Peak deconvolution for TXRF measurements

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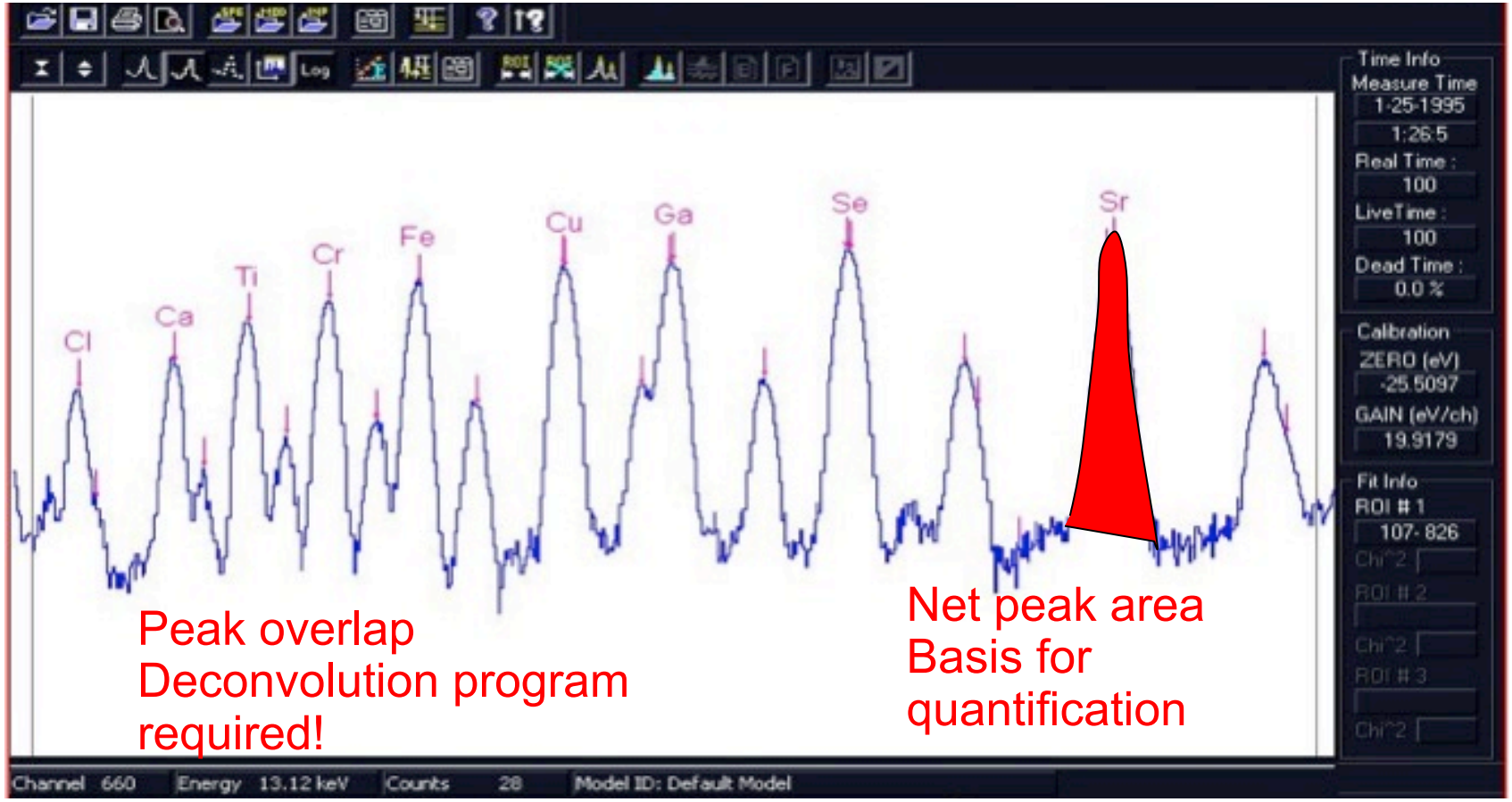
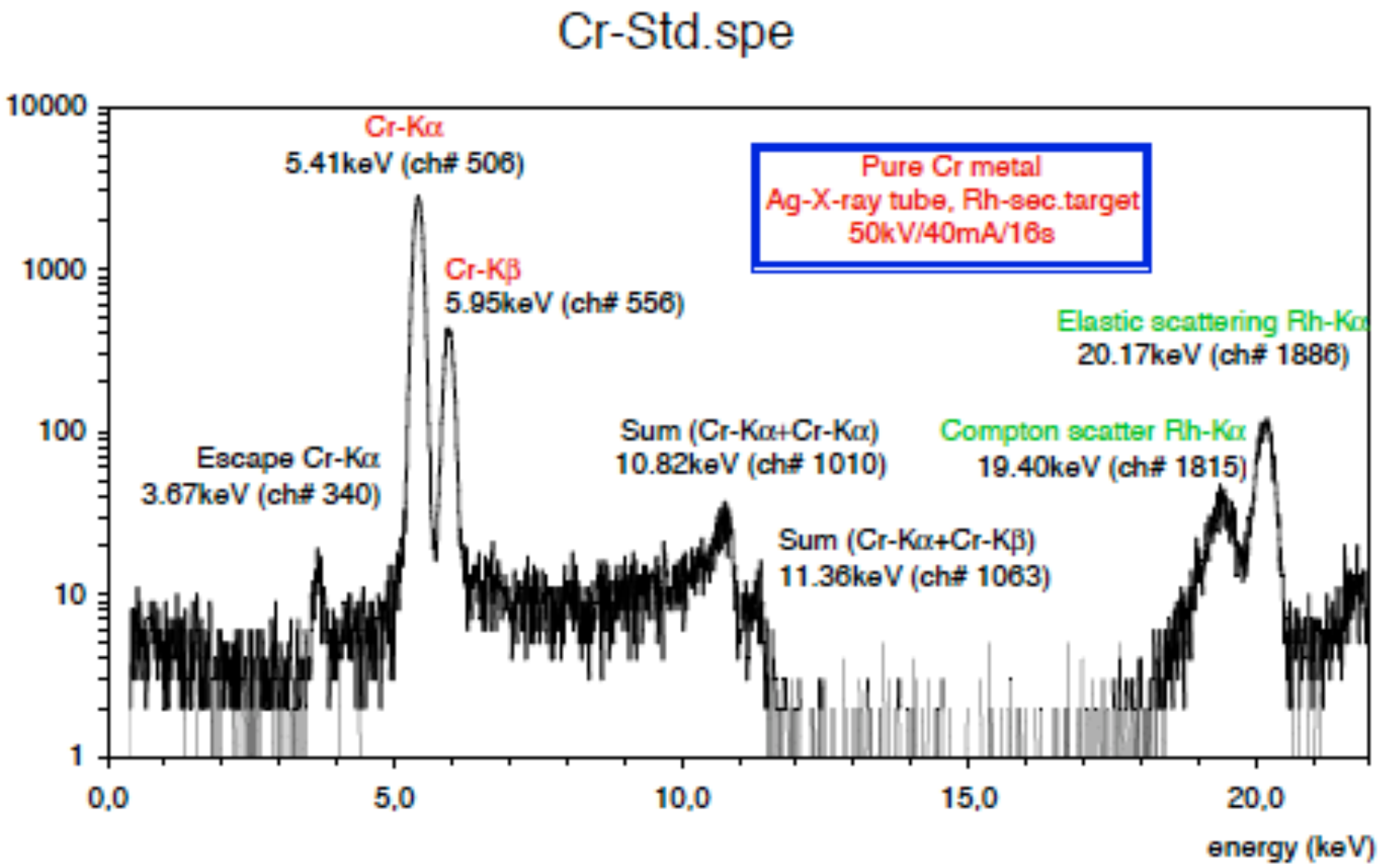
Enforce TXRF Training School 2022

Multielement spectrum



Escape & sum peaks



Peak resolution - ED

- The response function of a Si(Li)/SD detector is nearly Gaussian due the fact that Poisson statistics applies
- the natural line width is often neglected -> Voigt or Hypermet peak shape model
- The FWHM (**F**ull **W**idth at **H**alf **M**aximum) of a Gaussian peak is a function of the characteristic line energy *E* in (eV)
  - NOISE is the electronic contribution to the peak width (typically ~100 eV)
  - FANO is the Fano factor (typically ~0.115 for Silicon),

$$\mathrm{FWHM}(E) = \sqrt{NOISE^2 + 2.35 \cdot FANO \cdot E}$$

Freeware

- QXAS – developed and distributed by IAEA - ~1986
  https://nucleus.iaea.org/sites/nuclear-instrumentation/Software/Forms/AllItems.aspx
  + includes TXRF quantification module
  - DOS based -> requires emulator e.g. DOSBox, no further development, 8.3 filenames
- WinQXAS – developed under auspices and distributed by IAEA
  https://nucleus.iaea.org/sites/nuclear-instrumentation/Software/Forms/AllItems.aspx
  + Windows 32-bit program
  - setup needs some workarounds, no further development
- PyMCA – developed at the ESRF, open source
  http://pymca.sourceforge.net/index.html
  + active development, many options
  - no TXRF quantification, many options
- Detailed information on spectrum evaluation in the Handbook of X-ray Spectrometry:
  P. Van Espen; Chapter 4: Spectrum Evaluation; R. Van Grieken, A. Markowicz (Eds.), Handbook of X-ray Spectrometry, Marcel Dekker, New York (1993) 181-293.