector: JEOL8500F  
 QUAD SDD 5eV

Spectrum List:

- Cu\_10A\_BestRes20kV155kHz25DT5C
- K309\_1nA\_BestRes20kV9p1kHz5DTE
- K309\_20nA\_BestRes20kV180kHz30DT50s**

Spectrum Properties:

Name	Value
Acquisition time	8/18/08 1:23 PM
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 mm <sup>2</sup>
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)

KLM Lines:

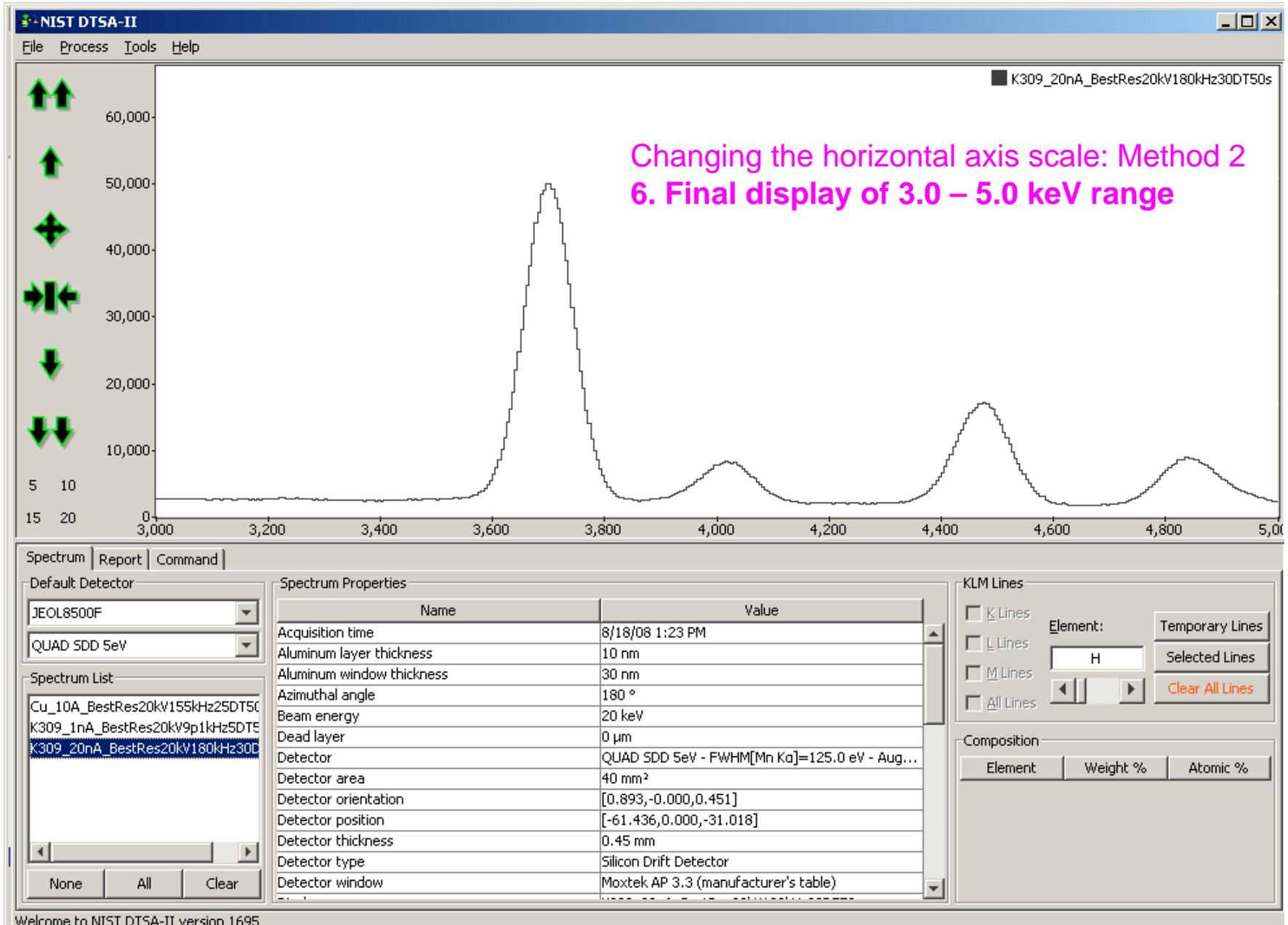
Element: He  
 Temporary Lines  
 Selected Lines  
 Clear All Lines

Composition:

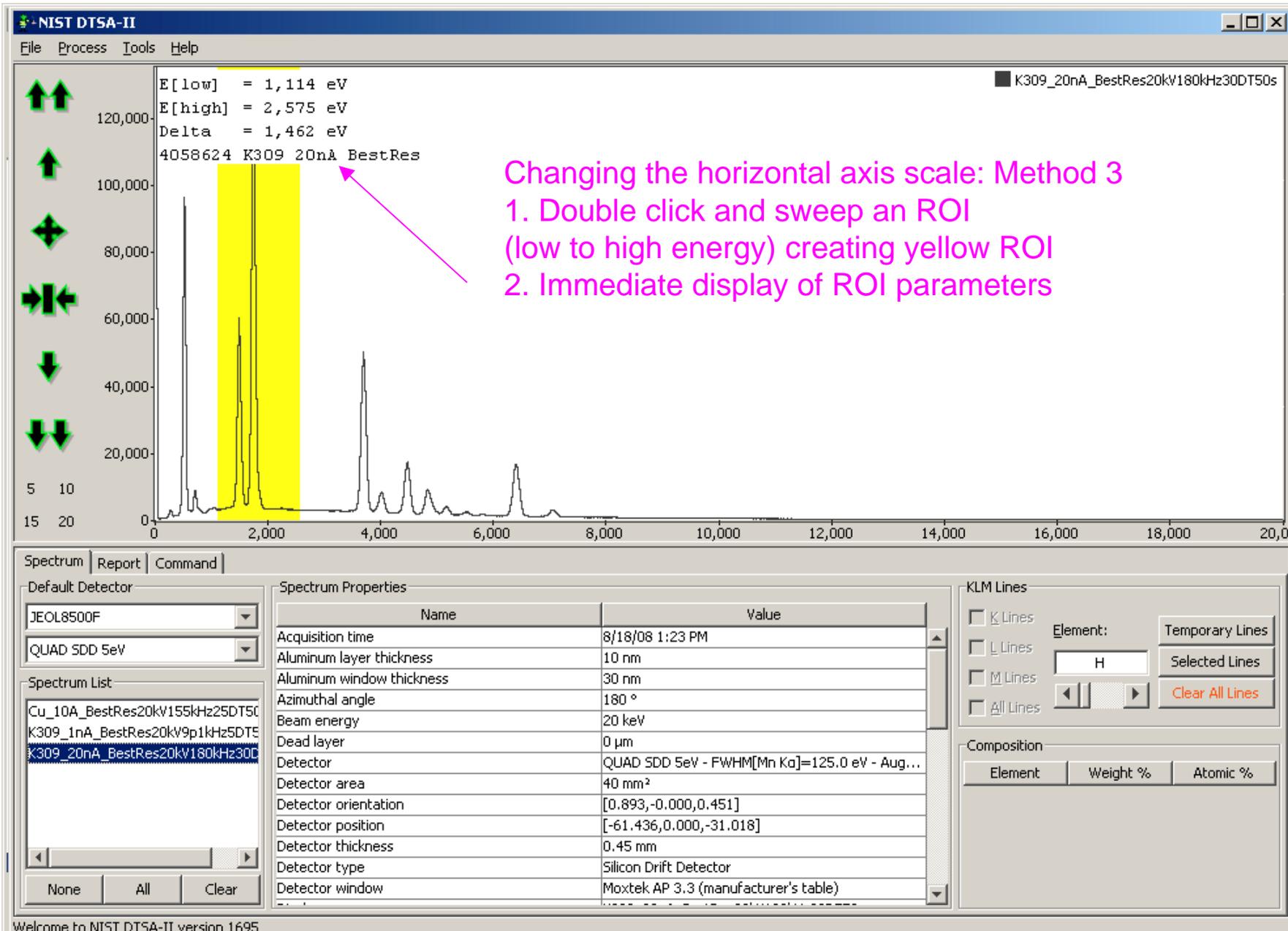
Element	Weight %	Atomic %

Welcome to NIST DTSA-II version 1695

# Basic display of single spectrum



# Basic display of single spectrum



# Basic display of single spectrum

The screenshot shows the NIST DTSA-II software interface. The main window displays a spectrum plot with a vertical axis representing counts (0 to 120,000) and a horizontal axis representing energy (0 to 20,000 eV). A yellow region of interest (ROI) is highlighted around a peak at approximately 2,000 eV. A context menu is open over the ROI, with the 'Zoom to region' option selected. The menu options are: Clear regions, Count events, Zoom to region, Zoom to all, and Copy Region(s) To Clipboard. The software title bar indicates the file name 'K309\_20nA\_BestRes20kV180kHz30DT50s'. The bottom panel shows the 'Spectrum Properties' table and the 'KLM Lines' section.

Changing the horizontal axis scale: Method 3

1. Double click and sweep an ROI (low to high energy) creating yellow ROI
2. Immediate display of ROI parameters
3. Click icon to expand

OR

4. Right click within yellow ROI
5. Select "zoom to region"

Name	Value
Acquisition time	8/18/08 1:23 PM
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 mm <sup>2</sup>
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)

KLM Lines

K Lines  
 L Lines  
 M Lines  
 All Lines

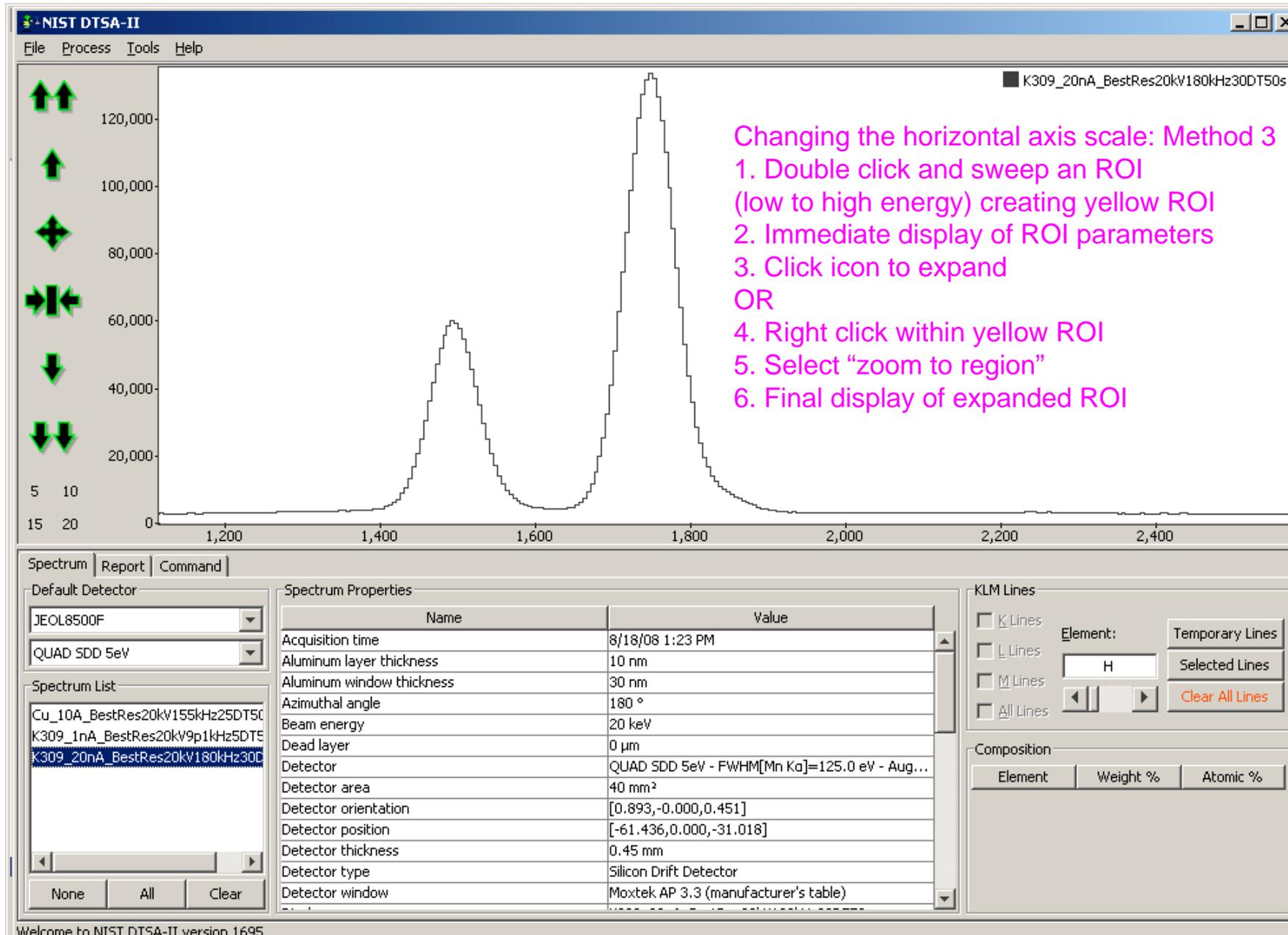
Element: H  
Temporary Lines  
Selected Lines  
Clear All Lines

Composition

Element	Weight %	Atomic %
---------	----------	----------

Welcome to NIST DTSA-II version 1695

# Basic display of single spectrum



- Changing the horizontal axis scale: Method 3
1. Double click and sweep an ROI (low to high energy) creating yellow ROI
  2. Immediate display of ROI parameters
  3. Click icon to expand
- OR
4. Right click within yellow ROI
  5. Select "zoom to region"
  6. Final display of expanded ROI

# Basic operations

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

# Peak Labeling

The screenshot displays the NIST DTSA-II software interface. The main window shows an XPS spectrum with intensity on the y-axis (0 to 120,000) and binding energy on the x-axis (0 to 10,000 eV). Several peaks are labeled with 'Fe' and 'YFe'. A pink arrow points to the 'KLM selection' panel on the right, which has a pink text label 'KLM selection' above it. The 'KLM Lines' panel includes checkboxes for K, L, and M lines, an 'Element' dropdown menu set to 'Fe', and buttons for 'Temporary Lines', 'Selected Lines', and 'Clear All Lines'. The 'Composition' table below is empty.

**Spectrum Properties**

Name	Value
Acquisition time	8/18/08 1:23 PM
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 mm <sup>2</sup>
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)

**Composition**

Element	Weight %	Atomic %
---------	----------	----------

One spectrum selected from list.

# Peak Labeling

The screenshot displays the NIST DTSA-II software interface. The main window shows an X-ray spectrum with several peaks labeled 'Fe'. The y-axis represents intensity (0 to 120,000) and the x-axis represents energy (0 to 10,000 eV). A pink arrow points from the text 'To make labels "stick" click these check boxes' to the 'K Lines' and 'L Lines' checkboxes in the 'KLM Lines' control panel.

**Default Detector:** JEOL8500F  
**QUAD SDD 5eV**

**Spectrum List:**  
Cu\_10A\_BestRes20kv155kHz25DT5C  
K309\_1nA\_BestRes20kv9p1kHz5DT5C  
K309\_20nA\_BestRes20kv180kHz30DT50s

**Spectrum Properties:**

Name	Value
Acquisition time	8/18/08 1:23 PM
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 mm <sup>2</sup>
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)

**KLM Lines:**  
 K Lines  
 L Lines  
 M Lines  
 All Lines

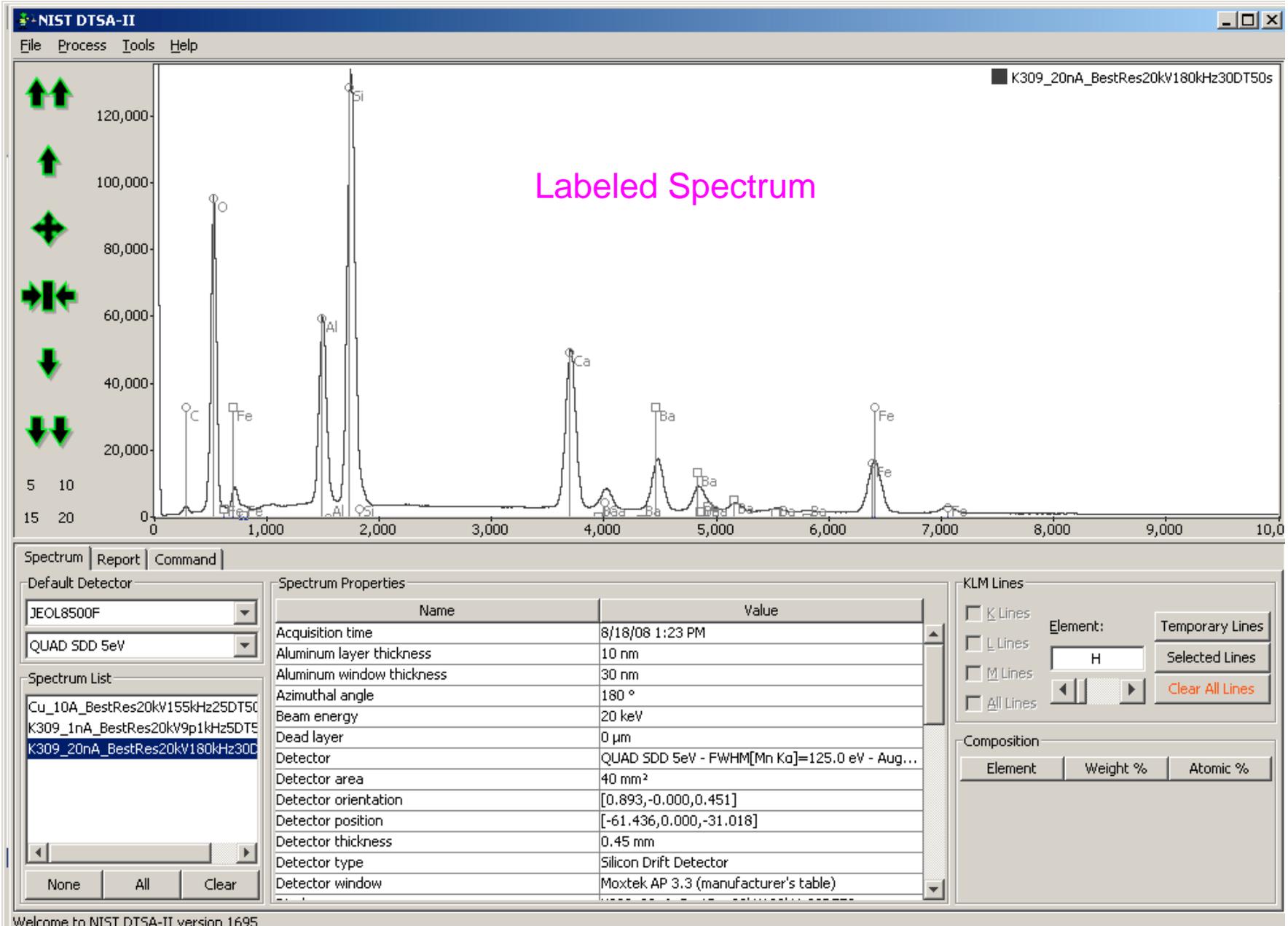
Element: Fe  
Buttons: Temporary Lines, Selected Lines, Clear All Lines

**Composition:**

Element	Weight %	Atomic %
---------	----------	----------

Welcome to NIST DTSA-II version 1695

# Peak Labeling



# Peak Labeling

**NIST DTSA-II** K309\_20nA\_BestRes20kV180kHz30DT50s

File Process Tools Help

Choosing the peak label style

120,000  
100,000  
80,000  
60,000  
40,000  
20,000  
0

0 1,000 2,000 3,000 4,000 5,000 6,000 7,000 8,000 9,000 10,000

Copy  
Save  
Print  
Zoom to all  
Zoom in by 2  
Zoom in by 5  
Zoom out by 2  
Zoom out by 5  
Ordinate Scale  
Spectrum Comparison  
KLM Labels  
Create an ROI...

Long labels  
Short labels  
Large labels  
Siegbahn labels

Spectrum | Report | Command

Default Detector: JEOL8500F  
QUAD SDD 5eV

Spectrum List:  
Cu\_10A\_BestRes20kV155kHz25DT50s  
K309\_1nA\_BestRes20kV9p1kHz5DT50s  
K309\_20nA\_BestRes20kV180kHz30DT50s

Spectrum Properties

Name	Value
Acquisition time	8/18/08 1:23 PM
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 mm <sup>2</sup>
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)

KLM Lines

K Lines  
 L Lines  
 M Lines  
 All Lines

Element: H  
Temporary Lines  
Selected Lines  
Clear All Lines

Composition

Element	Weight %	Atomic %

Welcome to NIST DTSA-II version 1695

# Peak Labeling

**NIST DTSA-II** File Process Tools Help

K309\_20nA\_BestRes20kv180kHz30DT50s

Choosing the peak label style  
IUPAC Long labels

5 10  
15 20

Spectrum | Report | Command

Default Detector: JEOL8500F  
QUAD SDD 5eV

Spectrum List:  
Cu\_10A\_BestRes20kv155kHz25DT50  
K309\_1nA\_BestRes20kv9p1kHz5DT50  
K309\_20nA\_BestRes20kv180kHz30DT50

Spectrum Properties:

Name	Value
Acquisition time	8/18/08 1:23 PM
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 mm <sup>2</sup>
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)

KLM Lines:  
 K Lines  
 L Lines  
 M Lines  
 All Lines  
 Element: H  
 Temporary Lines  
 Selected Lines  
 Clear All Lines

Composition:  

Element	Weight %	Atomic %

Welcome to NIST DTSA-II version 1695

# Peak Labeling

The screenshot displays the NIST DTSA-II software interface. The main window shows an XPS spectrum with several peaks labeled. A context menu is open over the spectrum, highlighting the 'KLM Labels' option. The menu options include: Copy, Save, Print, Zoom to all, Zoom in by 2, Zoom in by 5, Zoom out by 2, Zoom out by 5, Ordinate Scale, Spectrum Comparison, KLM Labels (highlighted), and Create an ROI... The 'KLM Labels' sub-menu is also visible, showing options: Long labels, Short labels, Large labels, and Siegbahn labels (highlighted).

Peak labels visible in the spectrum include: Si Ka2, Si Ka1; O Ka2, O Ka1; Al Ka2, Al Ka1; Ca Ka2, Ca Ka1; Ba La2, Ba La1; Fe Ka1; Fe Ka2; Fe Kb3, Fe Kb1; C Kα1; Fe Lα1, Fe Lβ1; Ba Lβ1; Ba Lα1; Fe Lβ3; Fe Lβ2; Fe Lβ1; Fe Lα1; Fe Lα2; Fe Lα3; Fe Lα4; Fe Lα5; Fe Lα6; Fe Lα7; Fe Lα8; Fe Lα9; Fe Lα10; Fe Lα11; Fe Lα12; Fe Lα13; Fe Lα14; Fe Lα15; Fe Lα16; Fe Lα17; Fe Lα18; Fe Lα19; Fe Lα20; Fe Lα21; Fe Lα22; Fe Lα23; Fe Lα24; Fe Lα25; Fe Lα26; Fe Lα27; Fe Lα28; Fe Lα29; Fe Lα30; Fe Lα31; Fe Lα32; Fe Lα33; Fe Lα34; Fe Lα35; Fe Lα36; Fe Lα37; Fe Lα38; Fe Lα39; Fe Lα40; Fe Lα41; Fe Lα42; Fe Lα43; Fe Lα44; Fe Lα45; Fe Lα46; Fe Lα47; Fe Lα48; Fe Lα49; Fe Lα50; Fe Lα51; Fe Lα52; Fe Lα53; Fe Lα54; Fe Lα55; Fe Lα56; Fe Lα57; Fe Lα58; Fe Lα59; Fe Lα60; Fe Lα61; Fe Lα62; Fe Lα63; Fe Lα64; Fe Lα65; Fe Lα66; Fe Lα67; Fe Lα68; Fe Lα69; Fe Lα70; Fe Lα71; Fe Lα72; Fe Lα73; Fe Lα74; Fe Lα75; Fe Lα76; Fe Lα77; Fe Lα78; Fe Lα79; Fe Lα80; Fe Lα81; Fe Lα82; Fe Lα83; Fe Lα84; Fe Lα85; Fe Lα86; Fe Lα87; Fe Lα88; Fe Lα89; Fe Lα90; Fe Lα91; Fe Lα92; Fe Lα93; Fe Lα94; Fe Lα95; Fe Lα96; Fe Lα97; Fe Lα98; Fe Lα99; Fe Lα100.

Below the spectrum, the 'Spectrum Properties' table is visible:

Name	Value
Acquisition time	8/18/08 1:23 PM
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 Ka]=125.0 eV - Aug...
Detector area	40 mm <sup>2</sup>
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)

The 'KLM Lines' section shows checkboxes for K Lines, L Lines, M Lines, and All Lines. The 'Element' field is set to 'H'. The 'Composition' table is also visible, with columns for Element, Weight %, and Atomic %.

Welcome to NIST DTSA-II version 1695

# Basic operations

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

# Exporting spectrum for publication as gnuplot

**NIST DTSA-II**

File Process Tools Help

K309\_20nA\_BestRes20kv180kHz30DT50s

120,000  
100,000  
80,000  
60,000  
40,000  
20,000  
0

0 1,000 2,000 3,000 4,000 5,000 6,000 7,000 8,000 9,000 10,0

5 10  
15 20

Copy  
Save  
Print  
Zoom to all  
Zoom in by 2  
Zoom in by 5  
Zoom out by 2  
Zoom out by 5  
Ordinate Scale  
Spectrum Comparison  
KLM Labels  
Create an ROI...

As displayed  
As gnuplot script

Spectrum | Report | Command

Default Detector: JEOL8500F  
QUAD SDD 5eV

Spectrum List:  
Cu\_10A\_BestRes20kv155kHz25DT50  
K309\_1nA\_BestRes20kv9p1kHz5DT50  
K309\_20nA\_BestRes20kv180kHz30DT50

Spectrum Properties:

Name	Value
Acquisition time	8/18/08 1:23 PM
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 mm <sup>2</sup>
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)

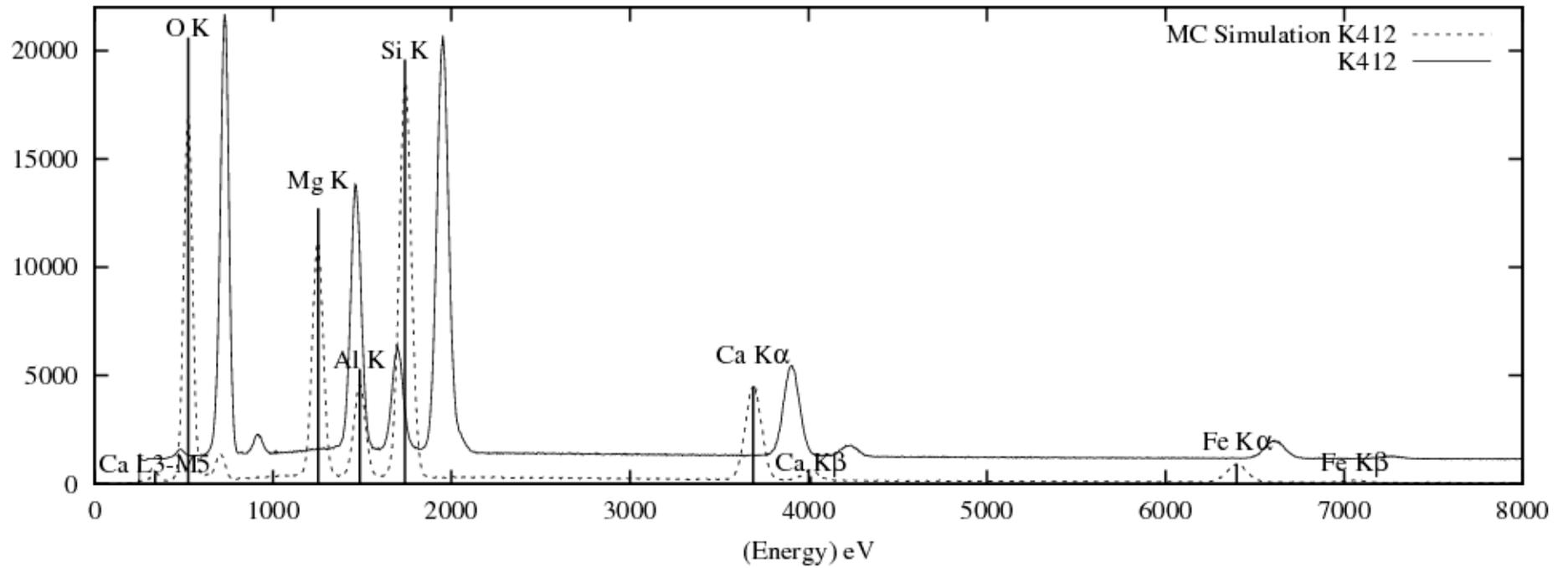
KLM Lines:  
 K Lines  
 L Lines  
 M Lines  
 All Lines  
 Element: H  
 Temporary Lines  
 Selected Lines  
 Clear All Lines

Composition:  

Element	Weight %	Atomic %

Welcome to NIST DTSA-II version 1695

# 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

When attempting to open a spectrum file with a different calibration, this message appears:

**Spectrum open**

The calibration of *K309\_10nA\_BestRes20kV90kHz17DT50s* does not seem to be similar to the default detector.

Apply the default detector none the less?

Yes No

Name	Value
Aluminum layer thickness	0 nm
Aluminum window thickness	30 nm
Azimuthal angle	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)
Elevation	40 °
Energy offset	0 eV

Default Detector: 8600 Probe, EDAX\_35mus

Spectrum List:

- K411-20kV750pA35mu-s500s
- K412\_20kV750pA35mu-s200s

KLM Lines:  K Lines,  L Lines,  M Lines,  All Lines. Element: Fe. Buttons: Temporary Lines, Selected Lines, Clear All Lines.

Composition: Element, Weight %, Atomic %

Welcome to NIST DTSA-II version 1695

# 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

We wish to match the spectra for the integral of  $\text{SiK}\alpha,\beta$   
Step 1: Click and swipe across  $\text{SiK}\alpha,\beta$  peak to define ROI for matching.

Legend:  
■ K411\_20kv750pA35mu-s100s  
■ K412\_20kv750pA35mu-s200s

Default Detector: 8600 Probe  
EDAX\_35mus

Spectrum List:  
K411\_20kv750pA35mu-s100s  
K412\_20kv750pA35mu-s200s

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)

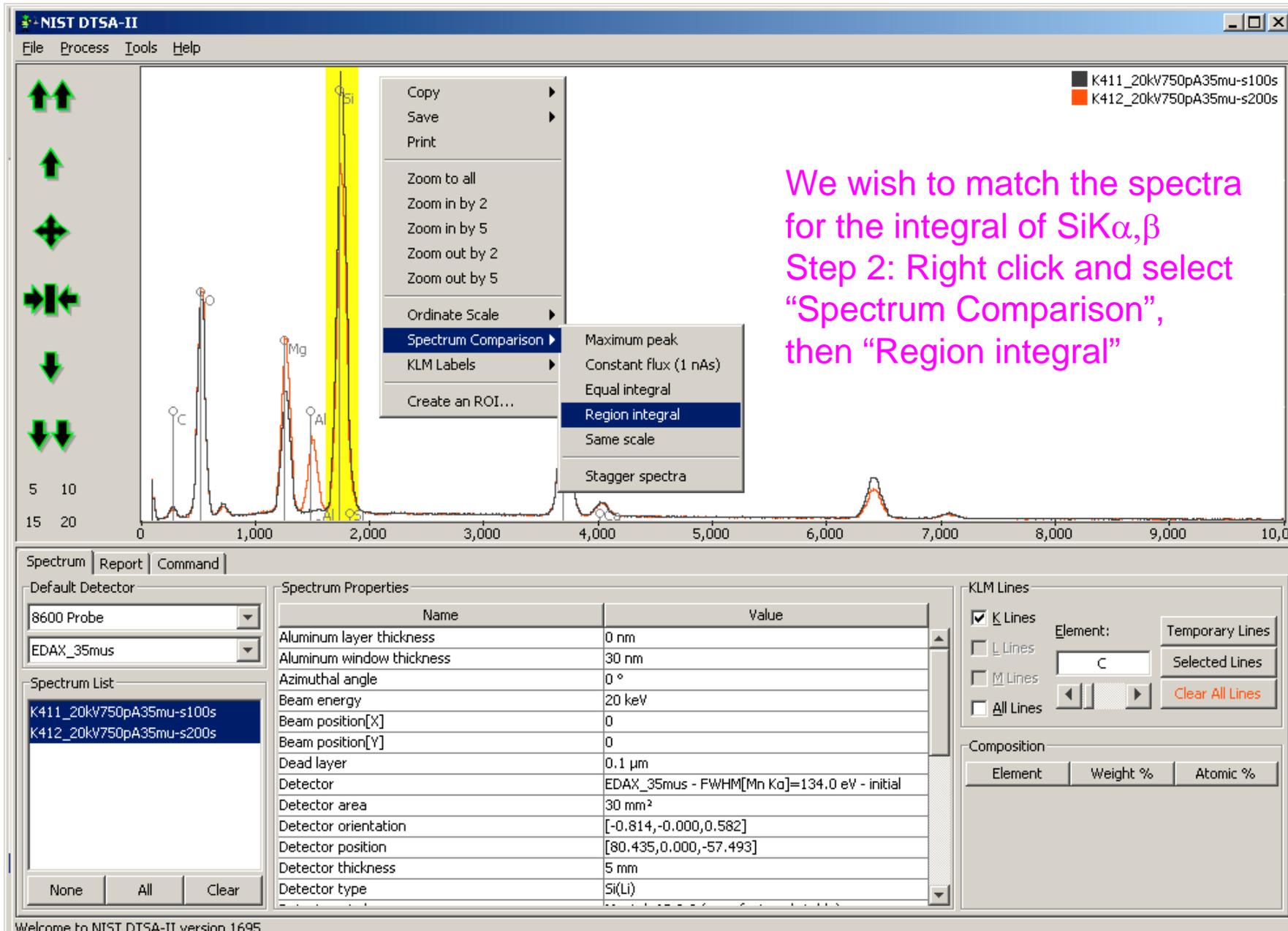
KLM Lines:  
 K Lines  
 L Lines  
 M Lines  
 All Lines

Element: [C] Temporary Lines Selected Lines Clear All Lines

Composition:  
Element Weight % Atomic %

Welcome to NIST DTSA-II version 1695

# Comparing multiple spectra



The screenshot shows the NIST DTSA-II software interface. The main window displays two overlaid spectra: K411\_20kV750pA35mu-s100s (black line) and K412\_20kV750pA35mu-s200s (orange line). The x-axis represents energy in eV, ranging from 0 to 10,000. The y-axis represents intensity. A yellow vertical band highlights the Si peak region around 1,700 eV. A context menu is open over this region, with 'Spectrum Comparison' and 'Region integral' selected. The 'Spectrum Comparison' sub-menu is also visible, showing options like 'Maximum peak', 'Constant flux (1 nAs)', 'Equal integral', 'Same scale', and 'Stagger spectra'.

We wish to match the spectra for the integral of SiK $\alpha,\beta$   
Step 2: Right click and select "Spectrum Comparison", then "Region integral"

**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 $\mu$ m
Detector	EDAX_35mus - FWHM[Mn K $\alpha$ ]=134.0 eV - initial
Detector area	30 mm <sup>2</sup>
Detector orientation	[-0.814,-0.000,0.582]
Detector position	[80.435,0.000,-57.493]
Detector thickness	5 mm
Detector type	Si(Li)

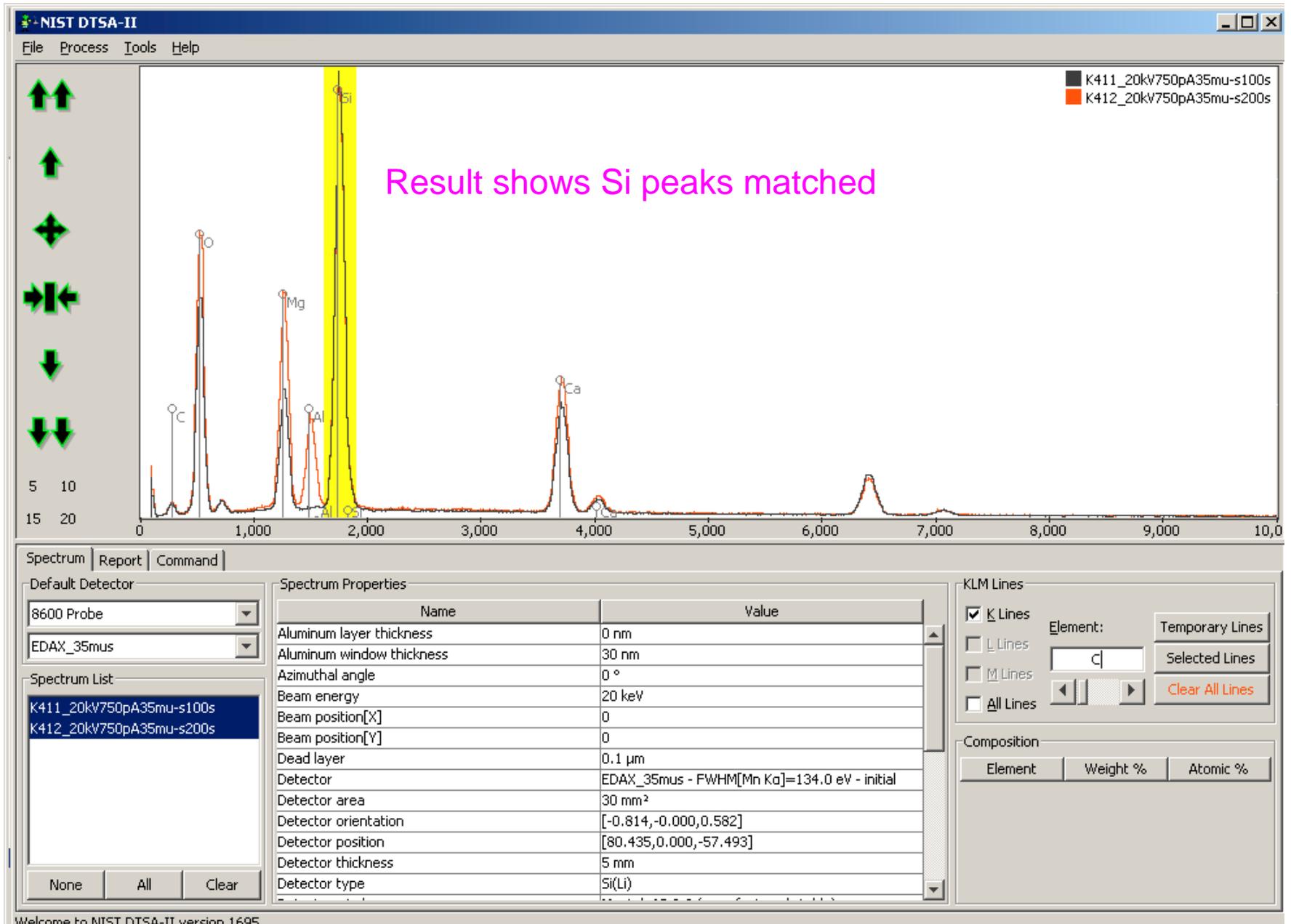
**KLM Lines**

K Lines    Element: C    Temporary Lines  
 L Lines    Selected Lines  
 M Lines    Clear All Lines  
 All Lines

**Composition**

Element	Weight %	Atomic %
---------	----------	----------

# 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

**Starting measured spectrum**

**Sub-sample spectrum**

- Fit background
- Linearize energy axis
- Smooth (Savitzky-Golay)
- Trim
- Peak search

**Spectrum Properties**

Name	Value
Operator	Bruker AXS
Optimal working distance	12.0 mm
Real time	71.1 seconds
Resolution	125 eV
Resolution measurement energy	5899 eV
Sample surface normal	[0.000,0.000,-1.000]
Solid angle	0.007111 sr
Source file	C:\Documents and Settings\newbury\Desktop\S...
Specimen-to-detector distance	75 mm
Spectrum description	Bruker AXS spectrum Cu_1nA
Spectrum index	1
Window type	Ultra-thin window
X Units	eV

**KLM Lines**

K Lines    Element: H    Temporary Lines

L Lines    Selected Lines

M Lines    Clear All Lines

All Lines

**Composition**

Element	Weight %	Atomic %

X Units = eV

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

**Random Number "seed"**

**Equivalent dose factor; set to 5% for this calculation**

**Number of synthesized spectra, each with different statistics**

**Sub-sample settings**

Scale: 0 20 40 60 80 100  
5.0%

Random Seed: 594

Duplicates: 3

Ok Cancel

Spectrum Report Command

Default Detector: JEOL8500F  
QUAD SDD 5eV

Spectrum List: K309\_20nA\_BestRes20kV180kHz30D...

Spectrum Properties

Name	Value
Acquisition time	8/18/08 1:23 PM
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 mm <sup>2</sup>
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)

KLM Lines

K Lines  
 L Lines  
 M Lines  
 All Lines

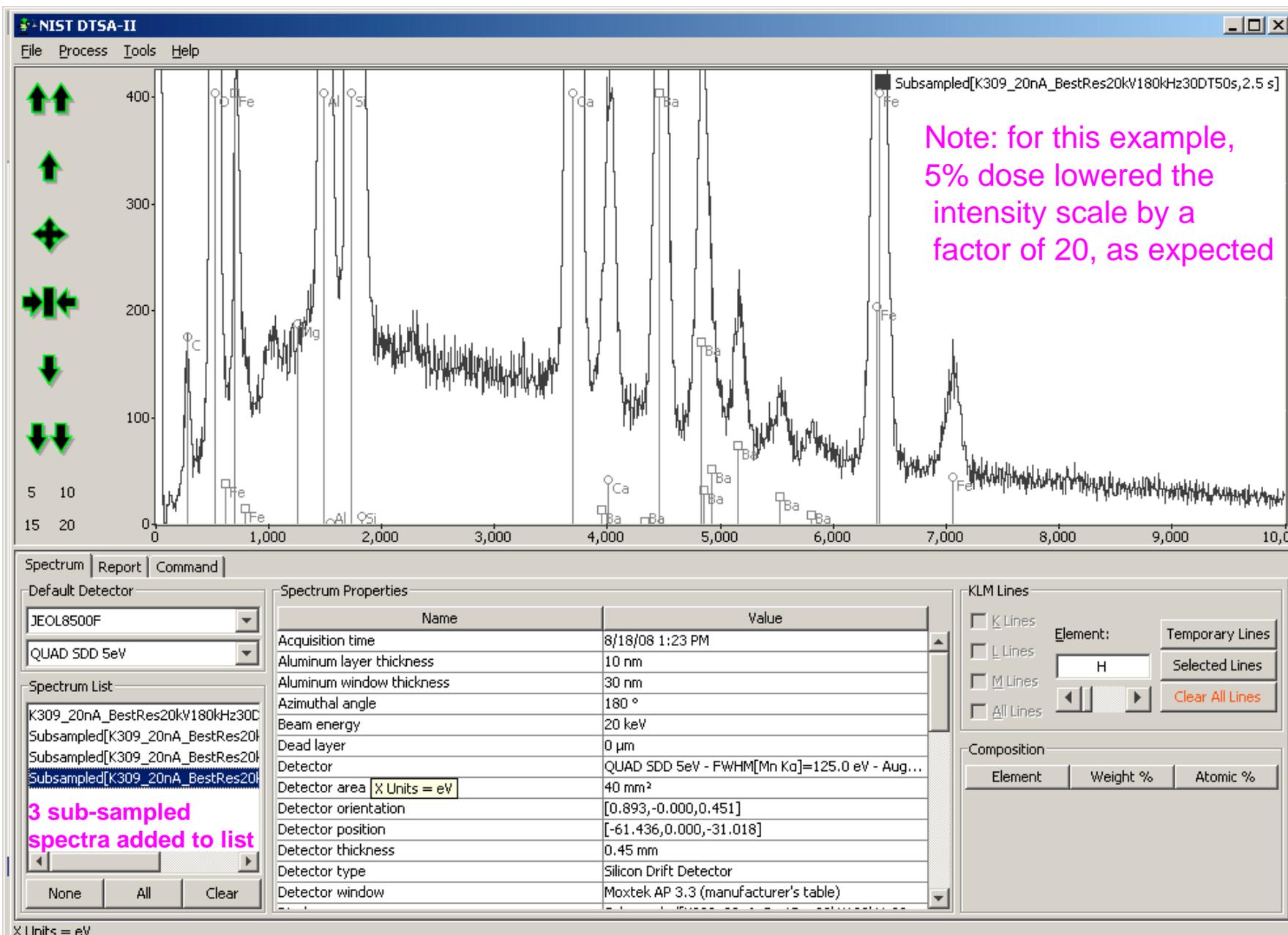
Element: H  
Temporary Lines  
Selected Lines  
Clear All Lines

Composition

Element	Weight %	Atomic %
---------	----------	----------

X Units = eV

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



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

Each sub-sampled spectrum is prepared with different random statistics.

Subsampled[K309\_20nA\_BestRes20kV180kHz30DT50s,2.5 s]  
 Subsampled[K309\_20nA\_BestRes20kV180kHz30DT50s,2.5 s]  
 Subsampled[K309\_20nA\_BestRes20kV180kHz30DT50s,2.5 s]

5 10  
15 20

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: JEOL8500F  
 QUAD SDD 5eV

Spectrum List:  
 K309\_20nA\_BestRes20kV180kHz30C  
 Subsampled[K309\_20nA\_BestRes20kV180kHz30DT50s,2.5 s]  
 Subsampled[K309\_20nA\_BestRes20kV180kHz30DT50s,2.5 s]  
 Subsampled[K309\_20nA\_BestRes20kV180kHz30DT50s,2.5 s]

None All Clear

Spectrum Properties

Name	Value
Acquisition time	8/18/08 1:23 PM
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 mm <sup>2</sup>
Detector orientation	[0.893,-0.000,0.451]
Detector position	[-61.436,0.000, X Units = eV]
Detector thickness	0.45 mm
Detector type	Silicon Drift Detector
Detector window	Moxtek AP 3.3 (manufacturer's table)

KLM Lines  
 K Lines  
 L Lines  
 M Lines  
 All Lines

Element: H  
 Temporary Lines  
 Selected Lines  
 Clear All Lines

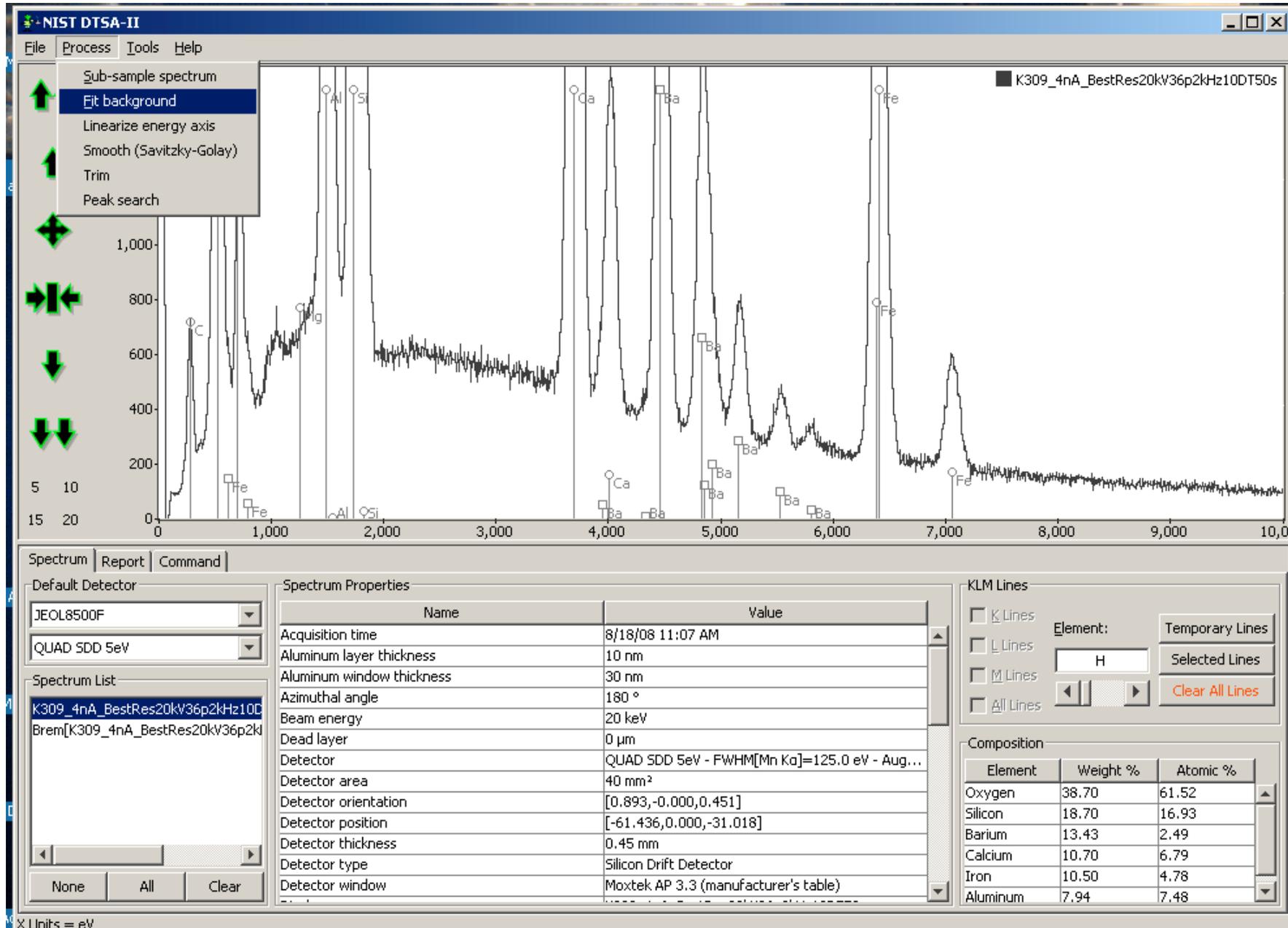
Composition  

Element	Weight %	Atomic %

X Units = eV

# Background fitting tool

# Background Fitting



# Background Fitting

The screenshot displays the NIST DTSA-II software interface. The main window shows an X-ray spectrum with several peaks labeled with elements: C, O, Fe, Al, Si, Ca, and Ba. The y-axis represents intensity (0 to 1,600) and the x-axis represents energy in eV (0 to 10,000). A 'Material Editor' dialog box is open in the center, with a pink arrow pointing to it from the text 'Enter material composition'. The dialog box contains the following fields and options:

- Material Name: [Empty text box]
- Density: 5.0 g/cm<sup>3</sup> (optional)
- Radio buttons:  Weight Fractions,  Atomic Proportions
- Text area: Your elements will appear here
- Element: [Empty text box] Quantity: 100%
- Buttons: Add, Delete, Clear, Ok, Cancel

At the bottom of the software window, there are several panels:

- Spectrum Properties:** A table listing various acquisition parameters.
- KLM Lines:** A section for selecting characteristic lines (K, L, M) with an 'Element' dropdown set to 'H' and buttons for 'Temporary Lines', 'Selected Lines', and 'Clear All Lines'.
- Composition:** A table with columns for 'Element', 'Weight %', and 'Atomic %'.

At the bottom left, it says 'X Units = eV'.

# Background Fitting

The screenshot displays the NIST DTSA-II software interface. The main window shows an X-ray spectrum with peaks labeled for elements like C, O, Fe, Al, Si, Ca, and Ba. A 'Material Editor' dialog box is open in the center, showing the material name 'K309' and a list of weight fractions for various elements. A pink arrow points to the 'Material Editor' dialog with the text 'Enter material composition'.

**Material Editor**

Material Name: K309  
Density: 4.5 g/cm<sup>3</sup> (optional)

Weight Fractions  Atomic Proportions

Ca 10.7% by weight  
Fe 10.5% by weight  
O 38.7% by weight  
Al 7.94% by weight  
Ba 13.43% by weight  
Si 18.78% by weight

Element:  Quantity: 0.03%

Buttons: Add, Delete, Clear, Ok, Cancel

**Spectrum Properties**

Name	Value
Acquisition time	
Aluminum layer thickness	
Aluminum window thickness	
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 mm <sup>2</sup>
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)

**KLM Lines**

K Lines  
 L Lines  
 M Lines  
 All Lines

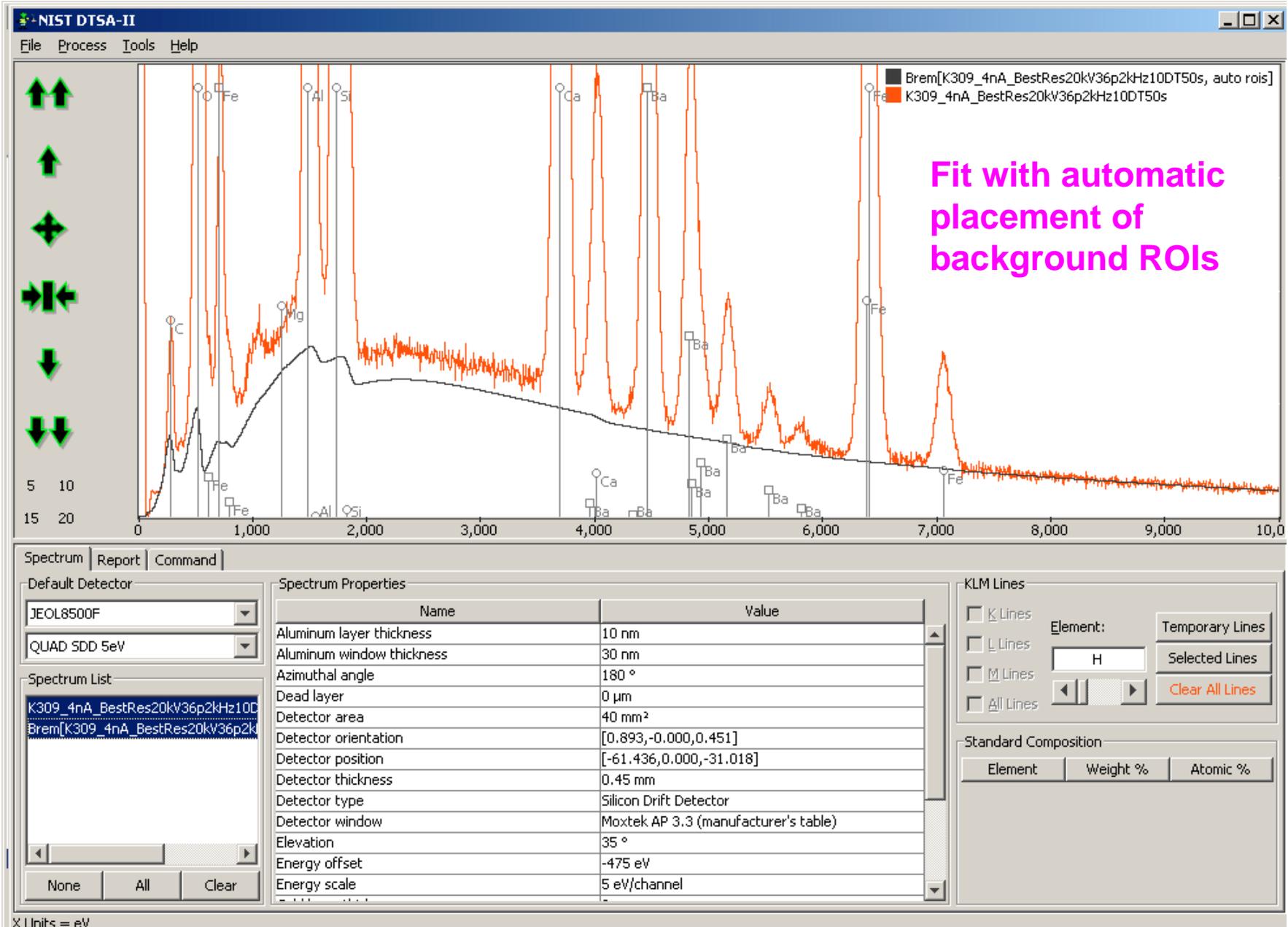
Element:  H  
Temporary Lines  
Selected Lines  
Clear All Lines

**Composition**

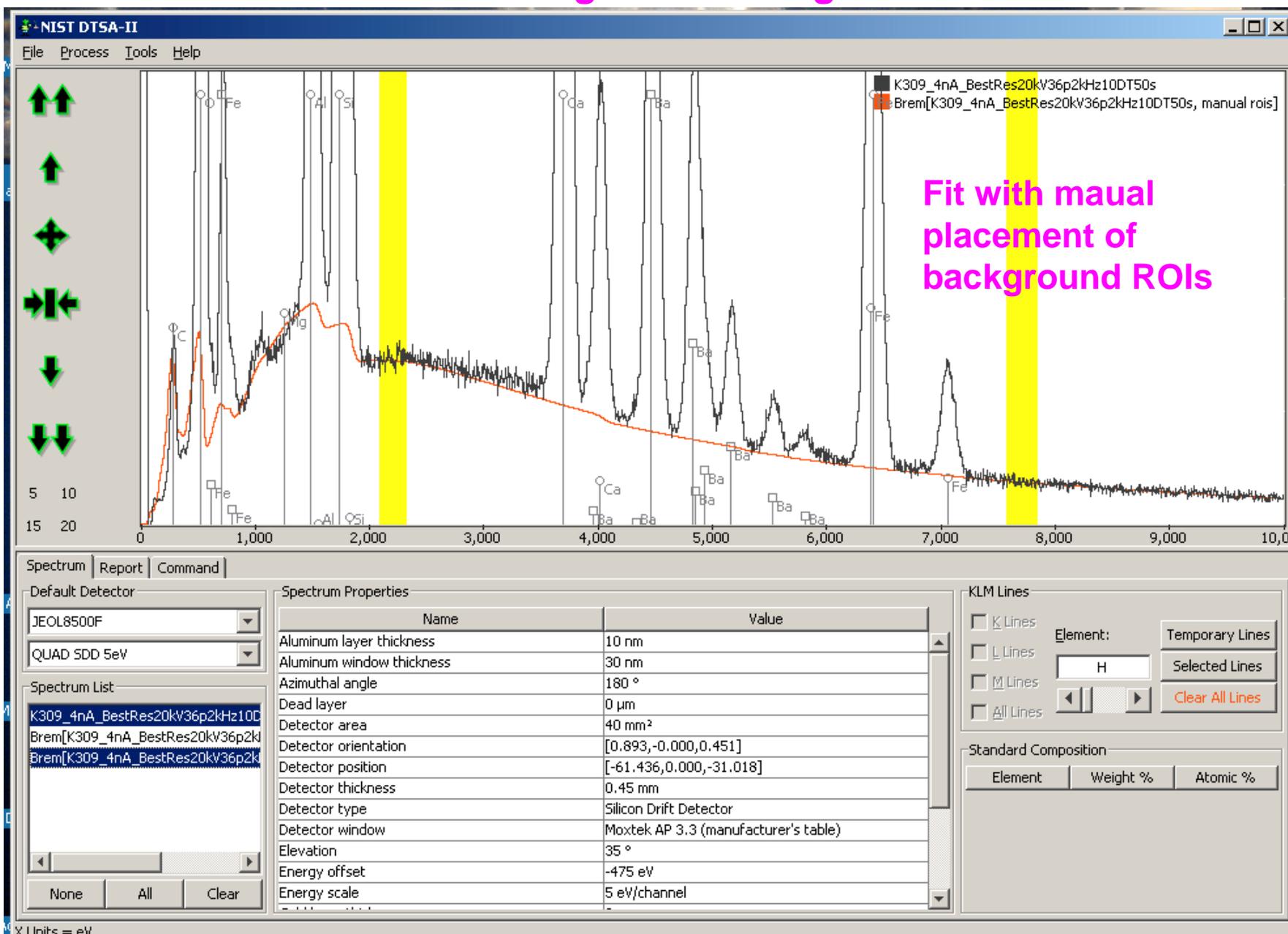
Element	Weight %	Atomic %

X Units = eV

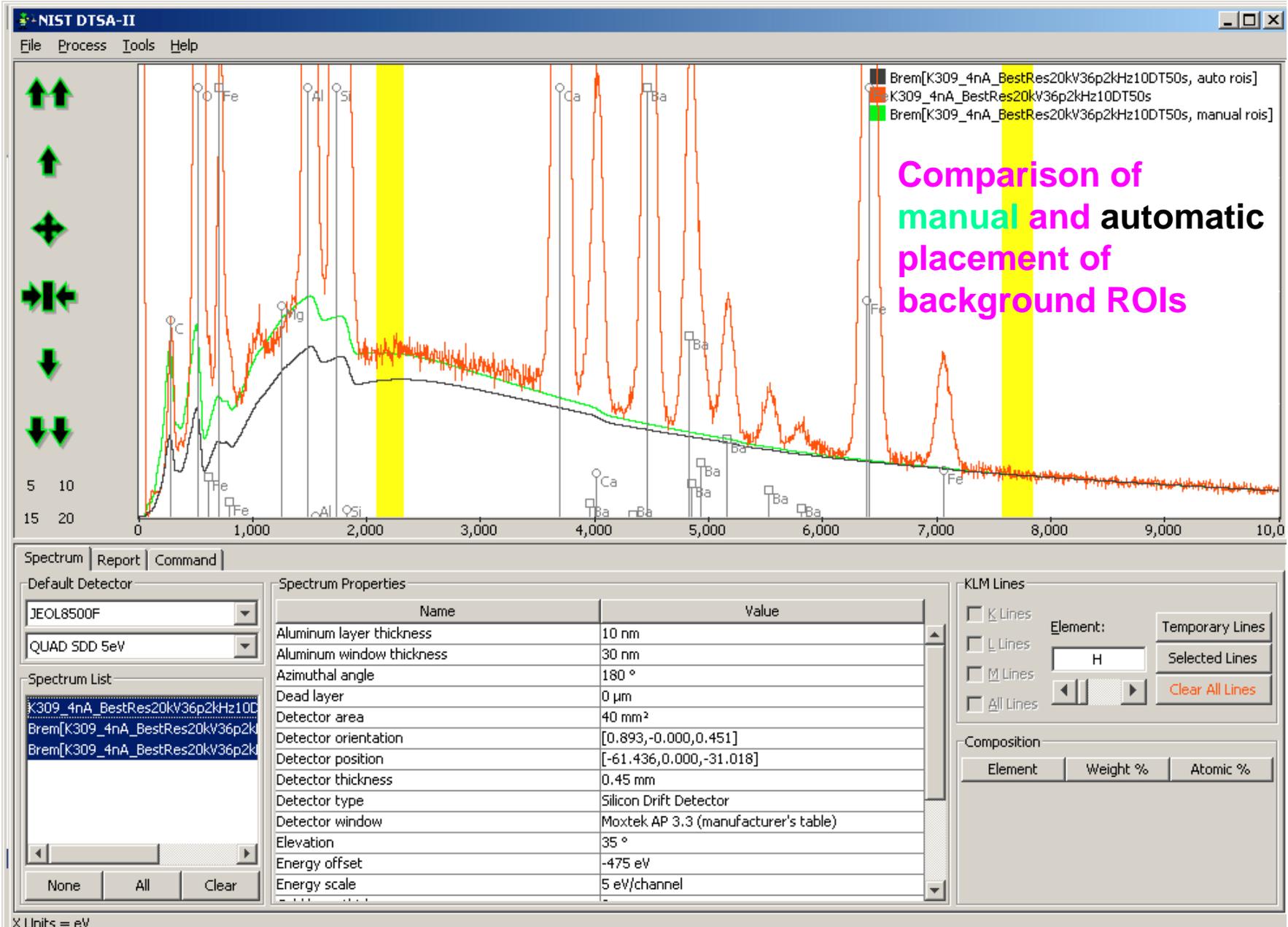
# Background Fitting



# 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

The screenshot displays the NIST DTSA-II software interface. The title bar reads "NIST DTSA-II". The menu bar includes "File", "Process", "Tools", and "Help". The "Tools" menu is open, showing options: "Edit spectrum properties", "Assign material", "Quantification alien", "Simulation alien" (highlighted), "Calibration alien", and "Report note".

On the left side, there are several green arrow icons for navigation: two up arrows, one up arrow, a four-way arrow, two left arrows, one down arrow, and two down arrows. Below these are numerical labels: "5 10" and "15 20".

The main area is a large empty plot with a y-axis labeled "5" and "0", and an x-axis labeled from "0" to "20,000" in increments of 2,000.

At the bottom, there are three tabs: "Spectrum", "Report", and "Command".

**Default Detector:** "8600 Probe" and "EDAX\_35mus".

**Spectrum List:** A list box with "None", "All", and "Clear" buttons below it.

**Spectrum Properties:** A large empty text area.

**KLM Lines:** Checkboxes for "K Lines", "L Lines", "M Lines", and "All Lines". An "Element:" field contains "H". Buttons for "Temporary Lines", "Selected Lines", and "Clear All Lines" are present.

**Composition:** A table with columns "Element", "Weight %", and "Atomic %".

At the bottom left, a status bar reads: "Welcome to NIST DTSA-II version 1698".

# Simulation Alien: selecting Analytical Simulation

The screenshot displays the NIST DTSA-II software interface. A central dialog box titled "Spectrum simulation" is open, showing the "Simulation Mode" screen. The dialog box includes a green alien character icon and the text "First page" and "Next: Configure sample".

The "Simulation Mode" dialog box contains two main sections:

- Analytical Simulation**:
  - Analytical model of a bulk, homogeneous material
- Monte Carlo Simulation**:
  - Monte Carlo model of a bulk, homogeneous material
  - Monte Carlo model of a film on a bulk, homogeneous substrate
  - Monte Carlo model of a sphere on a bulk, homogeneous substrate
  - Monte Carlo model of a cube on a bulk, homogeneous substrate
  - Monte Carlo model of an inclusion in a bulk, homogeneous substrate

At the bottom of the dialog box, there is a message: "Message: Select the type of spectrum simulation to perform." and a "More..." button. Below the message are four buttons: "Back", "Next", "Finish", and "Cancel".

The background software interface shows a menu bar with "File", "Process", "Tools", and "Help". A plot area on the left shows a spectrum with a y-axis from 0 to 15 and an x-axis from 0 to 2,000. Below the plot are controls for "Default Detector" (set to "8600 Probe" and "EDAX\_35mus") and a "Spectrum List" area with "None", "All", and "Clear" buttons. On the right side, there are controls for "Element:" (set to "H"), "Temporary Lines", "Selected Lines", and "Clear All Lines". At the bottom of the software window, it says "Welcome to NIST DTSA-II version 1698".

# Simulation Alien: specifying composition

The screenshot displays the NIST DTSA-II software interface. A central dialog box titled "Spectrum simulation" is open, with the sub-title "Configure sample". The dialog box includes a cartoon alien character holding a flask. It shows the previous step as "Simulation Mode" and the next step as "Instrument configuration". The main area of the dialog is titled "Materials and Scale" and contains a "Bulk material" dropdown menu currently set to "Stainless steel", with "Edit" and "None" buttons next to it. Below this, a message box says "Message: Specify the sample material and scale." with a "More..." button. At the bottom of the dialog are "Back", "Next", "Finish", and "Cancel" buttons.

The background software interface shows a menu bar with "File", "Process", "Tools", and "Help". On the left, there are several green arrow icons and a vertical scale from 0 to 15. Below that, there are two columns of numbers: "5 10" and "15 20". The main window area shows a plot with an x-axis from 0 to 2,000 and a y-axis from 0 to 15. On the right side, there are more plot axes with values "16,000", "18,000", and "20,0". At the bottom left, there are tabs for "Spectrum", "Report", and "Command". Below the tabs, there are dropdown menus for "Default Detector" (set to "8600 Probe") and "EDAX\_35mus". A "Spectrum List" area is empty. At the bottom left, there are "None", "All", and "Clear" buttons. At the bottom right, there are buttons for "Temporary Lines", "Selected Lines", and "Clear All Lines". Below these are "Weight %" and "Atomic %" options.

Welcome to NIST DTSA-II version 1698

# Simulation Alien: target composition

The screenshot displays the NIST DTSA-II software interface. A 'Material Editor' dialog box is open, showing the following details:

- Material Name:** 316F Stainless steel
- Density:** 7.8 g/cm<sup>3</sup> (required)
- Composition:** Weight Fractions (selected)
- Composition List:**
  - Fe 67% by weight
  - Mn 2% by weight
  - Cr 18% by weight
  - Si 1% by weight
  - Mo 2% by weight
  - Ni 10% by weight
- Element:** [Empty field] **Quantity:** 0%
- Buttons:** Add, Delete, Clear, Ok, Cancel, More...

The background shows a 'Spectrum simulation' window with a plot area and a 'Conf' (Configuration) panel on the left. The plot area has a y-axis from 0 to 15 and an x-axis from 0 to 2,000. The 'Conf' panel includes a 'Default Detector' dropdown set to '8600 Probe' and 'EDAX\_35mus', and a 'Spectrum List' area with 'None', 'All', and 'Clear' buttons.

# Simulation Alien: instrument configuration

The screenshot displays the NIST DTSA-II software interface. A central dialog box titled "Spectrum simulation" is open, showing the "Instrument configuration" step. The dialog includes a cartoon alien character and navigation options: "Previous: Configure sample" and "Next: Other options".

**Instrument Parameters:**

- Instrument: 8600 Probe
- Detector: EDAX\_35mus
- Calibration: FWHM[Mn K $\alpha$ ]=134.0 eV - initial
- Beam Energy: 20.0 keV
- Probe Flux (current·time): 100.0 nA·second
- Incident Angle: 0.0°

Buttons at the bottom of the dialog: Back, Next, Finish, Cancel.

The background software window shows a menu bar (File, Process, Tools, Help), a vertical toolbar with green arrows, a plot area with axes (0 to 2,000 on the x-axis, 0 to 15 on the y-axis), and a "Default Detector" dropdown menu set to "8600 Probe".

# Simulation Alien: Other options not invoked

The screenshot displays the NIST DTSA-II software interface. The main window shows a spectrum plot for a simulation of 316f Stainless steel. The plot has a y-axis from 0 to 1,000 and an x-axis from 0 to 1,000. Several peaks are labeled with elements: Si, Cr, Fe, Ni, Mn, and Ni. A zoomed-in view of the Ni peak is shown on the right, with the x-axis ranging from 8,000 to 10,000.

A dialog box titled "Spectrum simulation" is open, showing "Other options". The dialog box has a blue header and a close button. It contains the following options:

- Previous: *Instrument configuration*
- Next: *Perform Simulation*
- Noise parameters: \_\_\_\_\_
- Apply simulated count statistics
- Instance count:
- Extended output: \_\_\_\_\_
- X-ray generation images (takes ~2 x as long)

At the bottom of the dialog box, there is a "Message:" field, a "More..." button, and navigation buttons: "Back", "Next", "Finish", and "Cancel".

The background software interface includes a menu bar (File, Process, Tools, Help), a toolbar with green arrows, and a "Spectrum List" panel on the left. The "Spectrum List" panel shows a list of simulation entries, with "Simulation of 316f Stainless steel" selected. Below the list are "None", "All", and "Clear" buttons.

At the bottom right, there is a "Standard Composition" table:

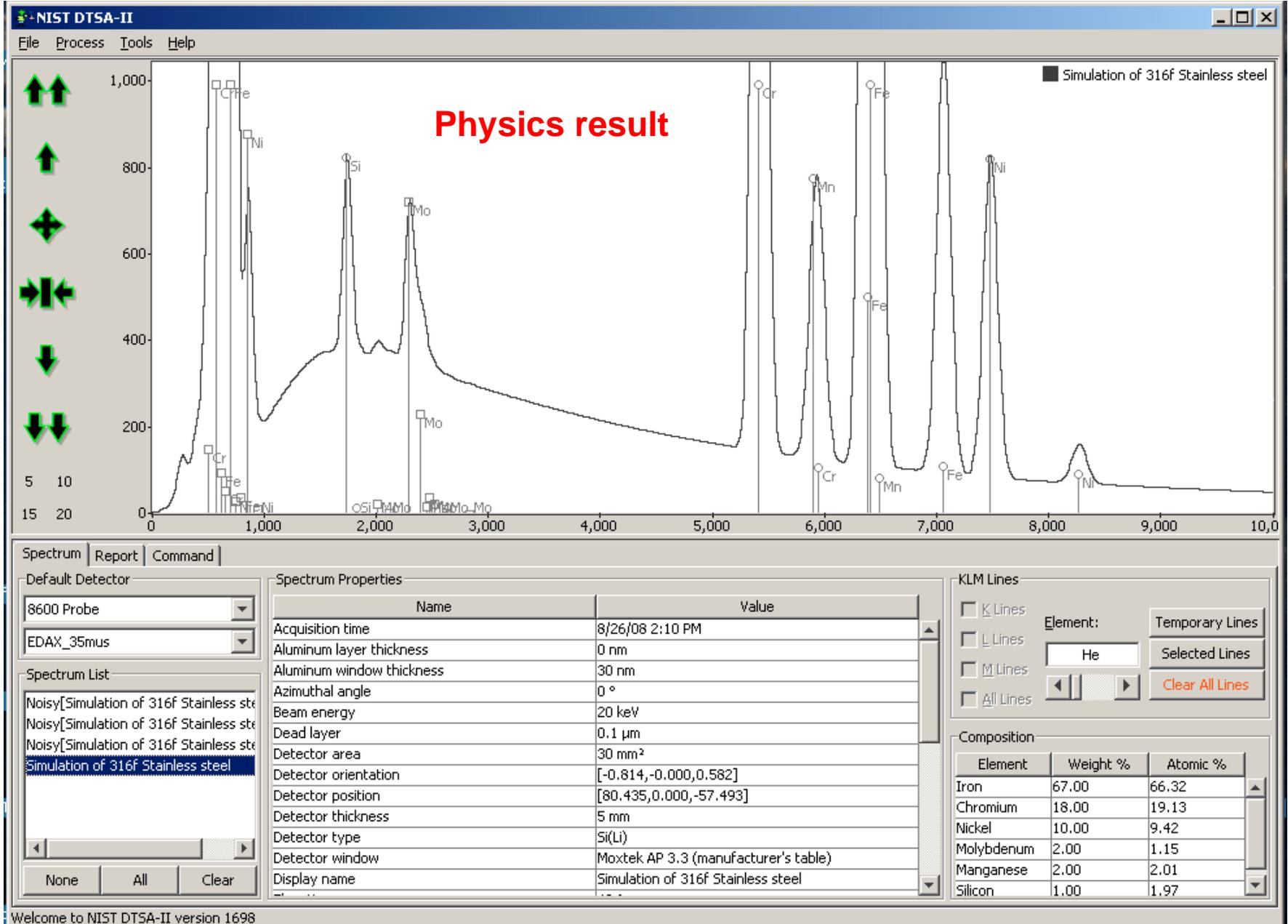
Element	Weight %	Atomic %
Iron	67.00	66.32
Chromium	18.00	19.13
Nickel	10.00	9.42
Molybdenum	2.00	1.15
Manganese	2.00	2.01
Silicon	1.00	1.97

## Simulation Alien

The screenshot shows the NIST DTSA-II software interface. A central dialog box titled "Spectrum simulation" is open, displaying "Perform Simulation". The dialog includes a progress bar labeled "Progress" which is almost completely filled with blue segments. Below the progress bar, a message reads "Message: Computing the requested spectra...". At the bottom of the dialog, there are buttons for "Back", "Next", "Finish", and "Cancel". A red arrow points to the "Finish" button. A white text box at the bottom of the image contains the instruction: "Hit 'Finish' when 'Progress' bar is filled".

Hit "Finish" when "Progress" bar is filled

# Simulation Alien



## Simulation Alien: Other options invoked

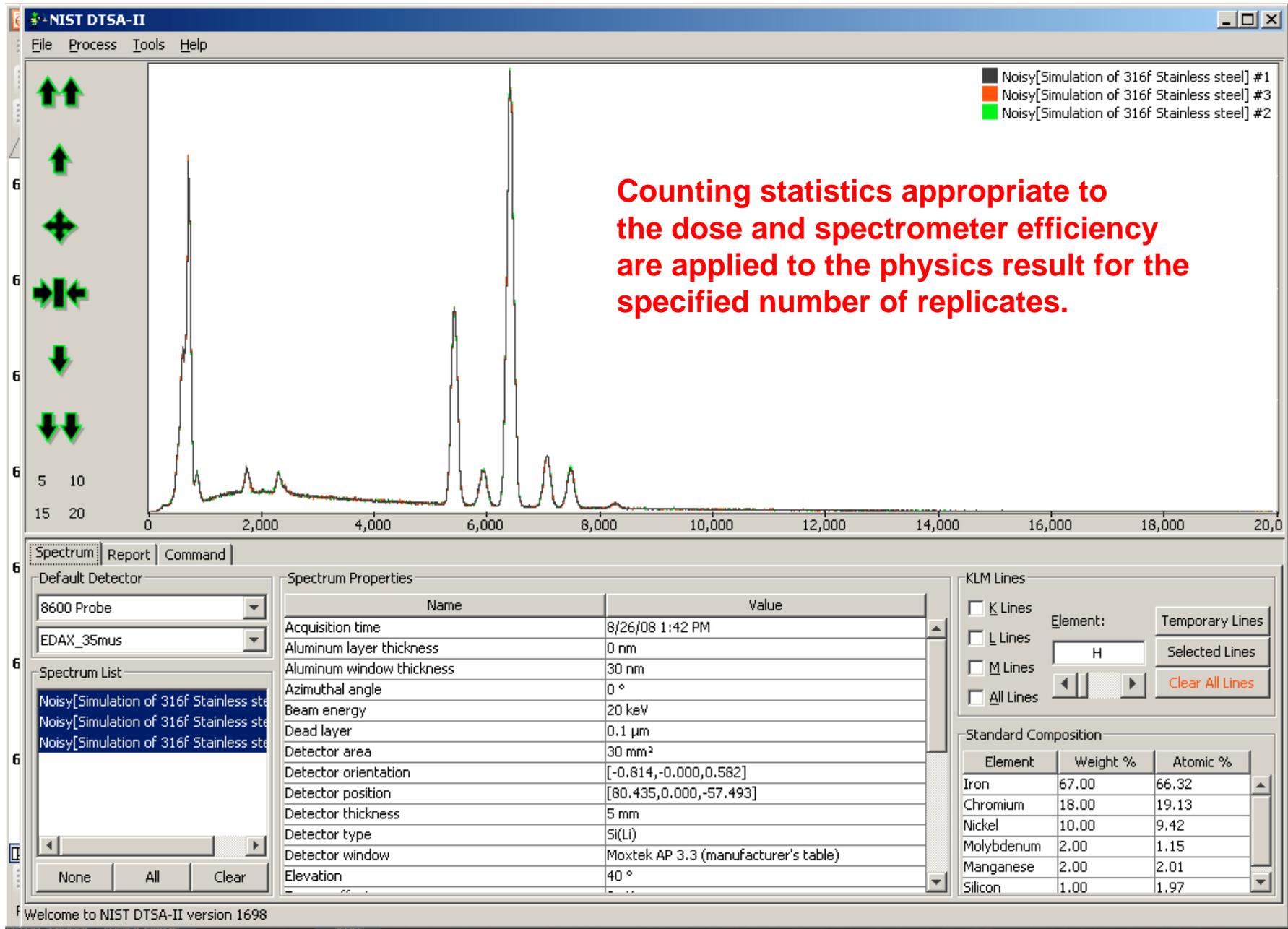
The screenshot shows the NIST DTSA-II software interface. A 'Spectrum simulation' dialog box is open, displaying the 'Other options' tab. The dialog box includes a progress indicator showing 'Previous: Instrument configuration' and 'Next: Perform Simulation'. The 'Other options' section contains the following settings:

- Noise parameters:  Apply simulated count statistics
- Instance count:  (highlighted by a red arrow)
- Extended output:  X-ray generation images (takes ~2. x as long)

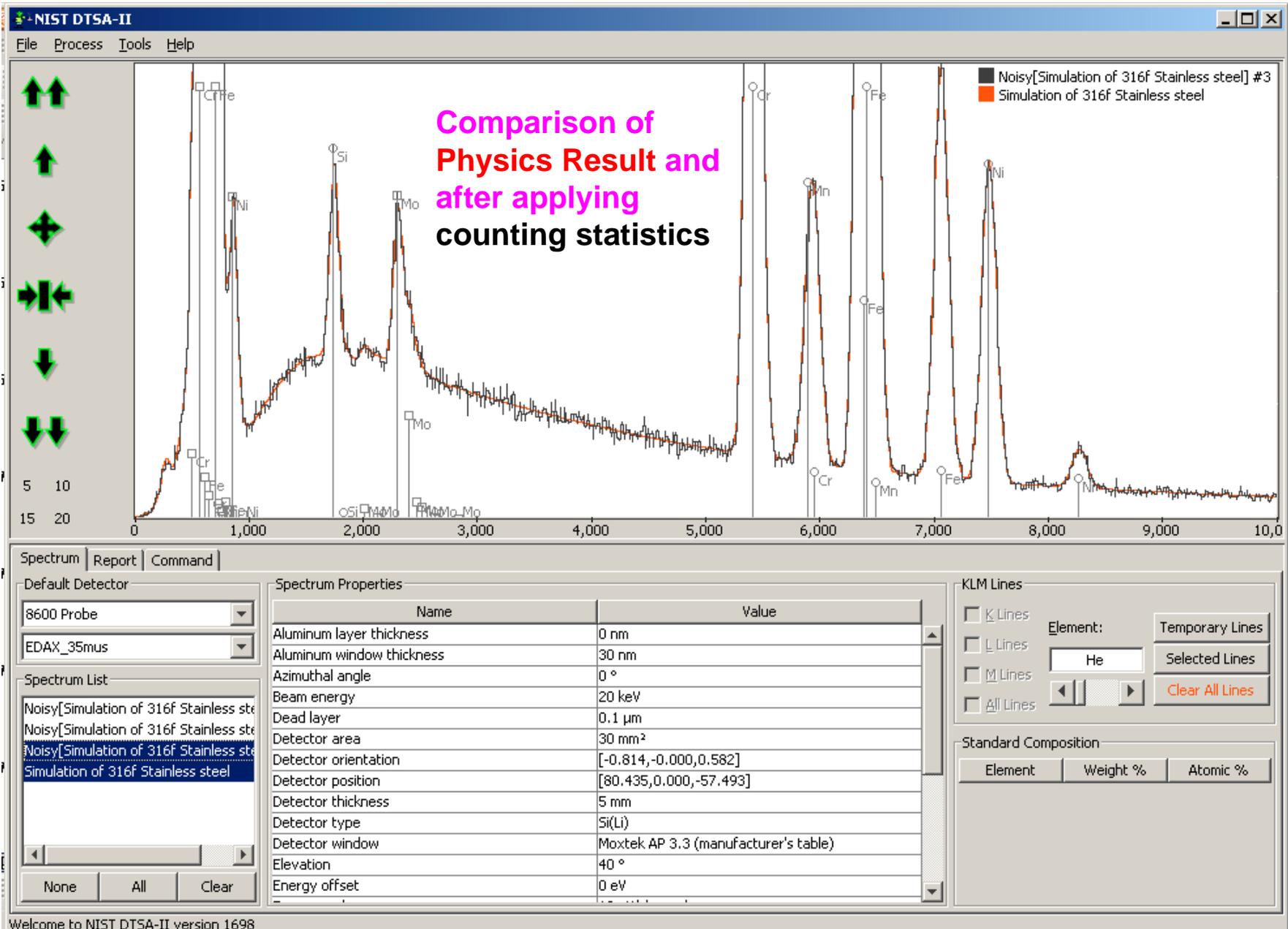
At the bottom of the dialog box, there are buttons for 'Back', 'Next', 'Finish', and 'Cancel'. A 'Message:' field with a 'More...' button is also present. The background shows a spectrum plot with a y-axis from 0 to 15 and an x-axis from 0 to 2,000. The 'Default Detector' is set to '8600 Probe' and 'EDAX\_35mus'. The 'Spectrum List' is empty. The 'Element:' field is set to 'H'. The 'Clear All Lines' button is visible. The status bar at the bottom reads 'Welcome to NIST DTSA-II version 1698'.

**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 $\mu\text{m}$ K411 glass sphere on a C substrate

**Spectrum simulation**

First page  
Next: *Configure sample*

**Simulation Mode**

Analytical Simulation

- Analytical model of a bulk, homogeneous material

Monte Carlo Simulation

- Monte Carlo model of a bulk, homogeneous material
- Monte Carlo model of a film on a bulk, homogeneous substrate
- Monte Carlo model of a sphere on a bulk, homogeneous substrate
- Monte Carlo model of a cube on a bulk, homogeneous substrate
- Monte Carlo model of an inclusion in a bulk, homogeneous substrate

Message: Select the type of spectrum simulation to perform. More...

Back Next Finish Cancel

Detector

Detector	EDAX_35mus - FWHM[Mn Ko]=134.0 eV - initial
Detector area	30 mm <sup>2</sup>
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)

Detector thickness = 5 mm

# Simulation Alien: Monte Carlo simulation of a 1 $\mu\text{m}$ K411 glass sphere on a C substrate

The screenshot displays the NIST DTSA-II software interface. A central dialog box titled "Spectrum simulation" is open, showing the "Configure sample" step. The dialog includes a cartoon alien character and navigation buttons for "Previous: Simulation Mode" and "Next: Instrument configuration".

**Materials and Scale**

- Substrate material: Carbon (Edit, None)
- Sphere material: K411 (Edit)
- Sphere diameter: 1.000  $\mu\text{m}$

Message: Specify the sample material and scale. (More...)

Navigation: Back, Next, Finish, Cancel

The background interface shows a plot area with a y-axis from 0 to 16 and an x-axis from 0 to 10,000. A vertical toolbar on the left contains green arrows for navigation. Below the plot, there are tabs for "Spectrum", "Report", and "Command". The "Default Detector" is set to "8600 Probe" and "EDAX\_35mus". A "Spectrum List" panel is empty. At the bottom, it states "Detector thickness = 5 mm".

# Simulation Alien: Monte Carlo simulation of a 1 $\mu\text{m}$ K411 glass sphere on a C substrate

The screenshot displays the NIST DTSA-II software interface. A central dialog box titled "Spectrum simulation" is open, showing the "Instrument configuration" step. The dialog includes a cartoon alien character and navigation text: "Previous: Configure sample" and "Next: Other options".

**Instrument Parameters:**

- Instrument: 8600 Probe
- Detector: EDAX\_35mus
- Calibration: FWHM[Mn K $\alpha$ ]=134.0 eV - initial
- Beam Energy: 20.0 keV
- Probe Flux (current·time): 100.0 nA·second
- Incident Angle: 0.0 °

Navigation buttons: Back, Next, Finish, Cancel, More...

Message: [Empty]

Bottom left: Spectrum List (None, All, Clear)

Bottom right: Element selection (Element: H, Temporary Lines, Selected Lines, Clear All Lines)

Bottom right table header: Composition (Element, Weight %, Atomic %)

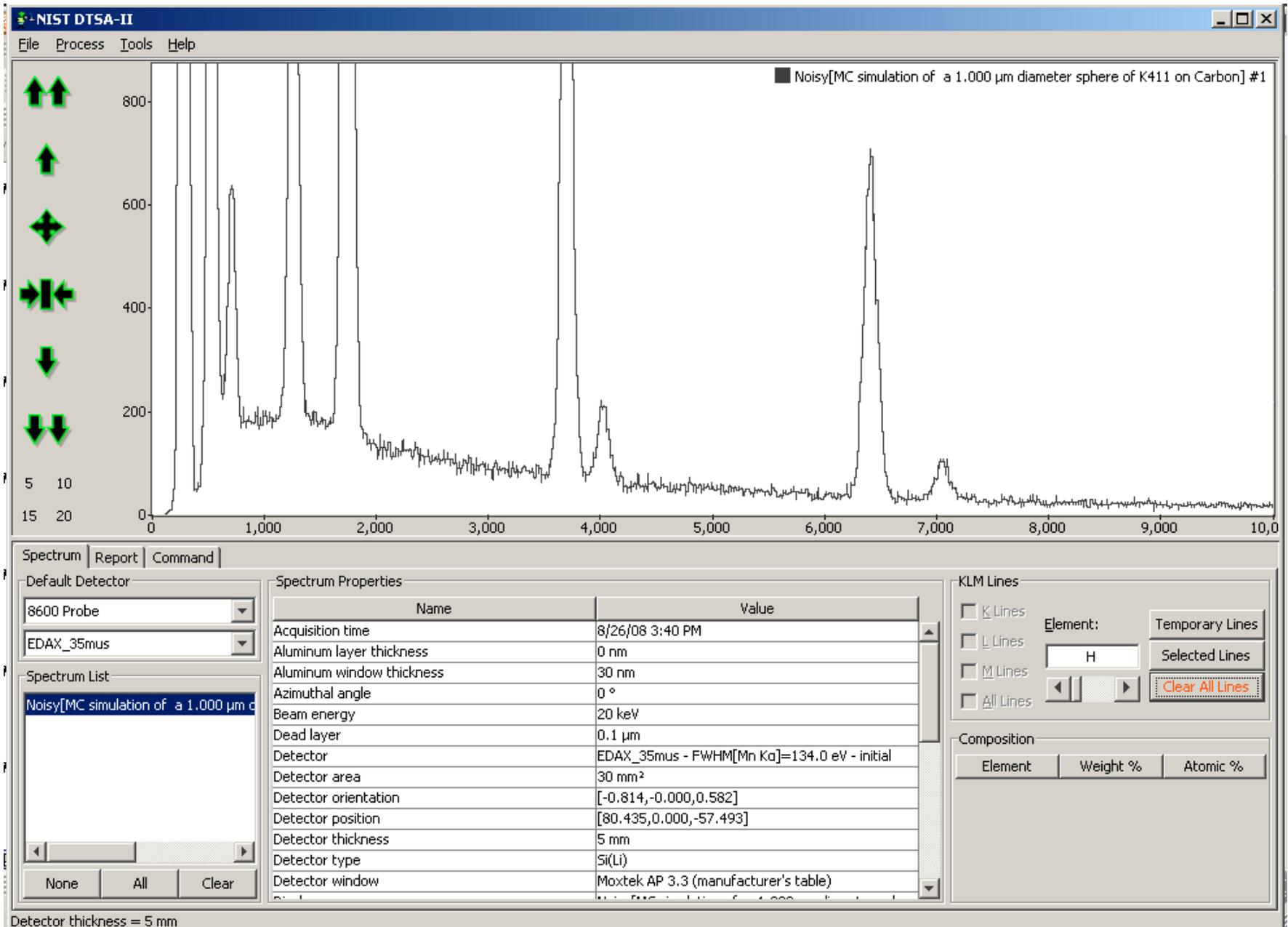
Bottom status bar: Detector thickness = 5 mm

## Simulation Alien: Monte Carlo simulation of a 1 $\mu\text{m}$ K411 glass sphere on a C substrate

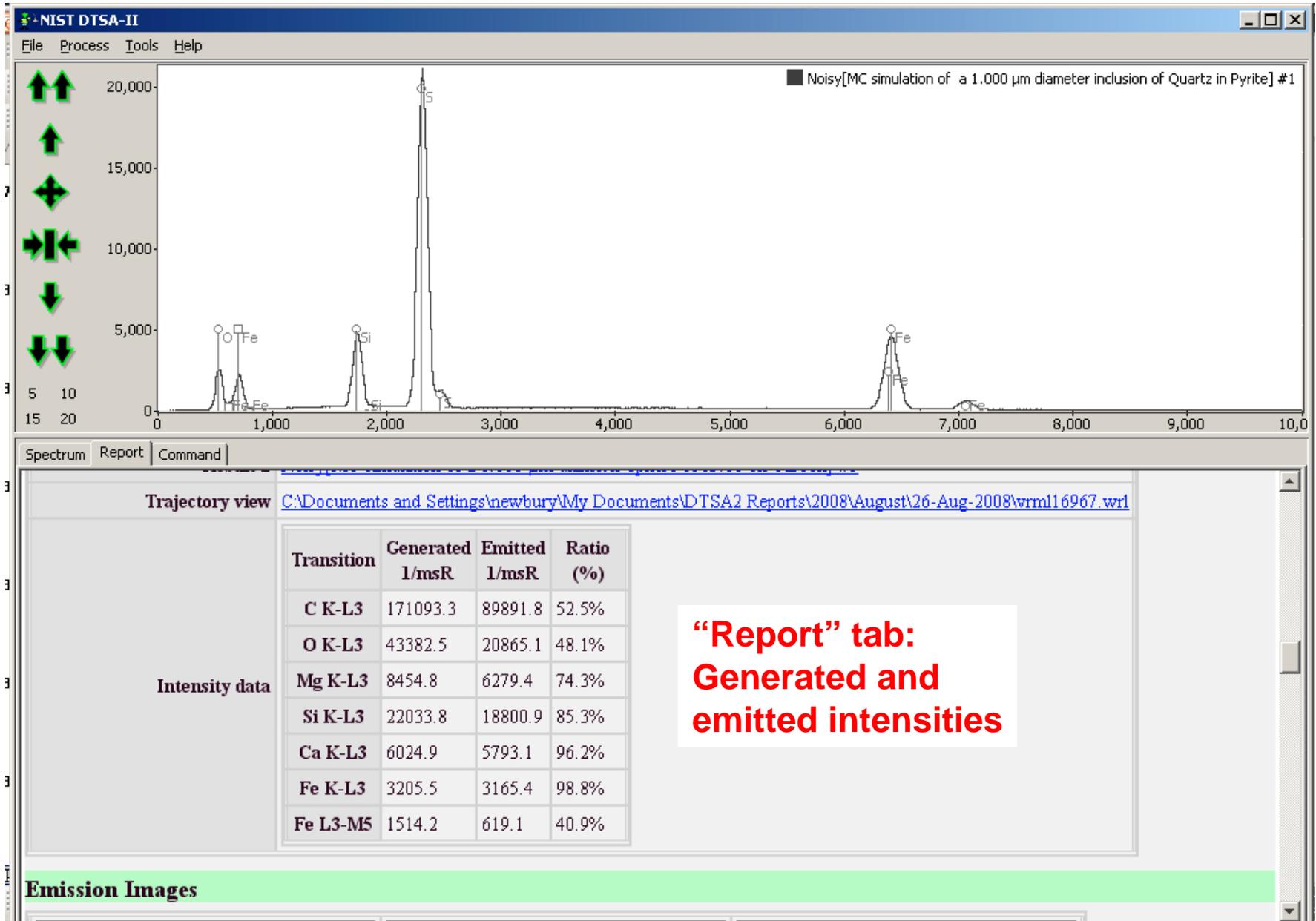
The screenshot shows the NIST DTSA-II software interface. A central dialog box titled "Spectrum simulation" is open, displaying "Other options". The dialog includes a cartoon alien character and navigation buttons: "Previous: Instrument configuration" and "Next: Perform Simulation". Under "Noise parameters", the checkbox "Apply simulated count statistics" is checked. The "Instance count" is set to 1. Under "Extended output", the checkbox "X-ray generation images (takes ~2 x as long)" is checked. A red arrow points from the text "Invoke x-ray generation images" to this checkbox. The background shows a plot area with a y-axis from 0 to 16 and an x-axis from 0 to 10,000. On the left, there are green navigation arrows and a "Spectrum List" panel. At the bottom, a status bar indicates "Detector thickness = 5 mm".

**Invoke x-ray generation images**

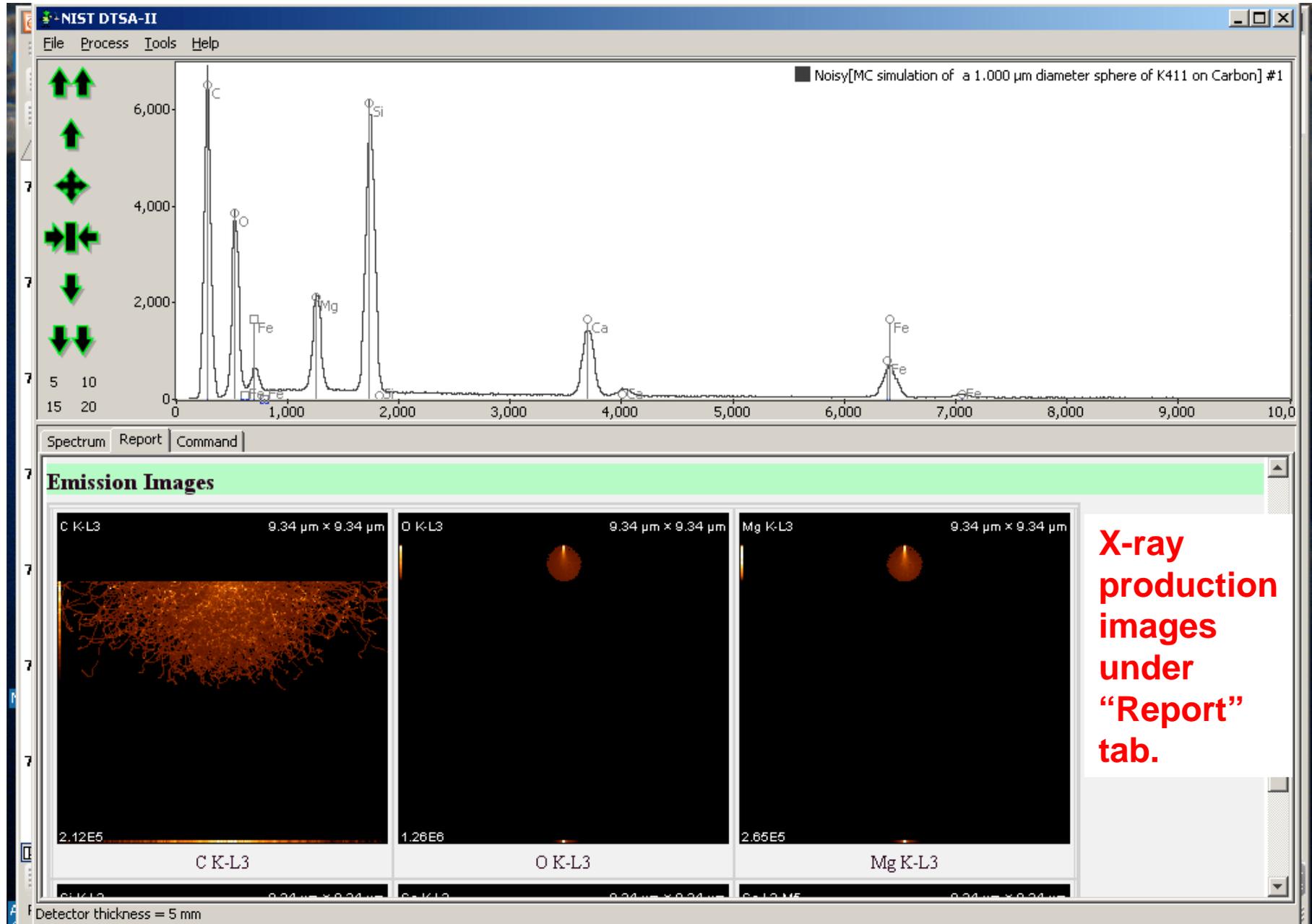
## Simulation Alien: Monte Carlo simulation of a 1 $\mu\text{m}$ K411 glass sphere on a C substrate



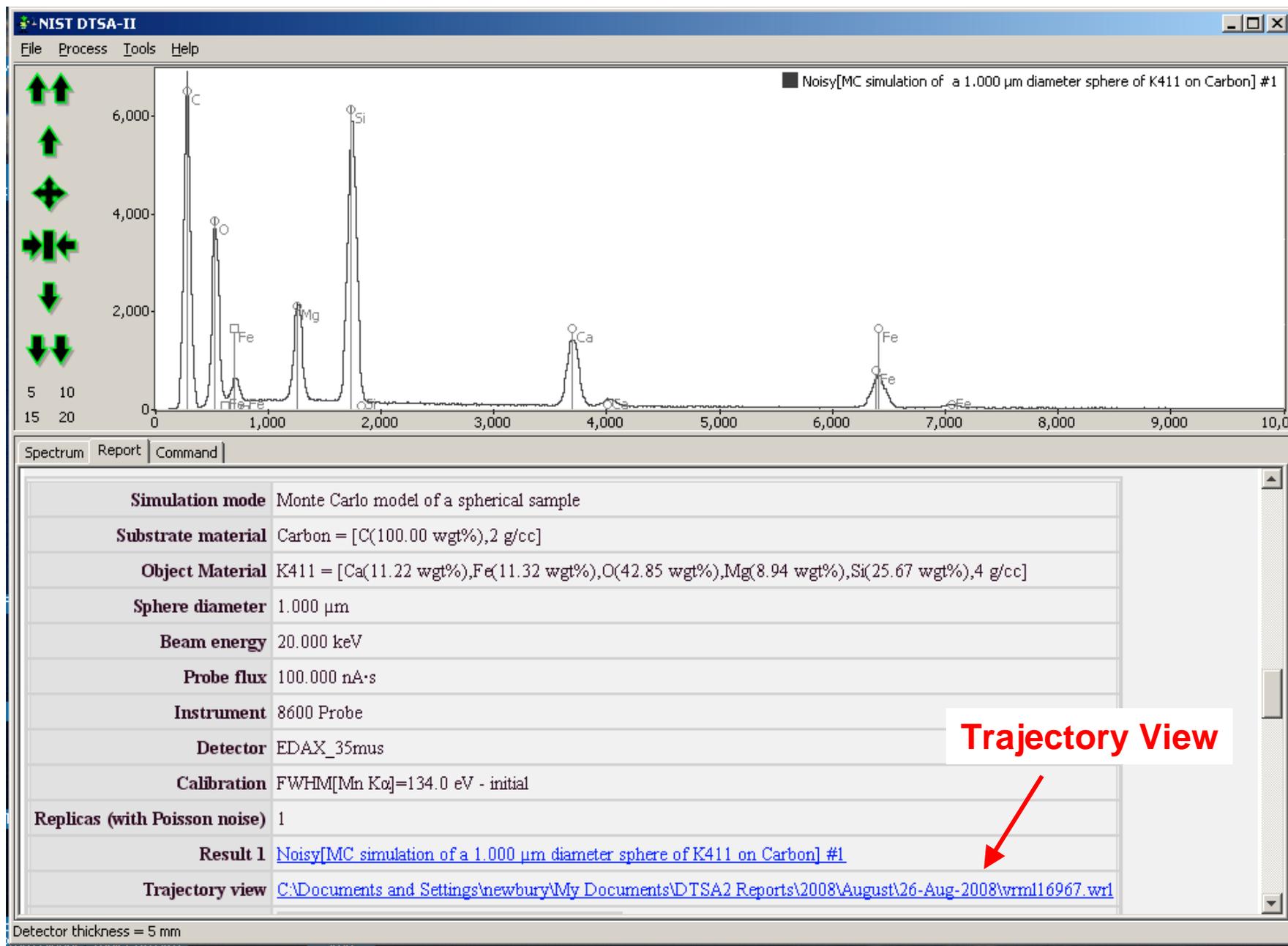
## Simulation Alien: Monte Carlo simulation of a 1 $\mu\text{m}$ K411 glass sphere on a C substrate



## Simulation Alien: Monte Carlo simulation of a 1 $\mu\text{m}$ K411 glass sphere on a C substrate



## Simulation Alien: Monte Carlo simulation of a 1 $\mu\text{m}$ K411 glass sphere on a C substrate



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

[Getting Started](#) [Quick Reference](#) [Going Further](#) [Release Notes](#) [About Cosmo Player](#)

[Getting Started with Cosmo Player 2.1.1](#)  
[On the Dashboard](#)  
[Moving Around in a World](#)  
[Examining Objects](#)  
[Changed Your Mind?](#)  
[Interacting with Active Objects](#)  
[Another Way of Moving Through a World](#)

# Getting Started with Cosmo Player 2.1.1

Copyright © 1997-1999 PLATINUM technology, inc. All rights reserved.

---

Cosmo Player plugs in to your Web browser to enable you to see and explore 3D worlds. With Cosmo Player you can visit any 3D world authored in the Virtual Reality Modeling Language (VRML). These 3D worlds often include other kinds of multimedia, like sound and movies.

This brief guide shows you the basics of the Cosmo Player main controls so you can get started right away.

You can find more in-depth information in [Cosmo Player 2.1.1 Quick Reference](#) and [Going Further with Cosmo Player 2.1.1](#).

You can find more technical information about installation and trouble-shooting in the [Release Notes](#).

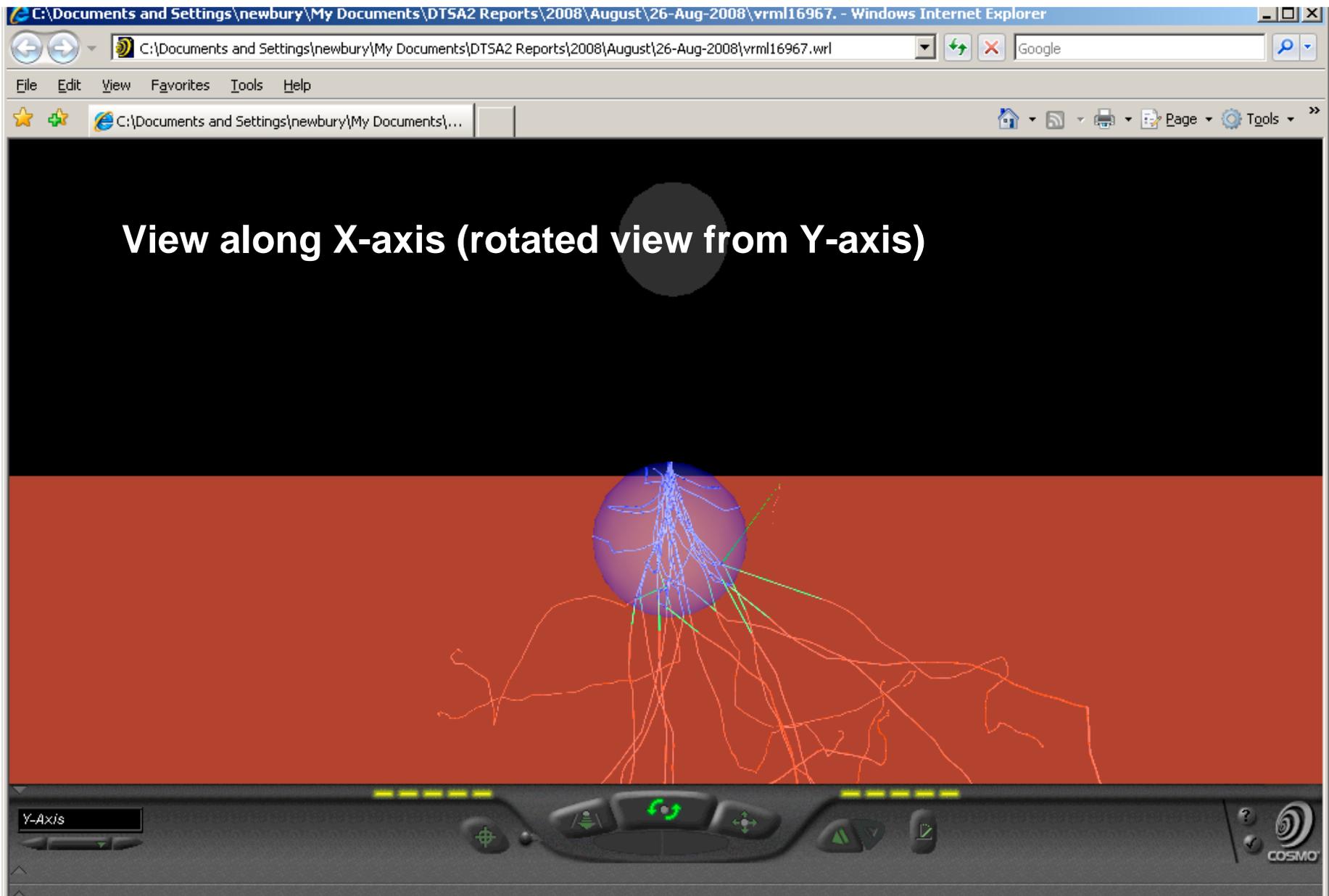
You can practice using Cosmo Player by playing , an interactive 3D game that teaches basic navigation.

---

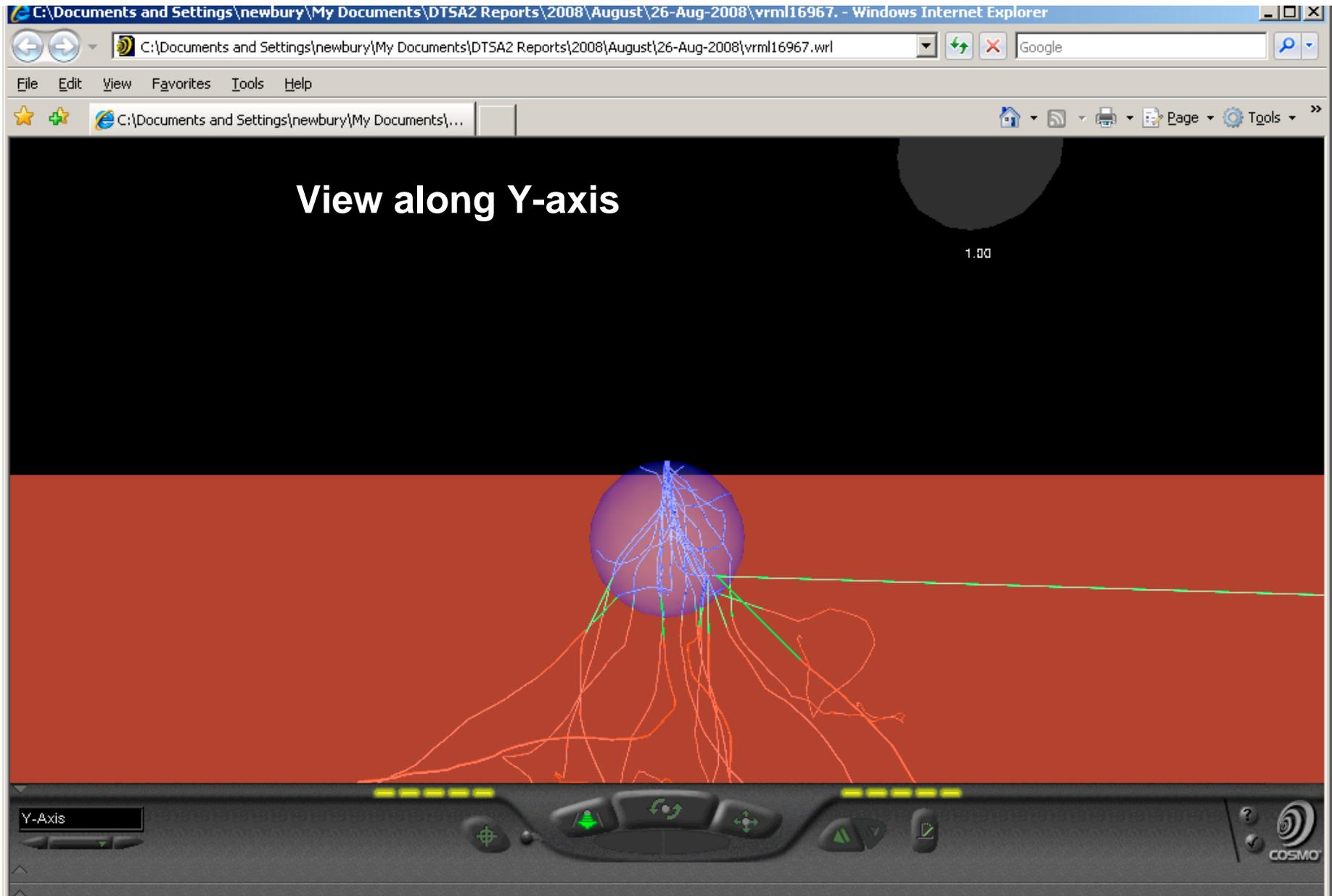
## On the Dashboard

You use the main controls on the Cosmo Player dashboard to do two things: move around in 3D worlds and examine objects in 3D worlds. (Some worlds don't display the dashboard, but they may provide on-screen cues to navigation.)

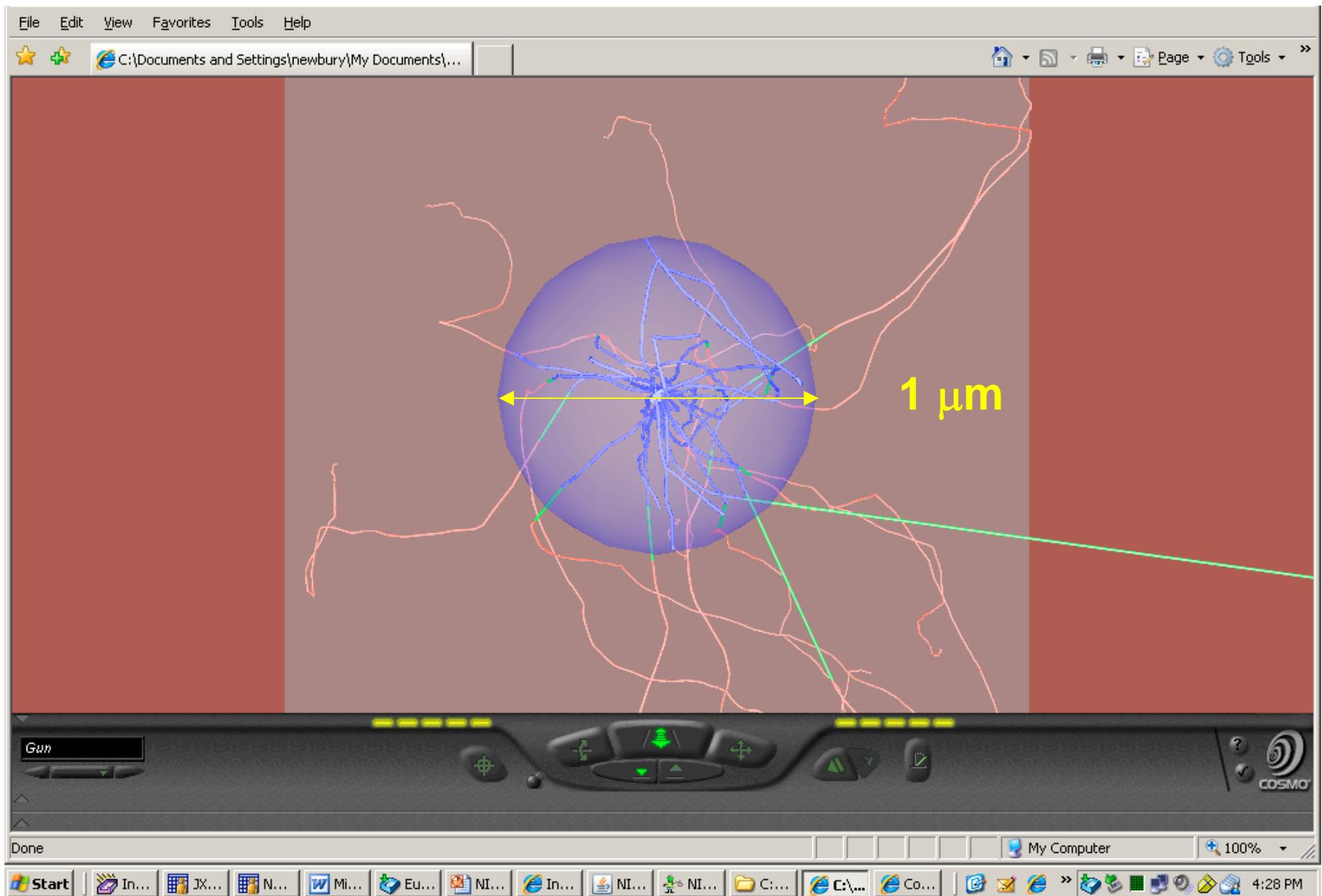
## Simulation Alien: Monte Carlo simulation of a 1 $\mu\text{m}$ K411 glass sphere on a C substrate



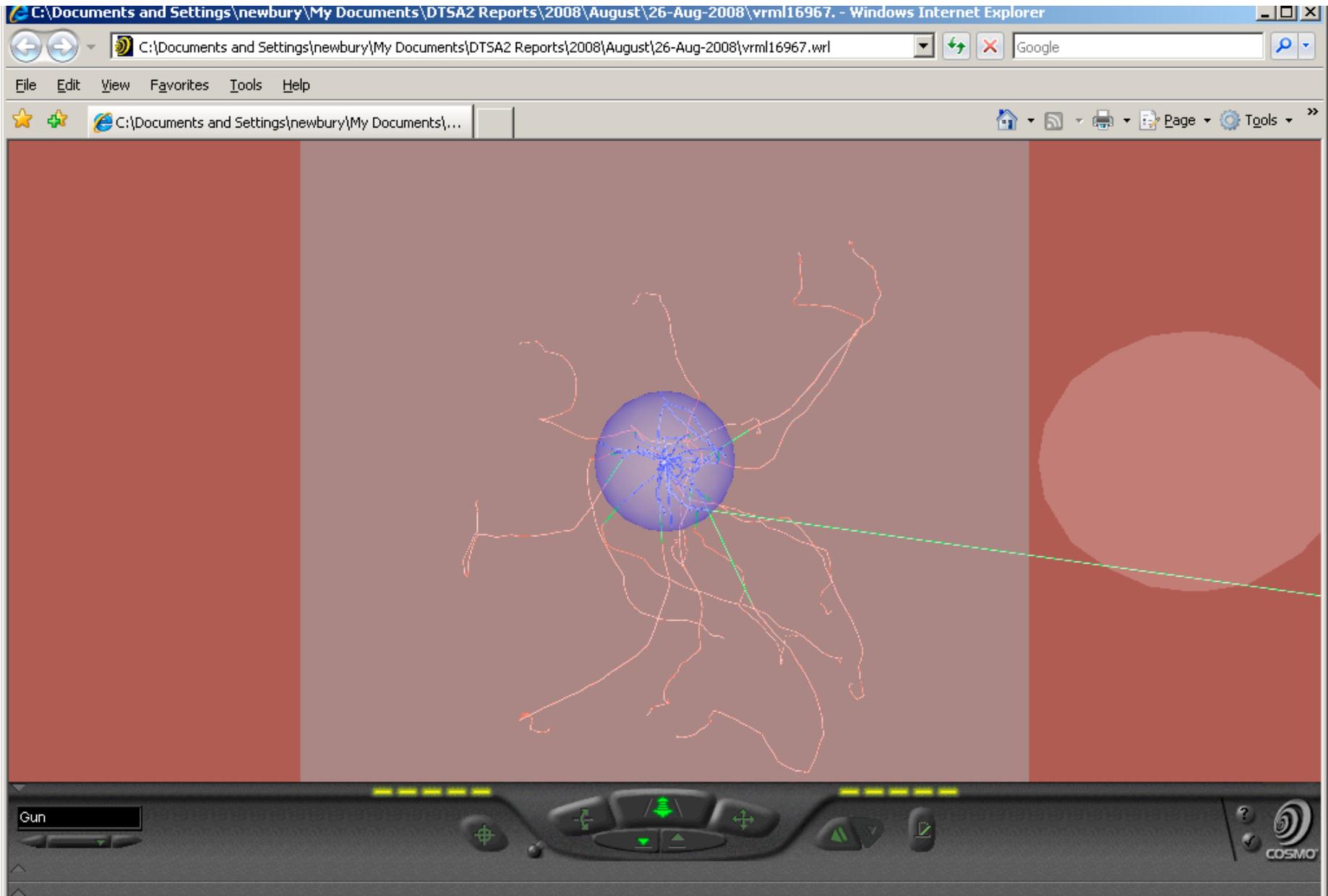
## Simulation Alien: Monte Carlo simulation of a 1 $\mu\text{m}$ K411 glass sphere on a C substrate



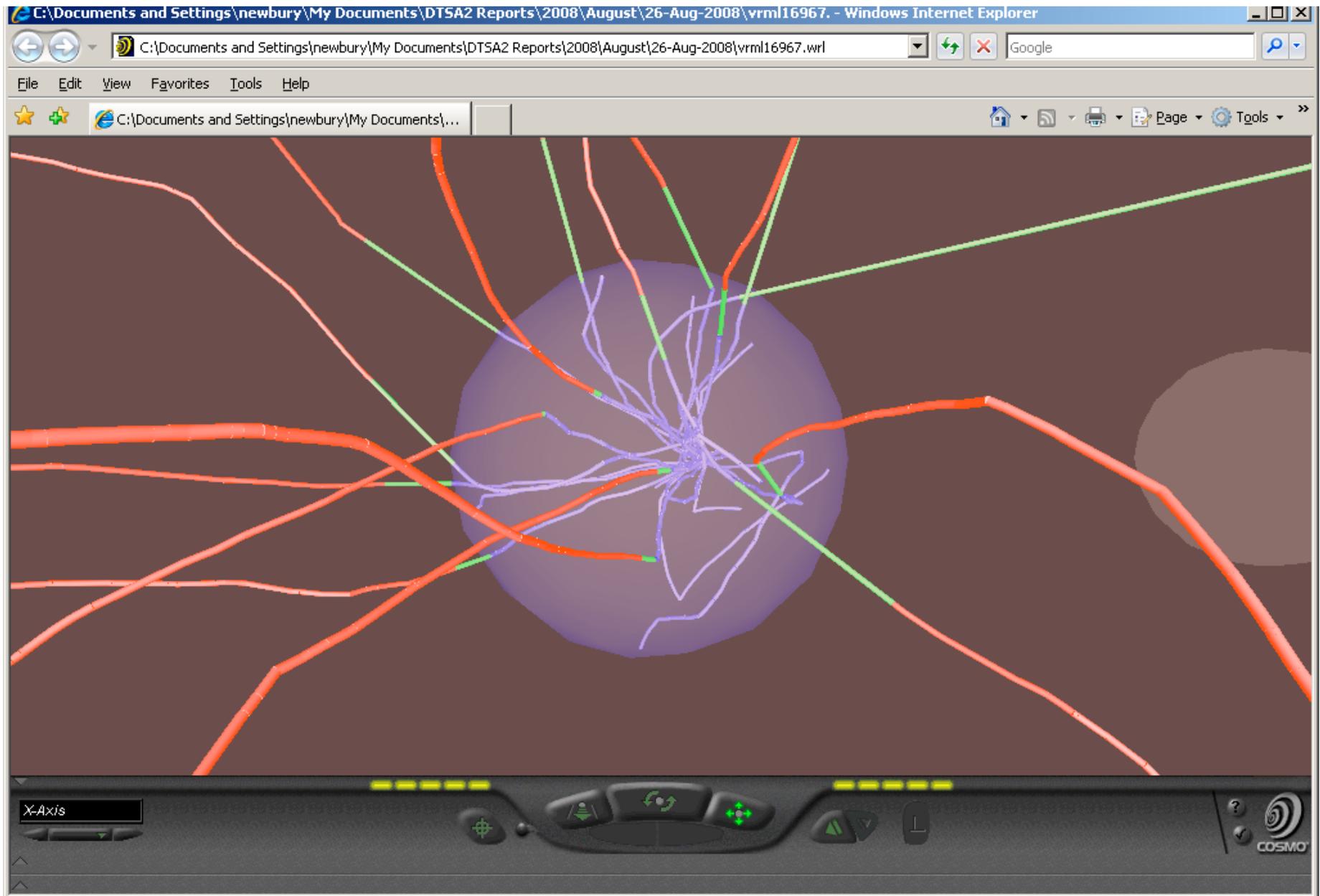
## View along the beam



## 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 $\mu\text{m}$ $\text{SiO}_2$ hemisphere in $\text{FeS}_2$

**Spectrum simulation** (First page)  
**Simulation Mode** (Next: Configure sample)

**Analytical Simulation**

- Analytical model of a bulk, homogeneous material

**Monte Carlo Simulation**

- Monte Carlo model of a bulk, homogeneous material
- Monte Carlo model of a film on a bulk, homogeneous substrate
- Monte Carlo model of a sphere on a bulk, homogeneous substrate
- Monte Carlo model of a cube on a bulk, homogeneous substrate
- Monte Carlo model of an inclusion in a bulk, homogeneous substrate

Message: Select the type of spectrum simulation to perform. More...

Buttons: Back, Next, Finish, Cancel

---

**Default Detector**

8600 Probe  
 EDAX\_35mus

**Spectrum List**

Noisy[MC simulation of a 1.000  $\mu\text{m}$  d...

None All Clear

---

Detector: EDAX\_35mus - FWHM[Mn K $\alpha$ ]=134.0 eV - initial  
 Detector area: 30 mm<sup>2</sup>  
 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)

---

Element: Fe  
 Temporary Lines  
 Selected Lines  
 Clear All Lines

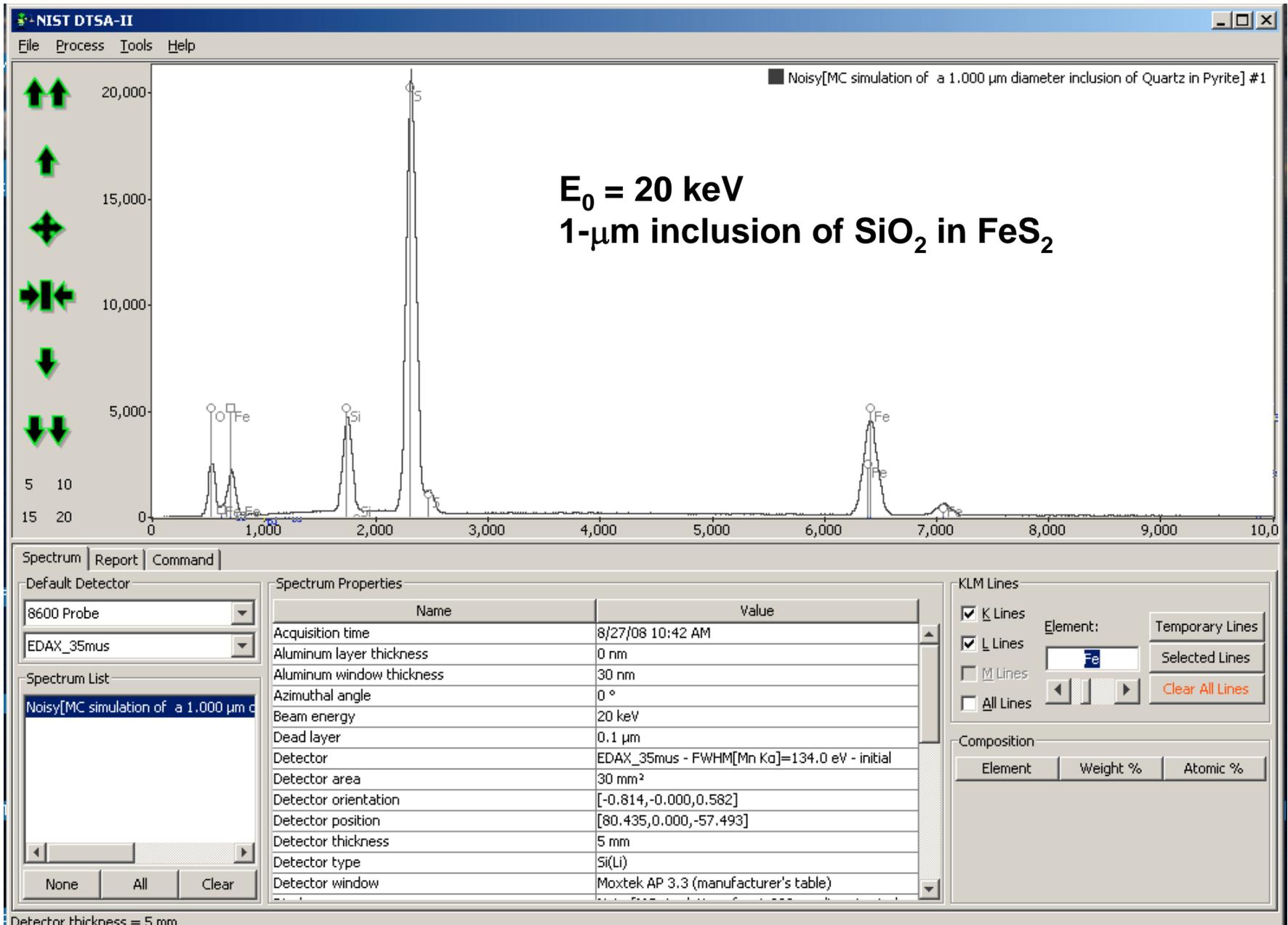
---

Composition

Element	Weight %	Atomic %

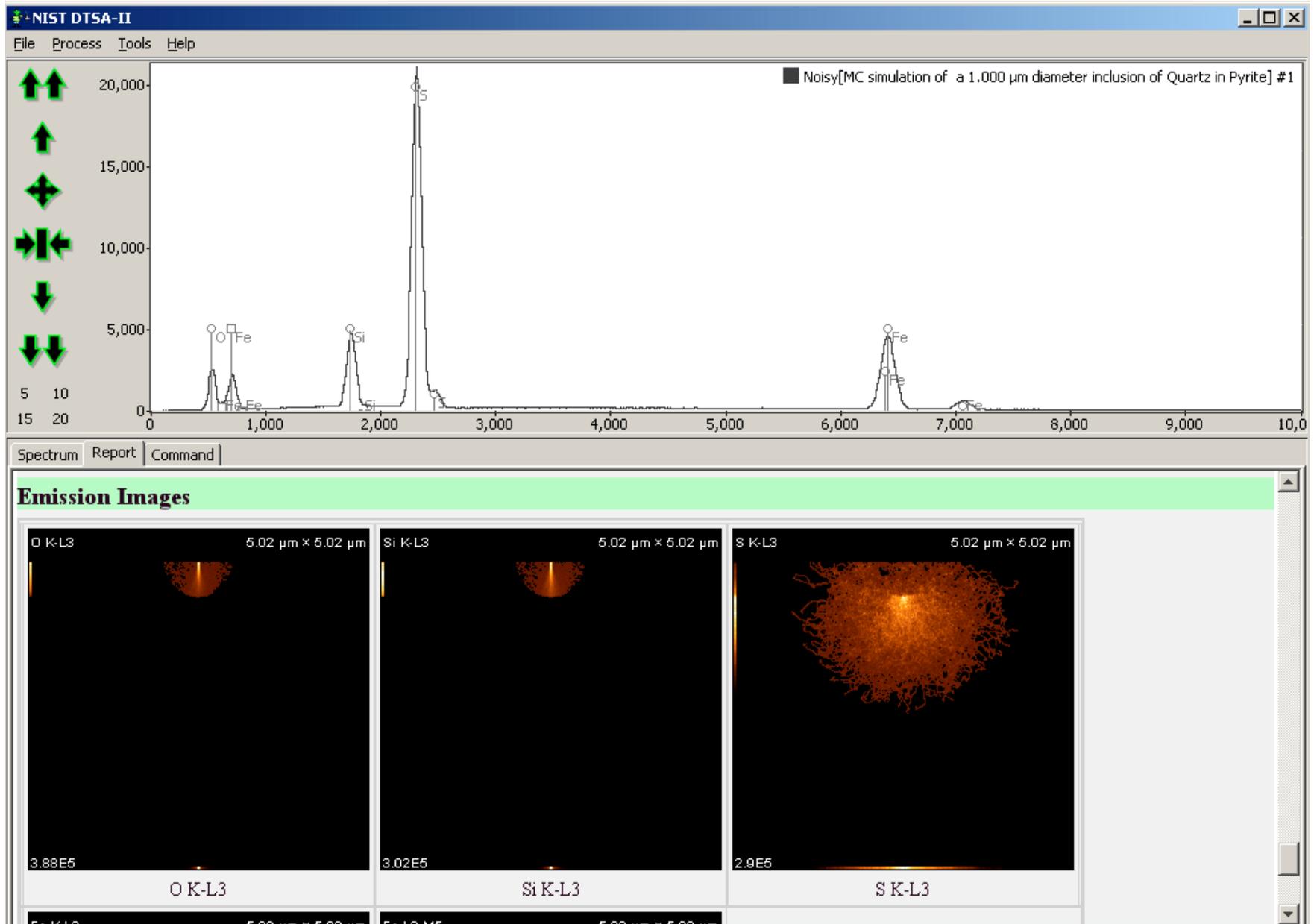
Detector thickness = 5 mm

# Simulation Alien: Monte Carlo simulation of a 1 $\mu\text{m}$ $\text{SiO}_2$ hemisphere in $\text{FeS}_2$

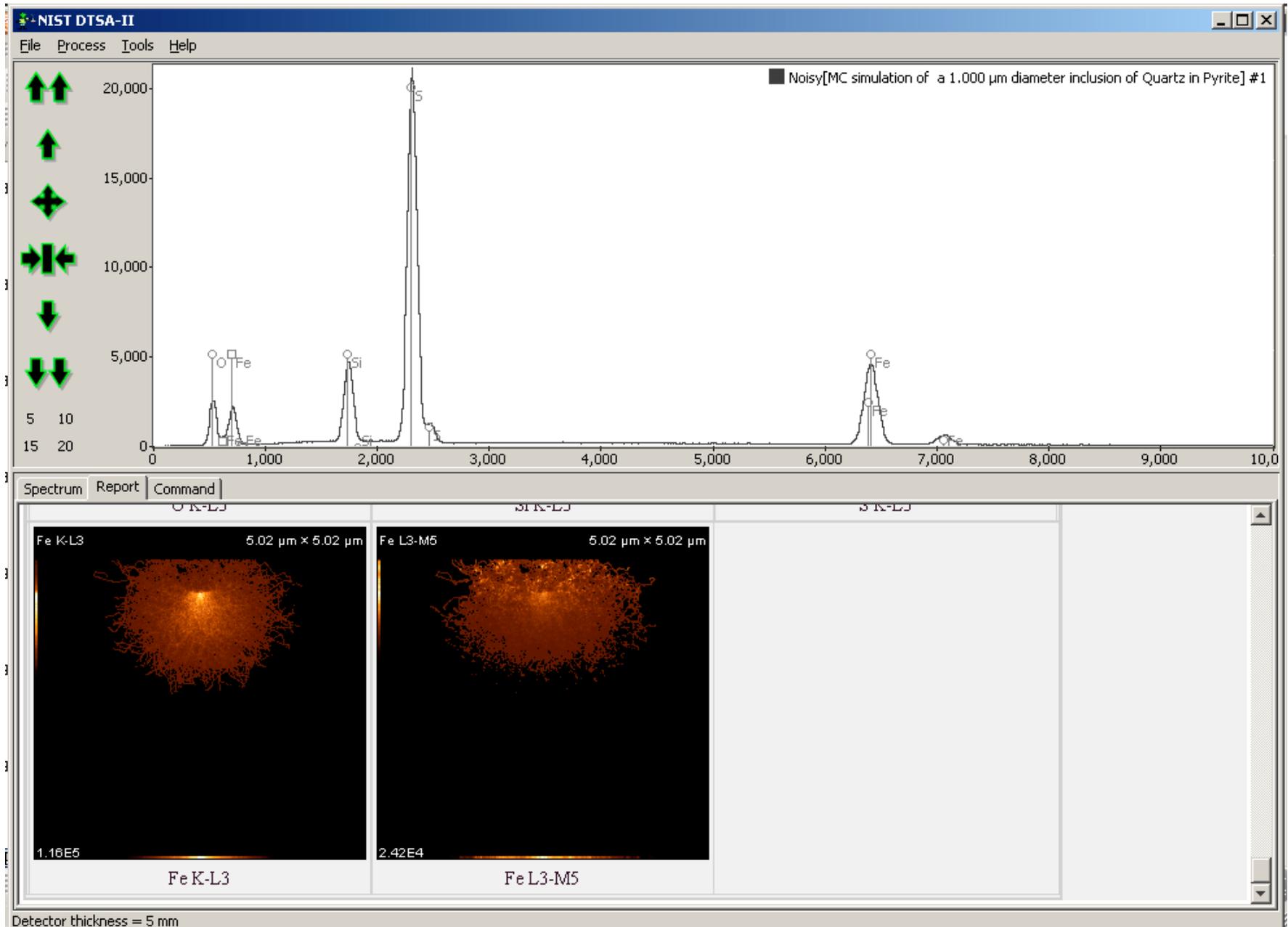


Detector thickness = 5 mm

# Simulation Alien: Monte Carlo simulation of a 1 $\mu\text{m}$ $\text{SiO}_2$ hemisphere in $\text{FeS}_2$



# Simulation Alien: Monte Carlo simulation of a 1 $\mu\text{m}$ $\text{SiO}_2$ hemisphere in $\text{FeS}_2$



# 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** [Window Title]

File Process **Tools** Help

↑ ↑  
↑  
↕  
← →  
↓  
↓ ↓

5 10  
15 20

10  
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

Cu\_20kV750pA35mu-s100s

Spectrum Report Command

Default Detector: 8600 Probe  
EDAX\_35mus

Spectrum List: Cu\_20kV750pA35mu-s100s

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 Ka]=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

10,000  
8,000  
6,000  
4,000  
2,000  
0

5 10  
15 20

0 2,000

16,000 18,000 20,0

Spectrum | Report | Command

Default Detector  
8600 Probe  
EDAX\_35mus

Spectrum List  
Cu\_20kV750pA35mu-s100s

None All Clear

Sp  
Ac  
Al  
Al  
Az  
Be  
Be  
Be  
De  
De  
De  
De

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 °

Element: Temporary Lines  
Fe Selected Lines  
Clear All Lines

Weight % Atomic %

**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

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

Detector \_\_\_\_\_

using the

with calibration

Setting \_\_\_\_\_

at a beam energy of  keV.

Message:

Spectrum | Report | Command

Default Detector

Spectrum List

None All Clear

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 °

Element:

Weight %  Atomic %

NIST DTSA-II

File Process Tools Help

Cu\_20kV750pA35mu-s100s

10,000  
8,000  
6,000  
4,000  
2,000  
0

0 2,000

5 10  
15 20

Spectrum Report Command

Default Detector  
8600 Probe  
EDAX\_35mus

Spectrum List  
Cu\_20kV750pA35mu-s100s

None All Clear

Ac  
Al  
Al  
Az  
Be  
Be  
De  
De  
De

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

**Quantification Alien**

Previous: Specify the instrument

**Specify standard spectra**

Next: Specify reference spectra

Spectrum	Elements	Probe (...)	Live time	Composition	File..	Database..	Remove	Clear

Message: Specify standard spectra and the associated elements and compo... More...

Back Next Finish Cancel

Select "File"

16,000 18,000 20,0

Element: Temporary Lines  
Fe Selected Lines  
Clear All Lines

Weight % Atomic %

**NIST DTSA-II**

File Process Tools Help

**Open a spectrum**

Look in: **Stds spc 20kv750pA35mu-s**

- My Recent Documents
- Desktop
- My Documents
- My Computer
- My Network Places

.AppleFileInfo	CaF2-20kv750pA35mu-s200s.spc	Fe5-20kv750pA35mu-s200s.spc
EDAX_20kv_1nA	Cd_20kv750pA35mu-s100s.spc	GaP_20kv750pA35mu-s100s.spc
Ag_20kv750pA35mu-s100s.spc	Ce_20kv750pA35mu-s100s.spc	GdF3_20kv750pA35mu-s100s.spc
Al_20kv750pA35mu-s100s.spc	Co_20kv750pA35mu-s100s.spc	Ge_20kv750pA35mu-s100s.spc
Al2O3_20kv750pA35mu-s100s.spc	Cr-20kv750pA35mu-s100s.spc	Hf_20kv750pA35mu-s100s.spc
Al_20kv750pA35mu-s100s.spc	Cr_20kv750pA35mu-s100s.spc	In_20kv750pA35mu-s100s.spc
As_20kv750pA35mu-s100s.spc	Cu-20kv750pA35mu-s100s.spc	Ir_20kv750pA35mu-s100s.spc
Au_20kv750pA35mu-s100s.spc	Cu-rep20kv750pA35mu-s100s.spc	K227_20kv750pA35mu-s100s.spc
B_20kv750pA35mu-s100s.spc	Cu_20kv750pA35mu-s100s.spc	K309_20kv750pA35mu-s500s.spc
Be_20kv750pA35mu-s100s.spc	<b>Cu5-20kv750pA35mu-s200s.spc</b>	K411-20kv750pA35mu-s500s.spc
Bi_20kv750pA35mu-s100s.spc	Dy_20kv750pA35mu-s100s.spc	K411_20kv750pA35mu-s100s.spc
C-20kv750pA35mu-s100s.spc	Er_20kv750pA35mu-s100s.spc	K412_20kv750pA35mu-s200s.spc
C_20kv750pA35mu-s100s.spc	Fe_20kv750pA35mu-s100s.spc	K961-20kv750pA35mu-s500s.spc

File name: **Cu5-20kv750pA35mu-s200s.spc**

Files of type: Common spectrum file

9,000 10,0

**Choose a spectrum file**

Temporary Lines  
Selected Lines  
Clear All Lines

Light % Atomic %

OK Cancel

Welcome to NIST DTSA-II version 1700

NIST DTSA-II

File Process Tools Help

16  
14  
12  
10  
8  
6  
4  
2  
0

5 10  
15 20

0 1,000

Spectrum Report Command

Default Detector

8600 Probe

EDAX\_35mus

Spectrum List

None All Clear

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

H	He
Li Be	B C N O F Ne
Na Mg	Al Si P S Cl Ar
K Ca Sc Ti V Cr Mn Fe Co Ni Cu Zn Ga Ge As Se Br Kr	
Rb Sr Y Zr Nb Mo Tc Ru Rh Pd Ag Cd In Sn Sb Te I Xe	
Cs Ba Hf Ta W Re Os Ir Pt Au Hg Tl Pb Bi Po At Rn	
La Ce Pr Nd Pm Sm Eu Gd Tb Dy Ho Er Tm Yb Lu	
Ac Th Pa U Np Pu Am Cm Bk Cf Es Fm Md No Lr	

Ok

Message: Specify standard spectra and the associated elements and compo... More...

Back Next Finish Cancel

Element: Temporary Lines  
Fe Selected Lines  
Clear All Lines

Composition

Element	Weight %	Atomic %
---------	----------	----------

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
Cu5-20kv750pA35mu-s200s	S	1.0	200.0	Cu5
Fe_20kv750pA35mu-s100s	Fe	1.0	100.0	Pure iron

Buttons: File.., Database.., Remove, Clear

Message: Fe\_20kv750pA35mu-s100s assigned as a reference for Fe

Buttons: Back, Next, Finish, Cancel

**Continue specifying needed spectra**

NIST DTSA-II

File Process Tools Help

15  
10  
5  
0

0 2,000

5 10  
15 20

Spectrum Report Command

Default Detector

8600 Probe

EDAX\_35mus

Spectrum List

None All Clear

16,000 18,000 20,0

Element: Fe

Temporary Lines

Selected Lines

Clear All Lines

Position

Weight % Atomic %

Quantification Alien

Previous: *Specify reference spectra*

Oxygen & other elements

Next: *Select the unknown spectrum*

No extra element

Element by difference

Oxygen by stoichiometry

Oxygen

Element	Cation	Anion	As
Sulfur	1	3	SO <sub>3</sub>
Iron	1	1	FeO

Message: Specify an element to be handled specially

More...

Back Next Finish Cancel

NIST DTSA-II

File Process Tools Help

15  
10  
5  
0

5 10  
15 20

0 2,000

Spectrum | Report | Command

Default Detector

8600 Probe

EDAX\_35mus

Spectrum List

None All Clear

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

Element: Fe

Temporary Lines

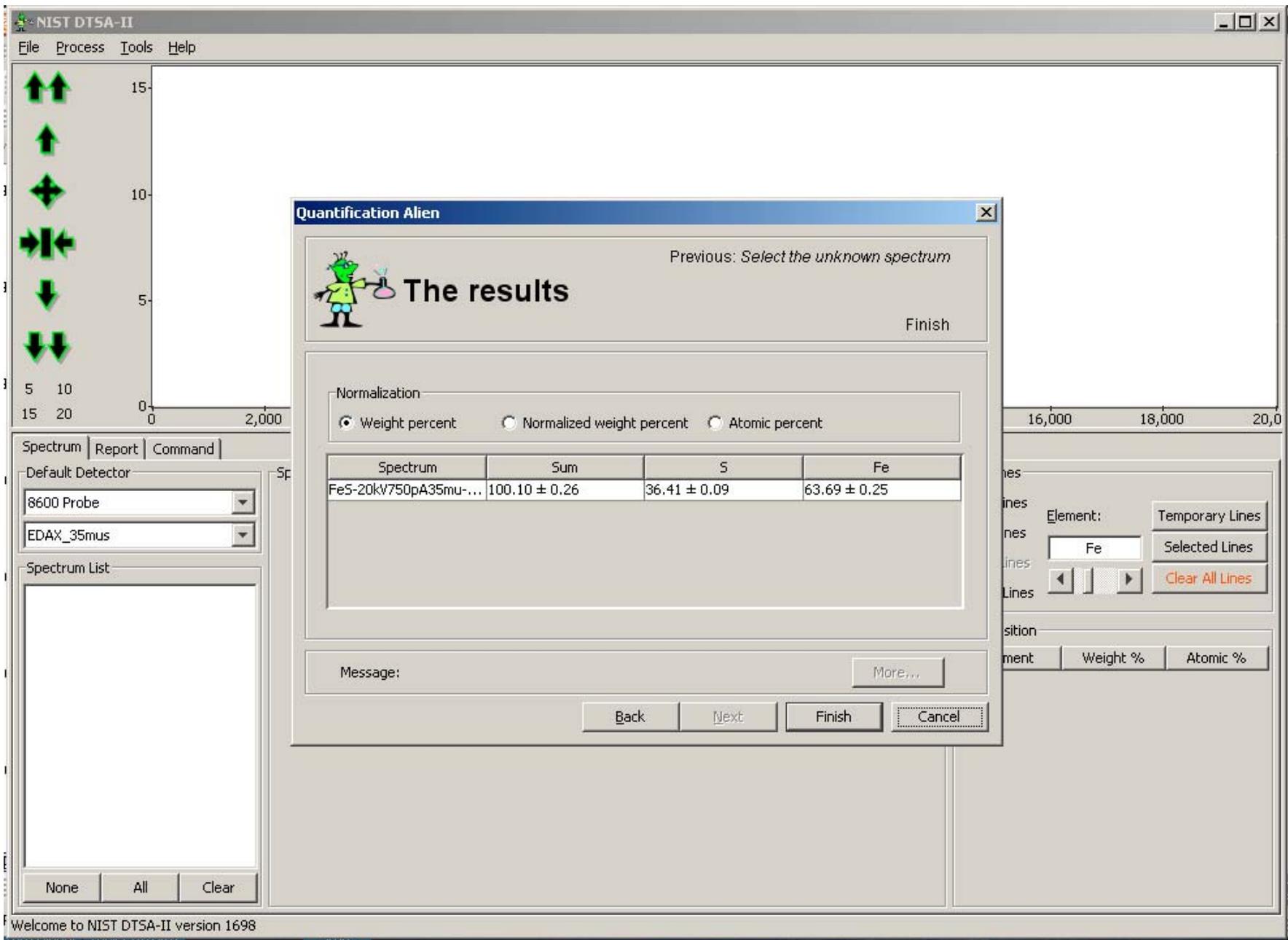
Selected Lines

Clear All Lines

Weight % Atomic %

Welcome to NIST DTSA-II version 1698

Access  
Finder  
to select  
spectra



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...

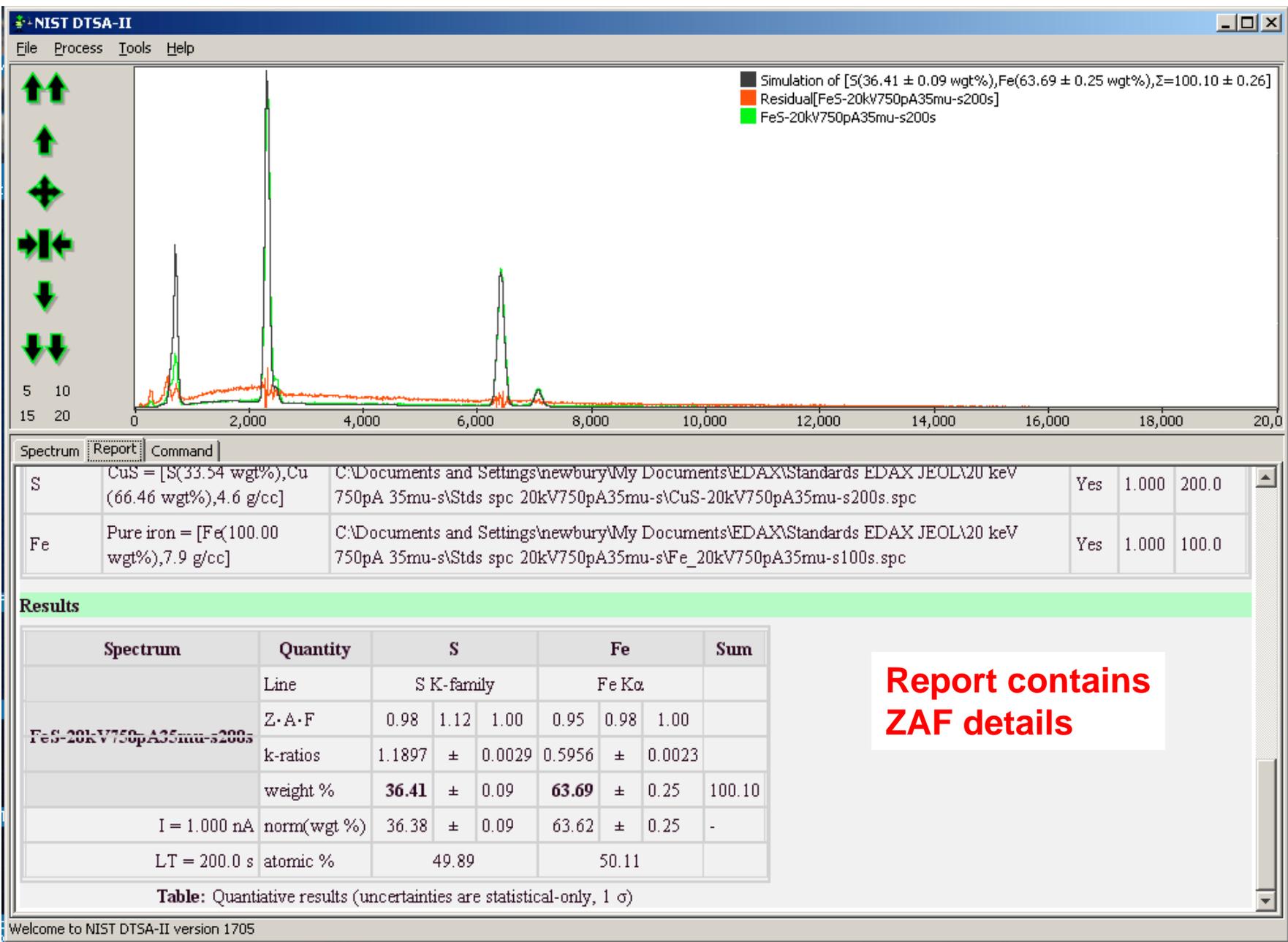
Back Next Finish Cancel

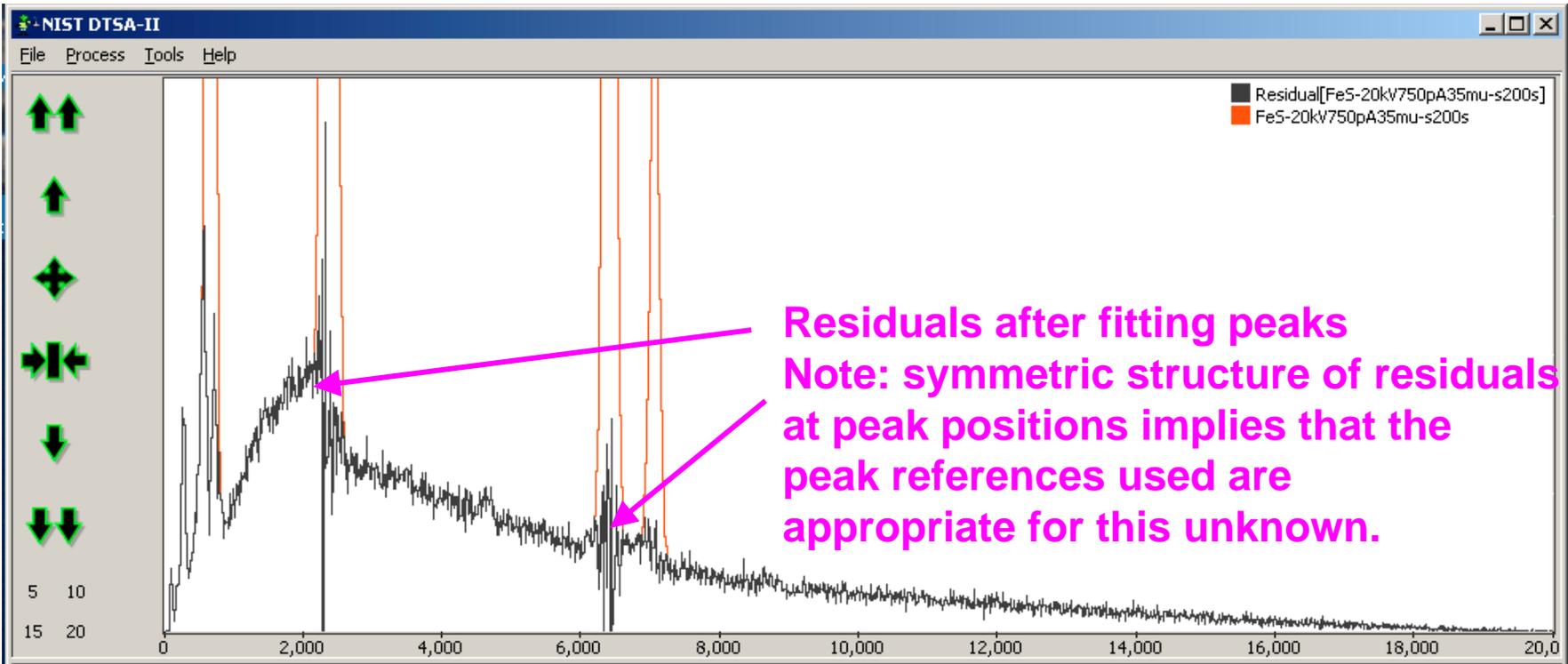
Element: Fe Temporary Lines Selected Lines Clear All Lines

Weight % Atomic %

None All Clear

Welcome to NIST DTSA-II version 1698





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 Ka]=134.0 eV - initial
Detector area	30 mm <sup>2</sup>
Detector orientation	[-0.814,-0.000,0.582]
Detector position	[80.435,0.000,-57.493]
Detector thickness	5 mm
Detector type	Si(Li)

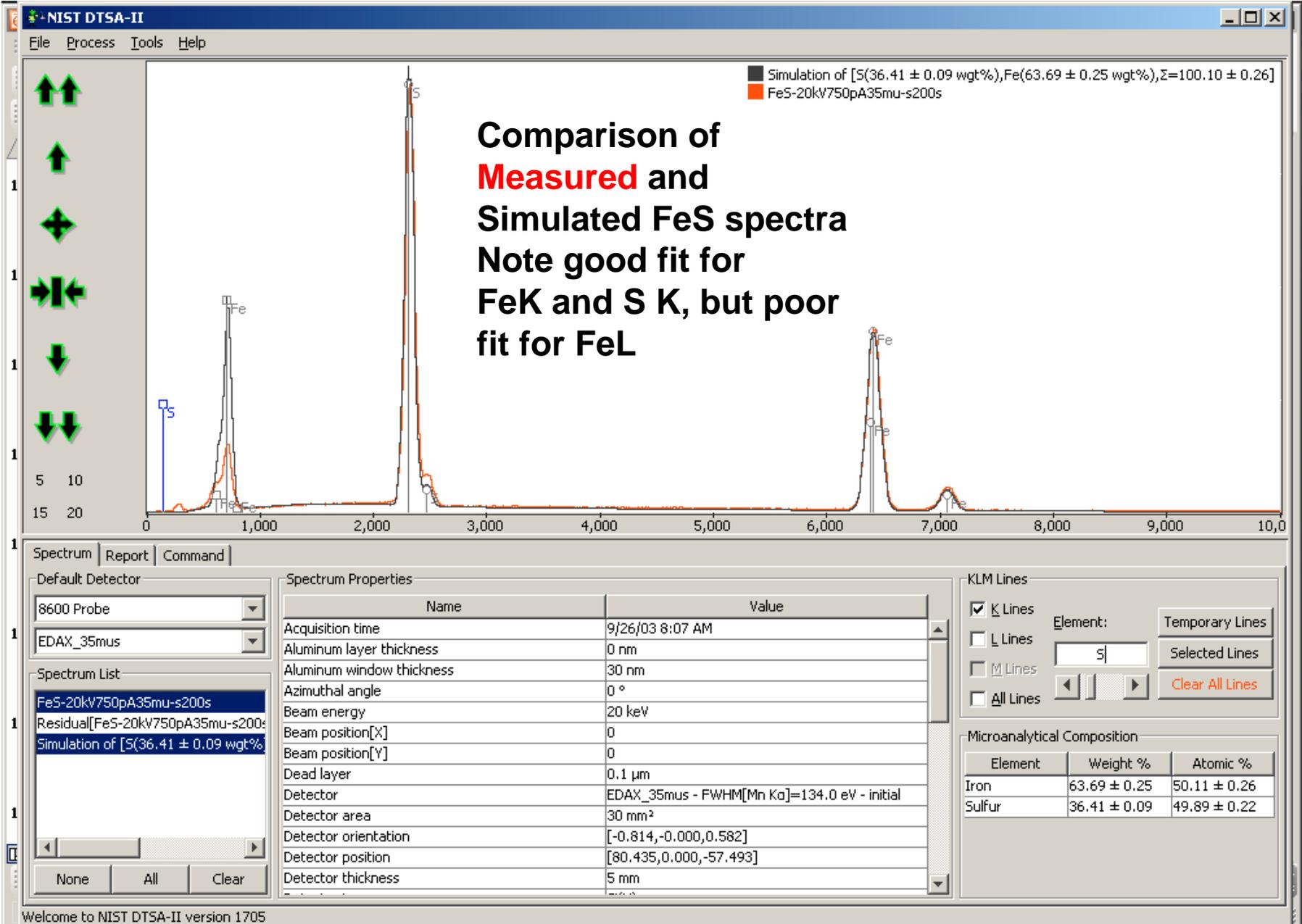
KLM Lines

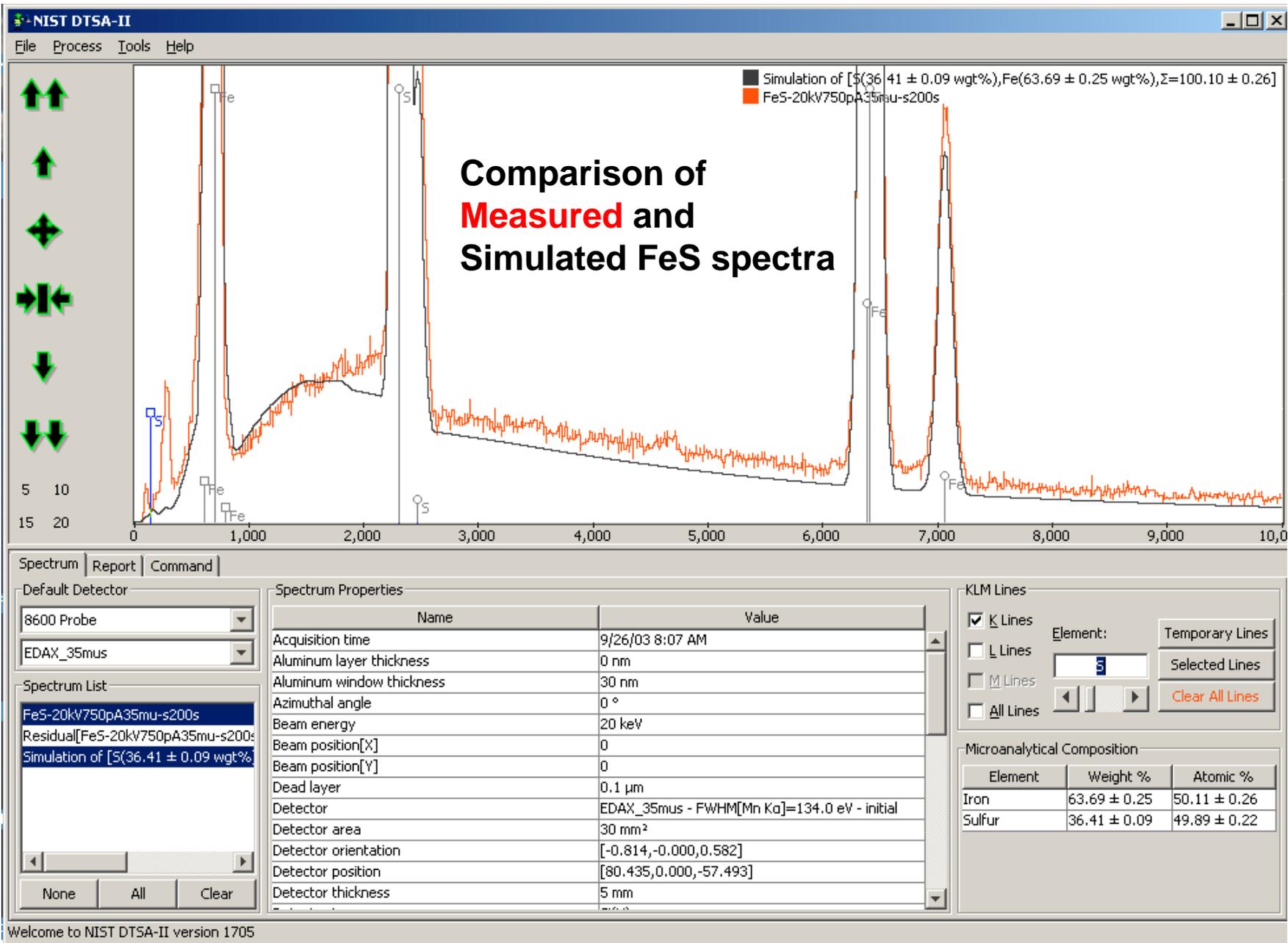
K Lines  
 L Lines  
 M Lines  
 All Lines

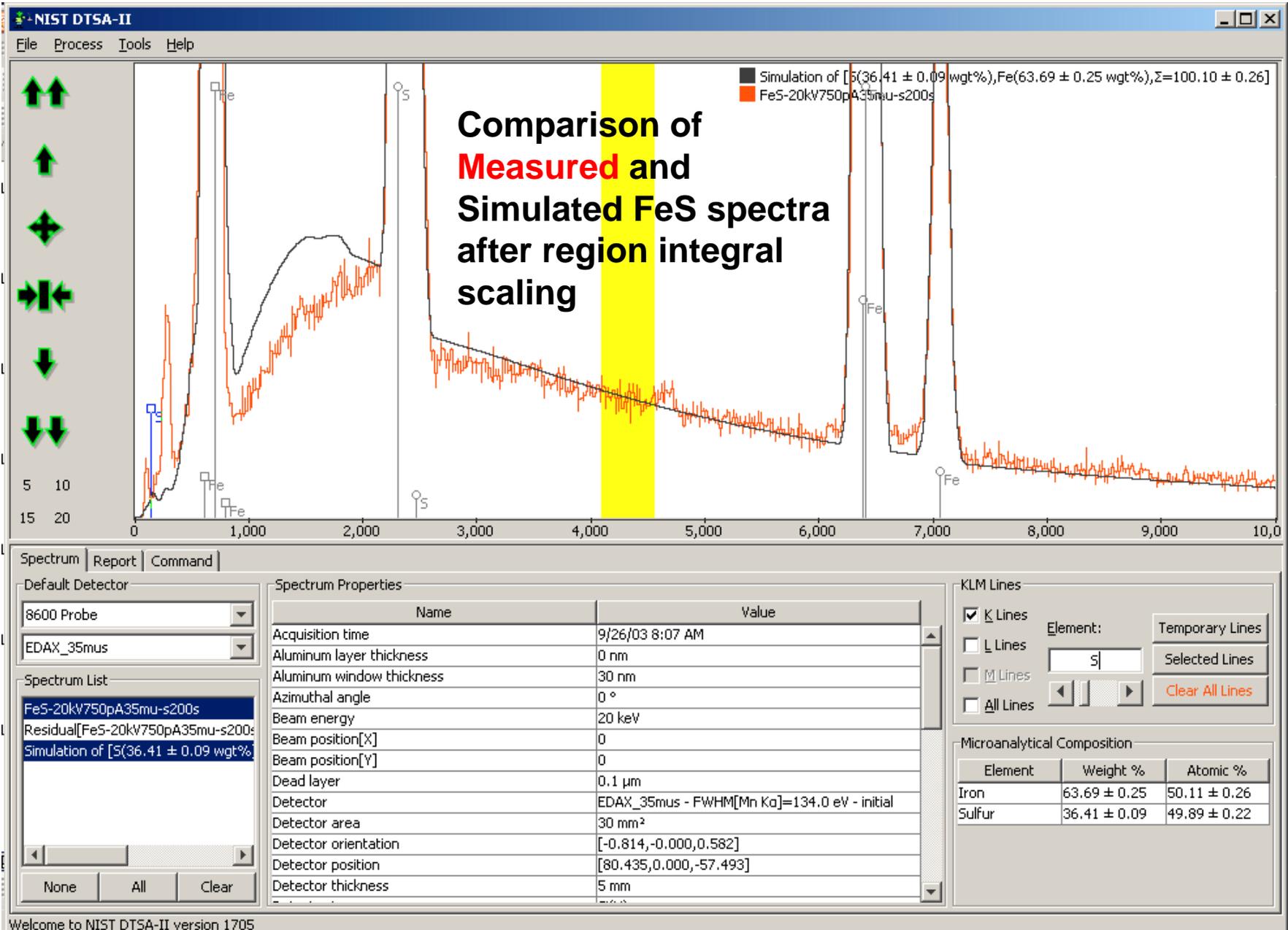
Element: Fe  
 Temporary Lines  
 Selected Lines  
 Clear All Lines

Microanalytical Composition

Element	Weight %	Atomic %







# Adding a new detector to the list under "Preferences"

The screenshot displays the NIST DTSA-II software interface. A 'DTSA-II - Preferences' dialog box is open, showing a tree view of 'Instruments and Detectors'. The 'JEOL8500F' folder is selected, and its contents are listed: 'Detector - QUAD SDD 5eV', 'Detector - BrukerQuadSDD-10eV', 'Probe', 'Detector - Si(Li)', '8600 Probe', and 'Detector - EDAX\_35mus'. The main area of the dialog shows the 'Instrument name' field set to 'JEOL8500F'. Below this are three buttons: 'Add Si(Li) detector', 'Add SDD detector', and 'Add microcalo...'. The background shows a spectrum plot with a peak at approximately 9,000 units. The 'Default Detector' is set to 'JEOL8500F' and the 'Spectrum List' contains 'Cu-stdB\_20kV20nAMed29'.

Parameter	Value
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)

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

**DTSA-II - Preferences**

Detector - BrukerQuadSDD\_145eV

Enable detector

Name  
Detector name: BrukerQuadSDD\_145eV

Import  
Import from spectrum

Window  
Window: No window

Position  
Elevation angle  
Azimuthal angle

Window options:  
Beryllium (8 µm)  
Beryllium (12 µm)  
Beryllium (25 µm)  
Moxtek AP 1.3  
Moxtek AP 1.7  
Moxtek AP 3.3 (model)  
Moxtek AP 3.3 (manufacturer's table)  
No window

Edit the properties of this detector.

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)

Default Detector: JEOL8500F  
BrukerQuadSDD-10eV

Spectrum List: Cu-stdB\_20kV20nAMed29

Buttons: None, All, Clear

Buttons: Temporary Lines, Selected Lines, Clear All Lines

Buttons: Light %, Atomic %

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

The screenshot shows the NIST DTSA-II software interface. A 'DTSA-II - Preferences' dialog box is open, displaying settings for a 'Detector - BrukerQuadSDD\_145eV'. The dialog is divided into several sections:

- User Information**: (Collapsed)
- Quantitative algorithms**: (Collapsed)
- Instruments and Detectors**: A tree view showing the hierarchy: JEOL8500F > BrukerQuadSDD\_145eV.
- Position**:
  - Elevation angle: 35.0 °
  - Azimuthal angle: 180.0 °
  - Optimal working distance: 12.0 mm
  - Sample-to-detector distance: 75.0 mm
- Crystal parameters**:
  - Detector Area: 40.0 mm<sup>2</sup>
  - Gold layer: 0.0 nm
  - Aluminum layer: 10.0 nm
  - Dead layer: 0.0 μm
  - Thickness: 0.4 mm

At the bottom of the dialog, there is a table with the following data:

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)

The background shows a spectrum plot with a peak at approximately 9,000 units. The status bar at the bottom left reads 'Welcome to NIST DTSA-II version 1705'.

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

The screenshot displays the NIST DTSA-II software interface. The main window shows a spectrum plot with a peak at approximately 9,000 eV. The 'DTSA-II - Preferences' dialog box is open, showing the configuration for the selected detector: 'Detector - BrukerQuadSDD\_145eV'. The dialog is divided into several sections: 'User Information', 'Quantitative algorithms', 'Instruments and Detectors', 'Configuration', and 'Base Performance'. The 'Instruments and Detectors' section shows a tree view with 'JEOL8500F' expanded, and 'Detector - BrukerQuadSDD\_145eV' selected. The 'Configuration' section includes fields for 'Aluminum layer' (10.0 nm), 'Dead layer' (0.0 μm), and 'Thickness' (0.4 mm). The 'Base Performance' section includes 'Energy scale' (5.0 eV/channel), 'Zero offset' (-475.0 eV), and 'Resolution' (145.0 eV at Mn Ka). The 'Default Detector' dropdown is set to 'BrukerQuadSDD-10eV'. The 'Spectrum List' shows 'Cu-stdB\_20kV20nAMed29' selected. The 'Temporary Lines', 'Selected Lines', and 'Clear All Lines' buttons are visible. The 'OK', 'Cancel', and 'Apply' buttons are at the bottom of the dialog. The status bar at the bottom left reads 'Welcome to NIST DTSA-II version 1705'.

**DTSA-II - Preferences**

- User Information
- Quantitative algorithms
- Instruments and Detectors
  - JEOL8500F
    - Detector - QUAD SDD 5eV
    - Detector - BrukerQuadSDD-10eV
    - Detector - BrukerQuadSDD\_128eV
    - Detector - BrukerQuadSDD\_145eV
  - Probe
  - 8600 Probe

**Detector - BrukerQuadSDD\_145eV**

Aluminum layer: 10.0 nm  
Dead layer: 0.0 μm  
Thickness: 0.4 mm

**Configuration**

Number of channels: 4096 channels  
Zero strobe discriminator: 50.0 eV

**Base Performance**

Energy scale: 5.0 eV/channel  
Zero offset: -475.0 eV  
Resolution: 145.0 eV at Mn Ka

Edit the properties of this detector.

OK Cancel Apply

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)

None All Clear

Welcome to NIST DTSA-II version 1705