U.S. DEPARTMENT OF ENERGY

Nuclear Energy

NEAMS

NUCLEAR ENERGY ADVANCED MODELING & SIMULATION PROGRAM

Hybrid K-Edge Densitometer Simulation Module for Safeguards Performance Modeling

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NEAMS PI meeting

Safeguards and Separations IPSC

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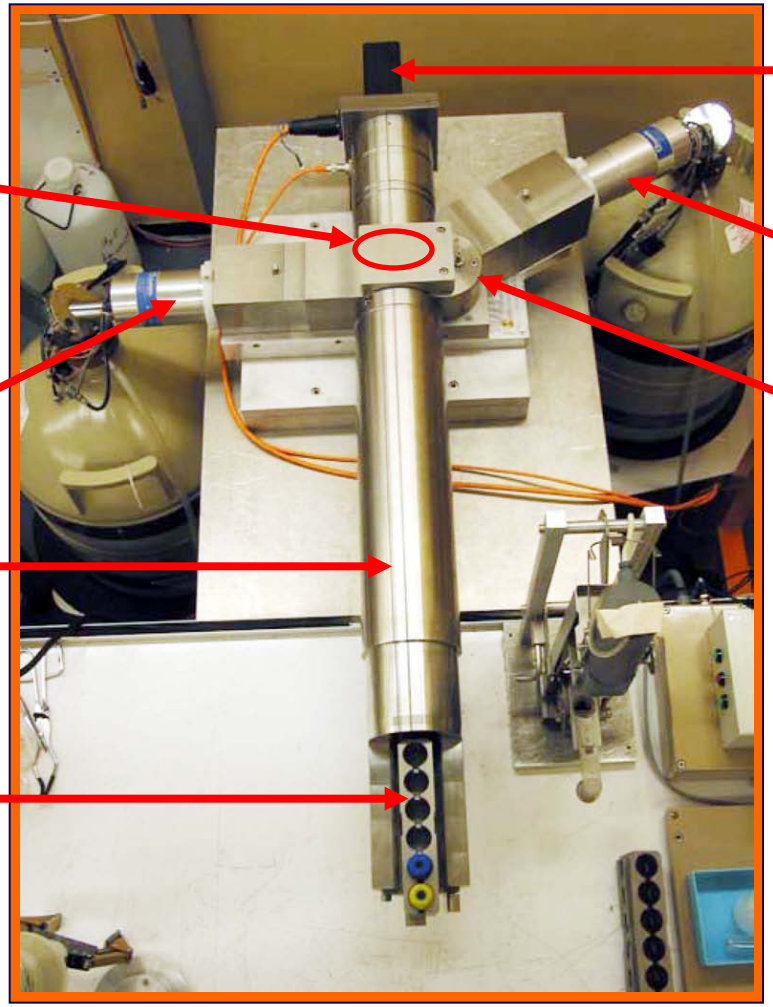
“Hybrid” K-Edge/XRF analytical technique

- **K-edge detector measures transmitted portion of x-ray beam**
  - continuous-energy x-ray beam; x-ray endpoint usually 145 to 150 kV
  - areal density of major element (usually U) is derived from prominence of K absorption edge in Ln(Ln(1/Transmission)) vs Ln(Energy) space
  - concentration (grams per liter) of major element is determined from areal density and sample thickness
- **XRF detector measures fluoresced x-rays emitted from sample face**
  - response function fitting is performed on Th, U, Np, Pu, Am, Cm x-rays
  - attenuation-corrected weight ratios (of any minor elements to the major element) are determined
- **“Hybrid” Technique: combination of KED and XRF data**
  - Major element concentration determined directly from KED data
  - Other concentrations determined by XRF weight ratio with major element

Overview of HKED System Components



Sample Changer Motor

Measurement Chamber

XRF Detector

K-Edge Detector

X-Ray Tube

Transport tube (penetrates hot cell shielding)

Multi-Slot Sample Tray in sample loading area

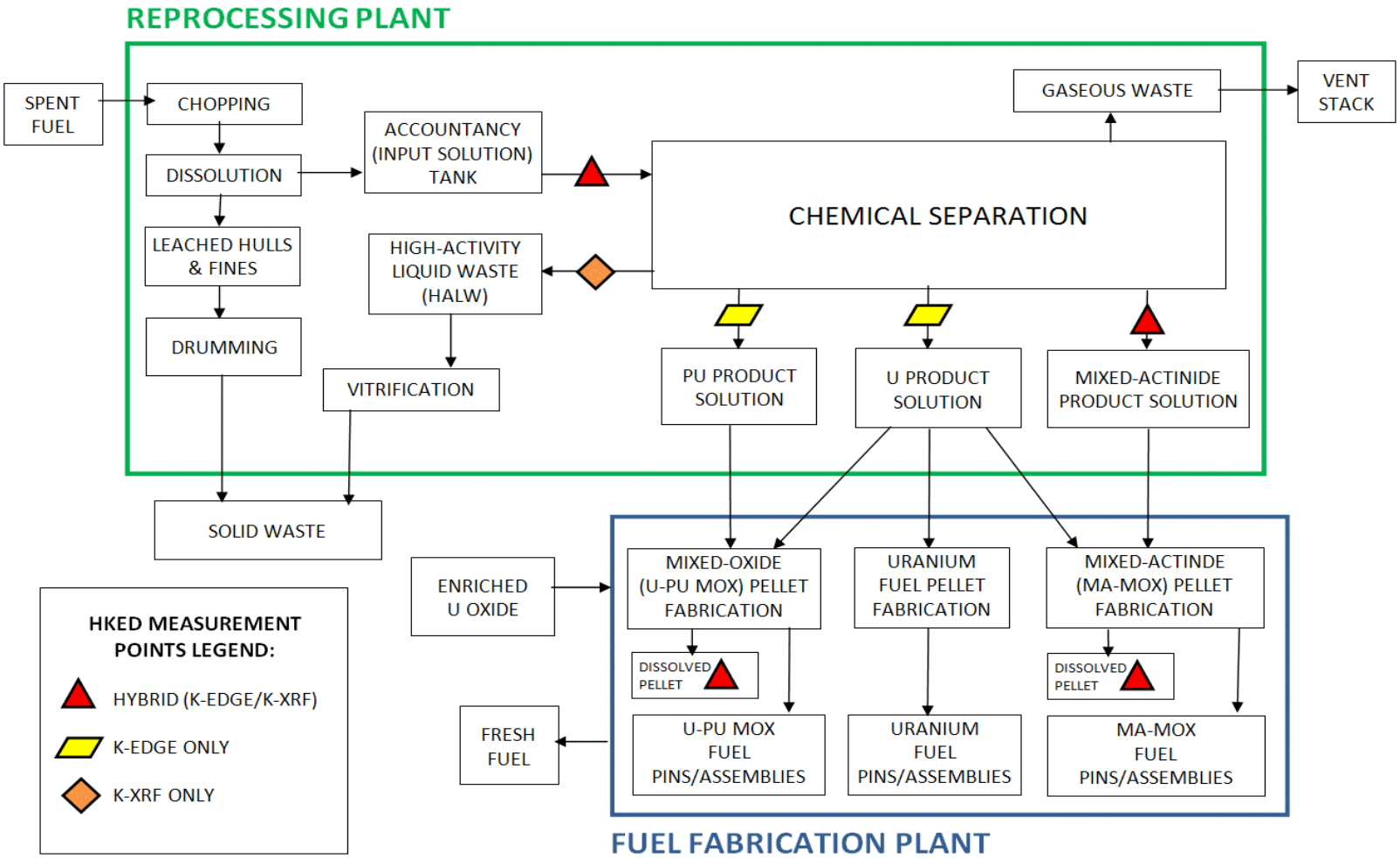
A commercial HKED system undergoes acceptance tests at ITU Karlsruhe, Germany before shipment to Rokkasho Japan

Photo courtesy CEC/JRC/ITU Karlsruhe

25 Years of HKED Developments at LANL

- 1986: LANL begins HKED collaboration with KFK (now ITU Karlsruhe)
- 1993: LANL-built HKED installed at JAERI NUCEF analytical lab
- 1994: LANL develops KED fitting with deattenuation (Hsue, Collins)
- 1997: LANL includes nonlinear fitting of broadened k-edges; begins collaborations with IAEA-SAL and NMCC-Japan
- 1998: First HKED determination of Neptunium (Collins, Hsue)
- 2000: LANL HKED software applicable to Th,U,Np,Pu,Am,Cm (Collins)
- 2001: LANL-designed HKED delivered for use inside Rokkasho, via commercial tech transfer agreement
- 2004-05: LANL HKED 2004 software in use by IAEA in Japan
- 2006-07: Low-Level XRF Densitometry added to LANL software
- 2007: Germanium X-ray Escape Peak fitting added to LANL software
- 2010: LANL HKED software licenses issued to Canberra, ORTEC
- 2010: SimHKED module functionality in HKED 2010 software
- 2011: LANL under contract with Seiko/ORTEC to deploy second HKED system inside Rokkasho

HKED Systems: “Multiple Instruments in One”



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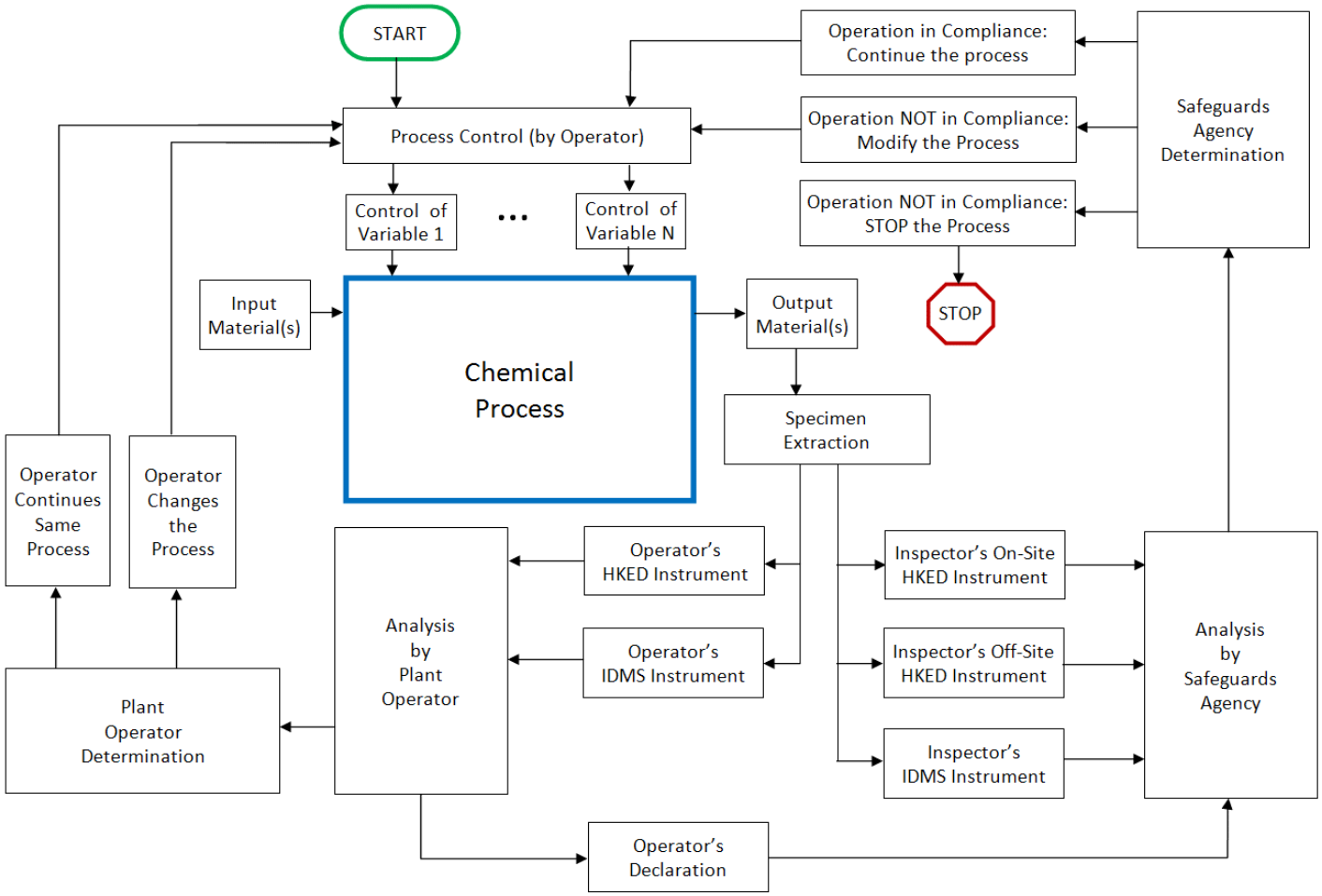
Safeguards Instruments result in Process Control "Feedback"



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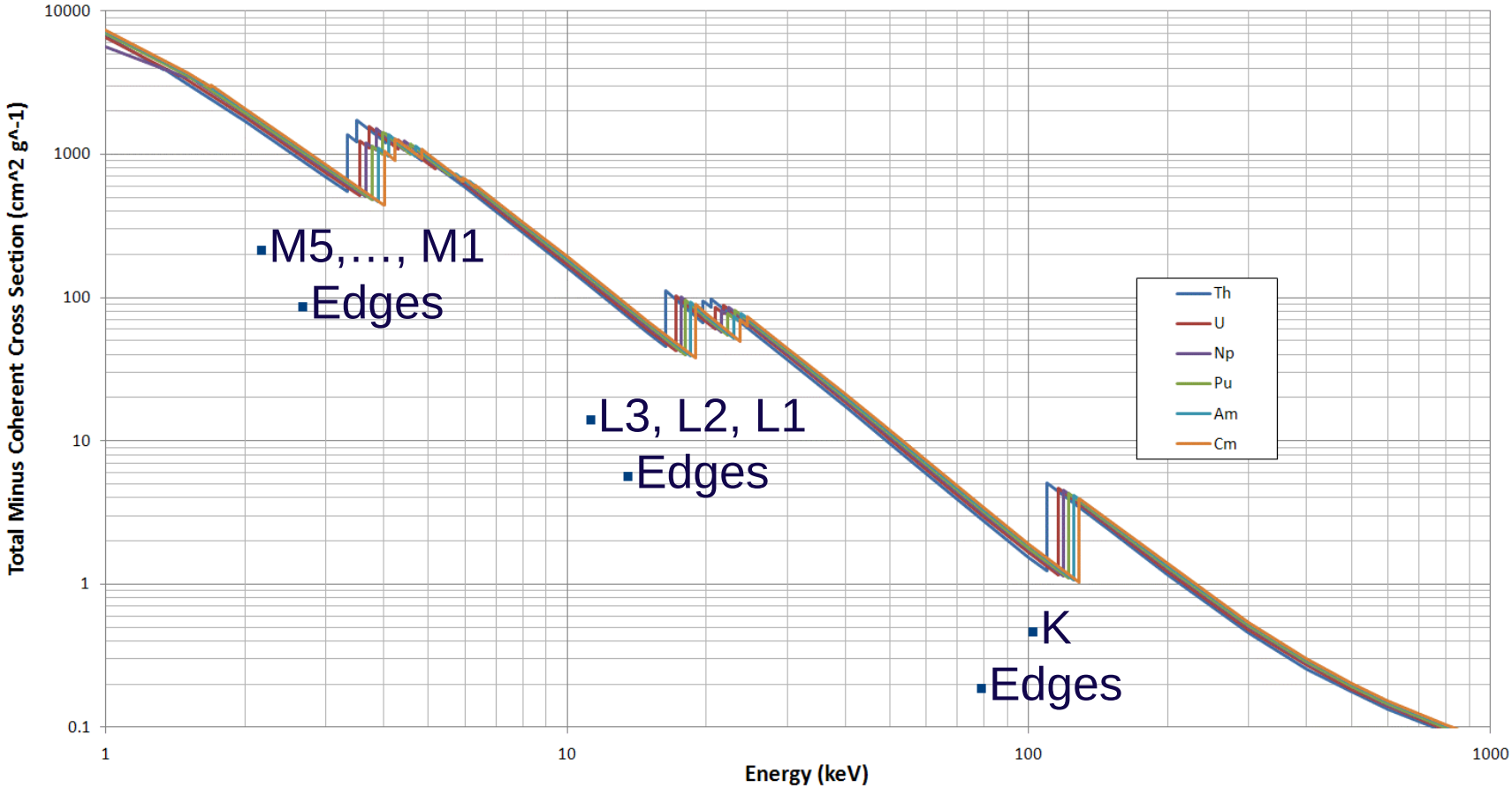
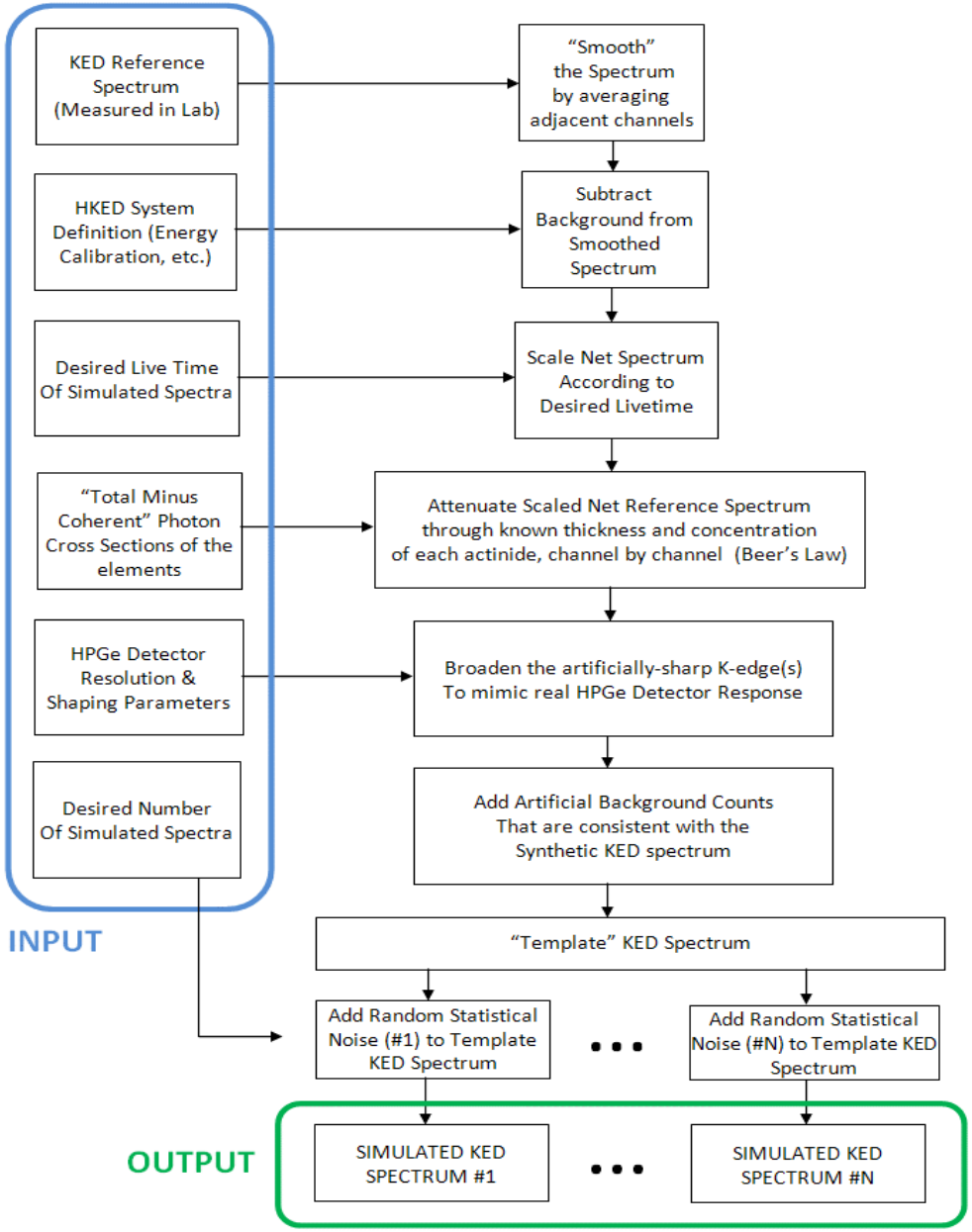
K-Edge Densitometry: Cast of Characters

(Mass Attenuation Coefficients of Th, U, Np, Pu, Am, Cm from Storm & Israel, 1970)



KED Simulation Information Flow



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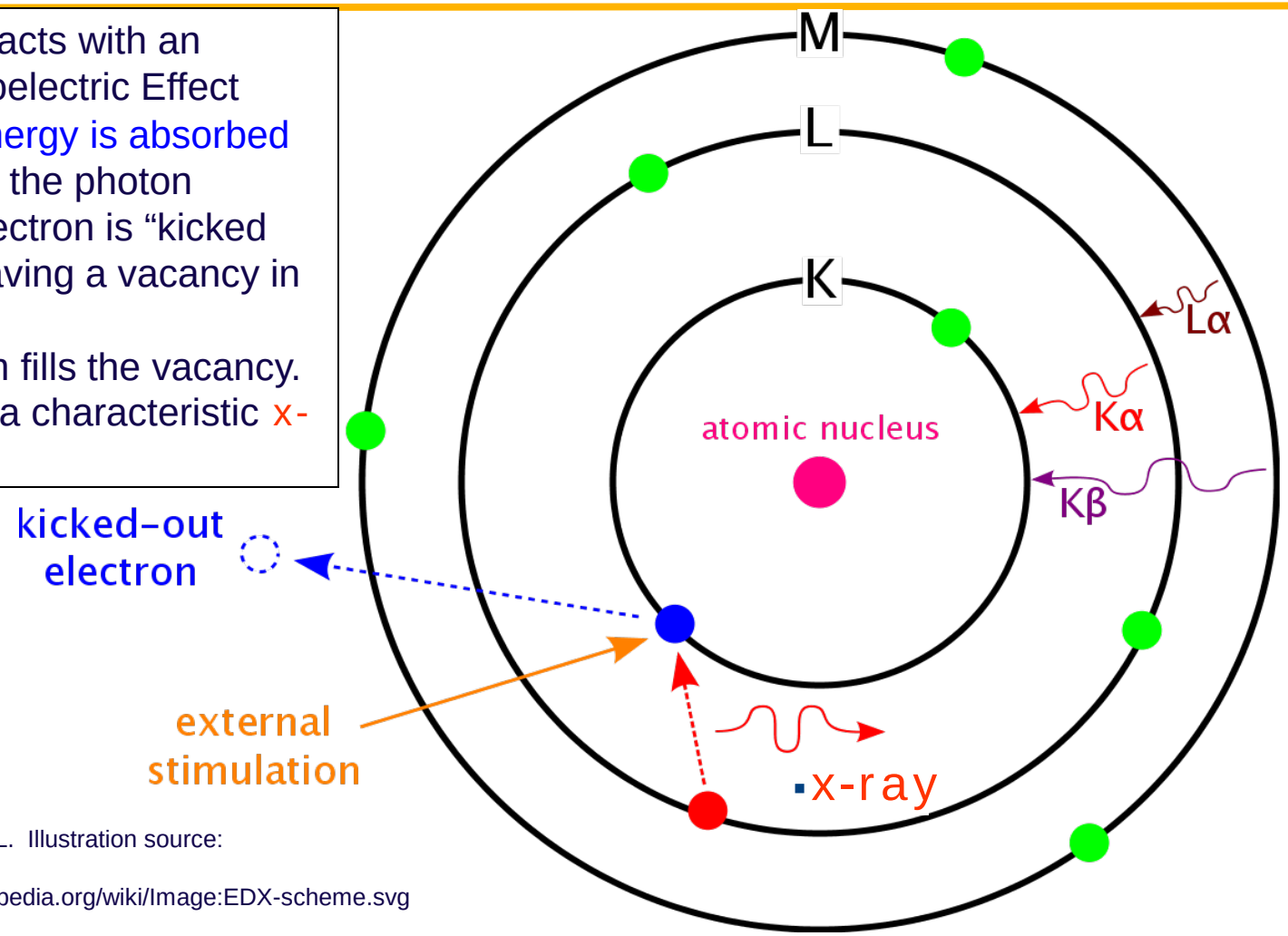
Energy-Dispersive X-Ray Fluorescence

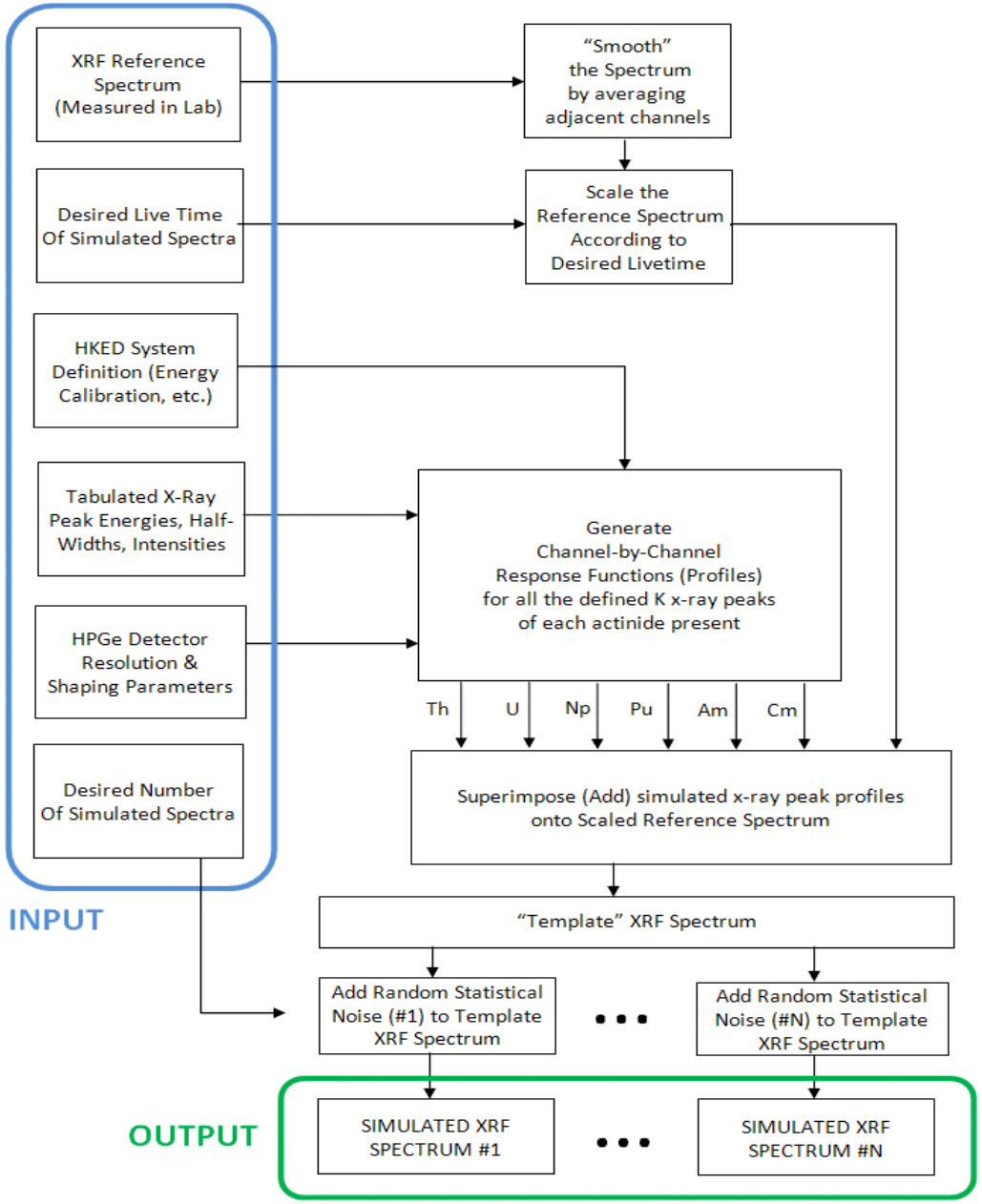
(1.) A photon interacts with an electron via Photoelectric Effect
(2.) The photon's energy is absorbed by the electron, and the photon disappears. The electron is "kicked out" of the atom, leaving a vacancy in its shell.
(3) Another electron fills the vacancy. That electron emits a characteristic x-ray photon



Text by LANL. Illustration source:

http://en.wikipedia.org/wiki/Image:EDX-scheme.svg

XRF Simulation Information Flow



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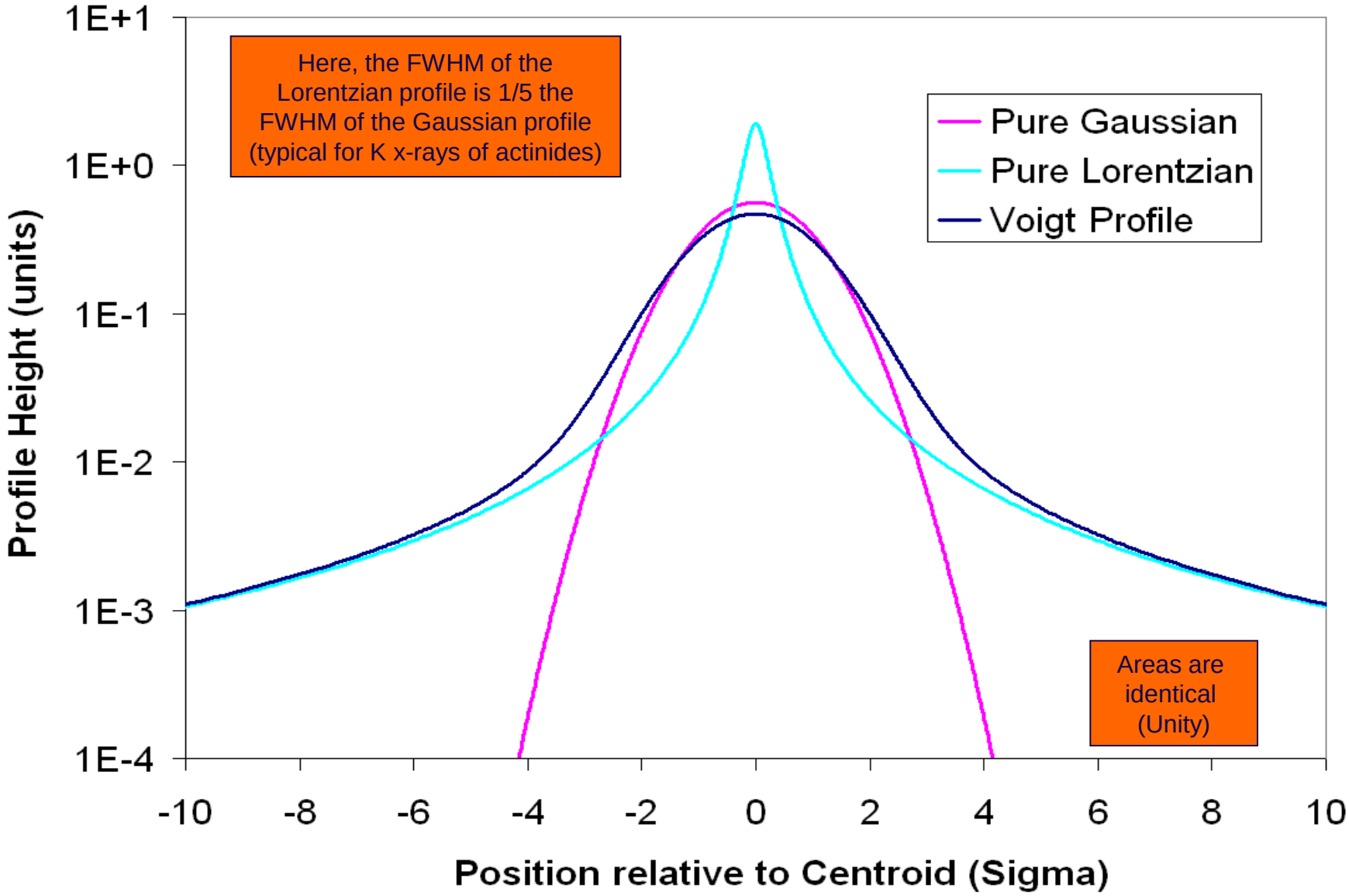
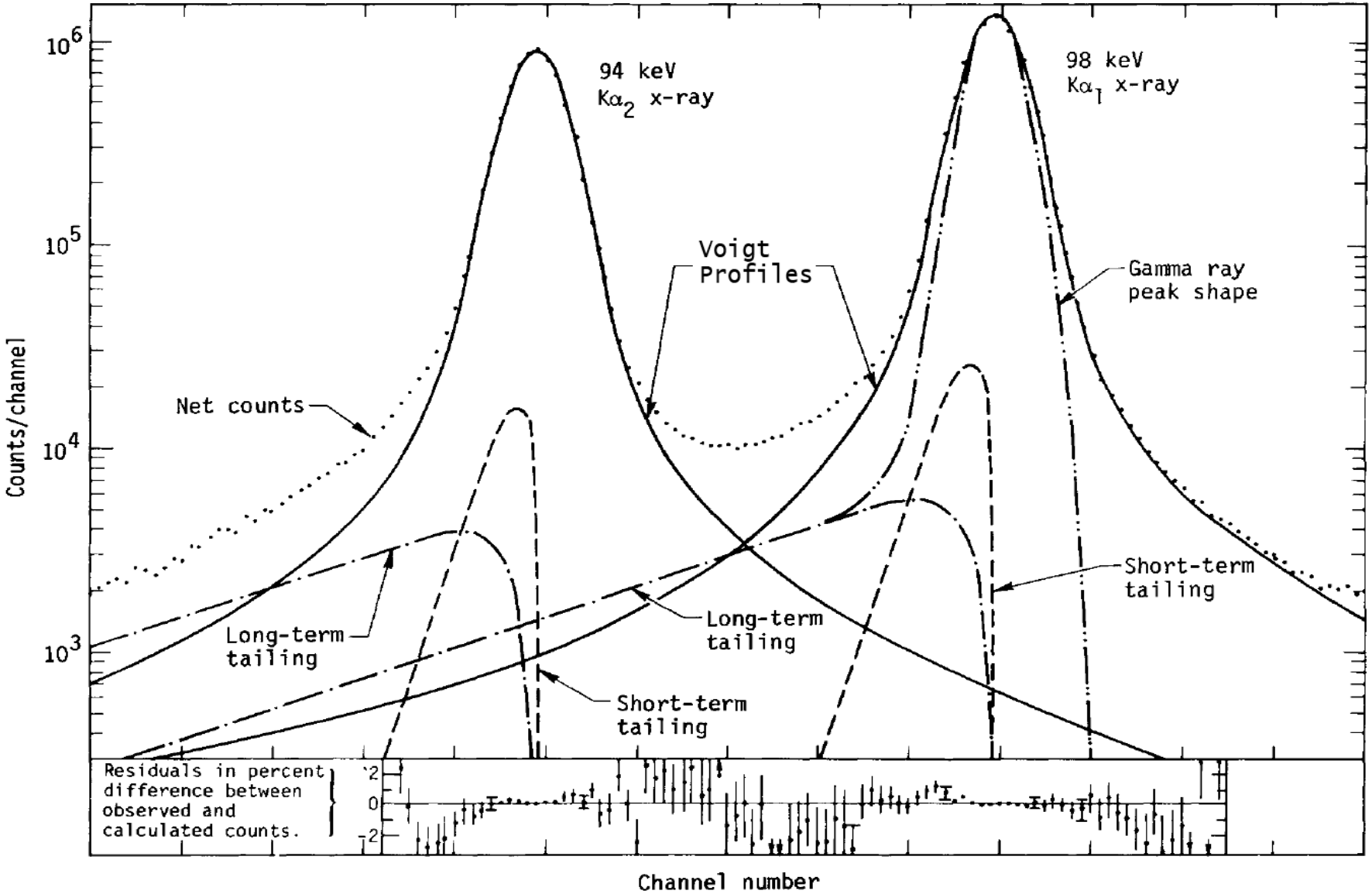
X-radiation is Lorentzian; the peak shapes are Voigtian

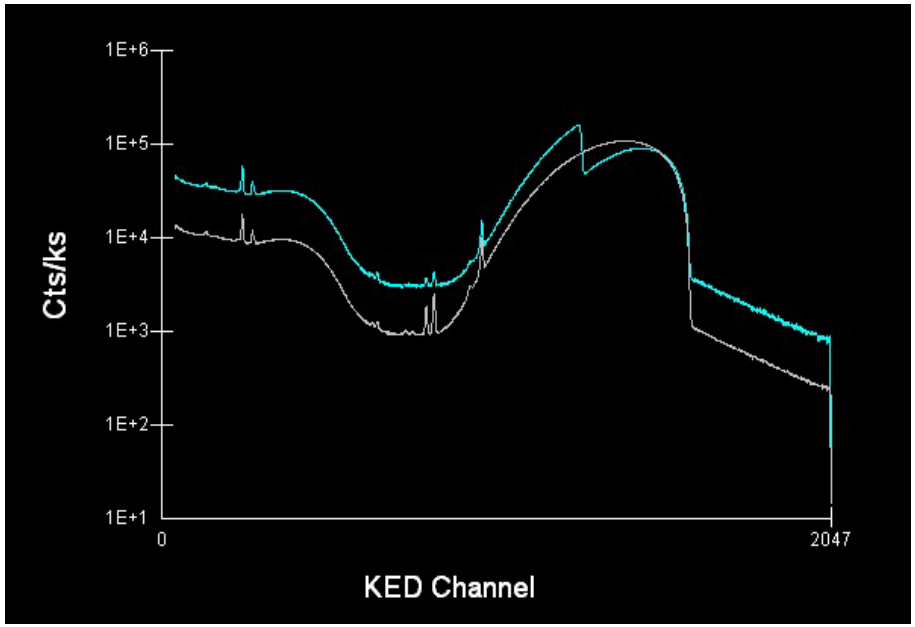


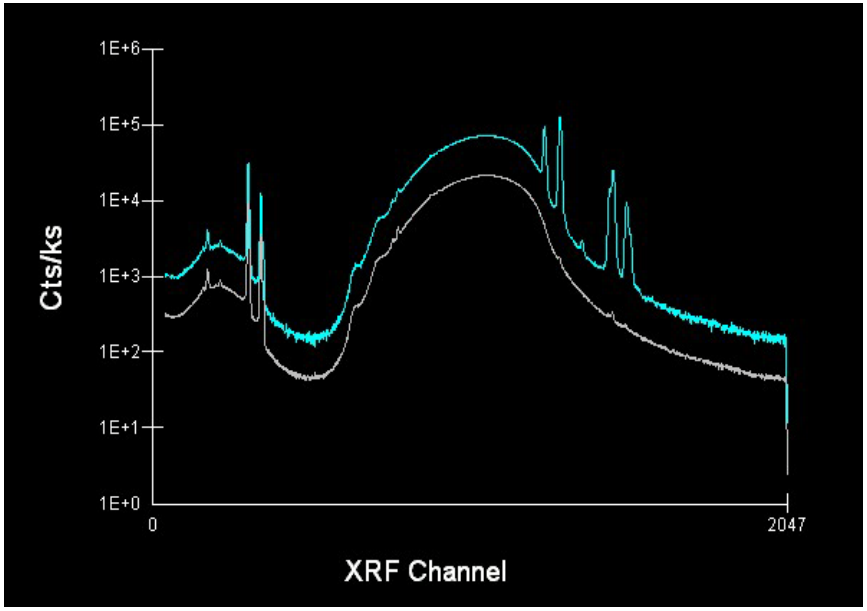
Response Function Profiles of XRF Peaks

Illustration from R. Gunnink, "An Algorithm for Fitting Lorentzian-Broadened, K-series X-ray Peaks of the Heavy Elements", NIM 143 (1977) p. 148, Figure 5.



Demonstration of SimHKED Module output in LANL HKED 2010





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Conclusions

- **Goals for FY2010 were met**
  - Sim Module for HKED
  - Report on Desired Features for MCNPX (INMM 2010 Baltimore)
  - Report on Module Development
- **SimHKED 2010 Module functionality was incorporated into LANL HKED 2010 software**
- **HKED Simulation is intended for Safeguards Performance Modeling in NEAMS**
- **Future work should integrate HKED Simulation and Analysis in "Batch Mode" or Black Box to make unified HKED Simulation Module**