UNDERSTANDING ENERGY RESOLUTION IN SOLID STATE DETECTORS

Energy resolution is one of the key parameters in a X-ray and gamma-ray spectrometers. This application note will answer two key questions:

1. What energy resolution should I expect, at a particular energy and under my operating conditions?
2. How can I optimize the energy resolution?

1) What energy resolution should I expect? What determines it?

In most cases, the energy resolution, δE, of a photopeak of energy E is approximately given by

$$(\delta E)^2 = K_F E + ENC^2 \qquad [1]$$

where *ENC* represents electronic noise and $K_F E$ represents statistical broadening.

The first term arises from quantum fluctuations in the charge generation process: even when X-rays deposit exactly the same amount of energy in a silicon detector, there will be fluctuations in the number of electron-hole pairs produced. This is a theoretical limit for any solid state detector. In silicon, $K_F E$ equals 119 eV FWHM at the 5.9 keV Mn K_α line and scales as the square root of energy.

The second term, *ENC*, is the input Equivalent Noise Charge. It is due to intrinsic noise in the detector and preamplifier: shot noise due to the detector's dark current, voltage noise from the input FET, etc. This electronic noise cannot be eliminated but its magnitude depends on many parameters: the pulse shaping amplifier's time constant, the detector temperature, the detector's capacitance, etc. There are many things one can do to reduce the noise to a minimum value. See section (3) for more details.

The two terms in Eqn. [1] really represent a lower limit to the energy resolution: additional factors will broaden the peak beyond this minimum. These two terms give rise to a purely Gaussian peak shape. In Si X-ray detectors and HPGe gamma-ray detectors, the observed resolution is usually quite close to that given by Eqn. [1] and the peaks are nearly Gaussian…but this is not always true!

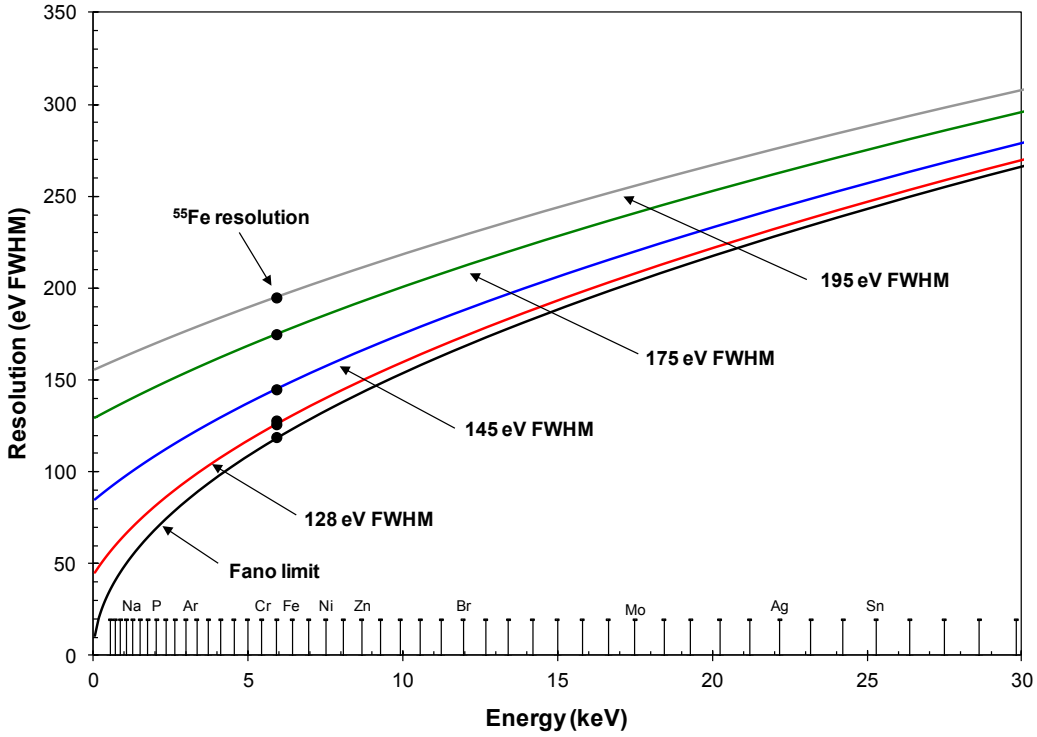
Other sources of resolution loss include electromagnetic interference, imperfect charge collection in the detector, ballistic deficit, and various others. These are discussed in section (4). In a Si X-ray detector, the other terms can be important when a system is not properly configured. In a CdTe X-ray detector, imperfect charge collection is often important, even dominant, even when a system is properly configured.

The X-rays emitted from a sample are not truly monoenergetic. This spreading does not contribute to the true resolution of the detector but may result in a peak which is broader than expected. This is discussed in section (5).

2) Energy resolution and X-ray energy for Si detectors

The energy resolution of an X-ray detector is usually specified at the 5.9 keV Mn K_α line. The plot and table below show how this value relates to the resolution at other energies, computed from [1]. The black curve shows Fano broadening only, i.e. the theoretical limit, given by Eqn. [1] with *ENC* equal to zero. The red curve shows the result when the resolution at 5.9 keV is 128 eV FWHM (i.e. for an SDD near optimum conditions) . It is quite close to the Fano limit, except at the lowest energies.

At low energies, the electronic noise dominates. This means that minimizing electronic noise is important when measuring low energies. At high energies, the statistical fluctuations dominate. Minimizing electronic noise is less important at high energy.



	Energy	Fano Limit	Resolution				
	keV	eV FWHM					
Noise		0.0	41.4	47.1	82.8	128.3	154.5
C	0.3	26.1	48.9	53.9	86.9	130.9	156.7
Mg	1.3	54.8	68.7	72.3	99.3	139.5	163.9
Al	1.5	59.8	72.7	76.2	102.2	141.6	165.7
Si	1.7	64.6	76.8	80.0	105.1	143.7	167.5
Ar	3.0	84.3	93.9	96.6	118.2	153.5	176.0
Ti	4.5	104.0	112.0	114.2	133.0	165.2	186.2
Cr	5.4	114.0	121.2	123.3	140.9	171.6	192.0
Mn	**5.9**	**119.0**	**126.0**	**128.0**	**145.0**	**175.0**	**195.0**
Fe	6.4	123.9	130.7	132.6	149.1	178.4	198.1
Ni	7.5	134.0	140.2	142.0	157.5	185.5	204.5
Cu	8.1	139.0	145.0	146.8	161.8	189.2	207.8
Zn	8.6	144.0	149.8	151.5	166.1	192.9	211.2
Zr	15.8	194.6	198.9	200.2	211.5	233.1	248.4
Mo	17.5	204.8	209.0	210.2	221.0	241.7	256.6
Rh	20.2	220.2	224.1	225.2	235.3	254.9	269.0
Pd	21.2	225.5	229.2	230.3	240.2	259.4	273.3
Ag	22.2	230.6	234.3	235.4	245.1	263.9	277.6
Cd	23.2	235.8	239.4	240.5	250.0	268.5	281.9
In	24.2	241.1	244.6	245.6	254.9	273.1	286.3
Sn	25.3	246.3	249.7	250.7	259.8	277.7	290.7

Table 1. Resolution at common X-ray energies. Find the Mn row in the above table and locate the resolution of the detector (bold). The column with that resolution lists the resolutions of that detector for these comon energies. A detector specified as 145 eV FWHM at the Mn K_α line will have a resolution of 102 eV FWHM for the Al K_α line (1.49 keV) and 221 eV FWHM at 17.5 keV (Mo K_α line)

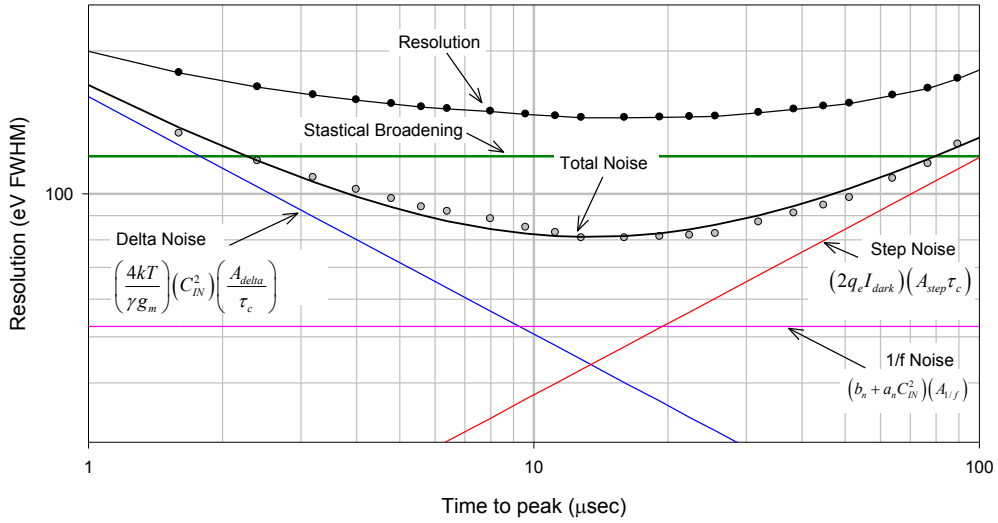
3) Energy resolution and electronic noise

The magnitude of Fano broadening is a theoretical limit; there is nothing a user can do to change it. Electronic noise, on the other hand, depends strongly on the detector which was selected and the system configuration, specifically detector temperature, peaking time, and pulse shaping. You can make the intrinsic much better or much worse by how you operate the spectrometer.

Quantitatively, the magnitude of intrinsic noise is given by

$$ENC^2 = \left(2q_e I_{dark}\right)\left(A_{step}\tau_c\right) + \left(b_n + a_n C_{IN}^2\right)\left(A_{1/f}\right) + \left(\frac{4kT}{\gamma g_m}\right) C_{IN}^2 \left(\frac{A_{delta}}{\tau_c}\right) \qquad [3]$$

where τ_c is the time constant of the shaping amplifier, I_{dark} is the dark current through the detector, C_{IN} is the preamplifier's input capacitance, T is the FET temperature, k is the Boltzmann constant, g_m is the FET's transconductance, γ characterizes the FET's thermal noise, b_n and a_n characterize low frequency (or 1/f noise), and A_{step}, $A_{1/f}$, and A_{delta} characterize the noise filtering properties of the shaping amplifier. The figure below shows noise versus peaking time for a typical detector.



Plot showing the energy resolution of a Si detector versus peaking time, showing the components to the resolution: statistical broadening (a.k.a. Fano limit) and noise, including delta noise, 1/f noise, and step noise.

Equation [3] may seem complicated but there are a few key points:

1. **The noise depends strongly on the peaking time.** There is an optimum peaking time (the noise corner) at which the noise is minimal, where the step and delta noise contributions are equal. If one uses a shorter peaking time, there will be more electronic noise. Resolution will be degraded, but if the statistical fluctuations dominate, the total resolution loss may not be significant. Shorter peaking times permit one to operate at a higher count rate and still maintain a low dead time fraction. In most practical applications of XRF, the best system performance (defined as the precision and accuracy of the analytical results) are found at peaking time shorter than the noise corner, at higher count rates. But the optimum depends strongly on the spectrum and on the analysis algorithms.
2. **The noise increases with detector area.** In a planar Si-PIN detector, C_{IN} scales with area: larger area detectors are more sensitive but have more delta noise. In a SDD, C_{IN} is much smaller than in the Si-PIN and is independent of detector area. The reduced delta noise is the primary advantage

of an SDD: it yields lower noise at the corner and much lower noise at short peaking times, allowing higher count rates while maintaining good energy resolution. The 1/f noise also has a component proportional to C_{IN}. The dark current increases with detector volume so also increases for large area detectors, for both SiPIN and SDD. Clearly, small detectors will yield lower noise.

3. **The noise increases with detector temperature.** The delta noise in [3] is proportional to $\sqrt{T}$ so change slowly for normal operation. However, the dark current is an exponential function of temperature, so step noise changes rapidly with detector temperature. The plot below shows typical results. At elevated temperatures, the noise corner shifts to shorter peaking times. At the noise corner, where resolution is best, the change with temperature is clear. At short peaking times (which is usually optimal from a system perspective, including count rate effects), the noise increase slightly with temperature, and so the total resolution changes little.

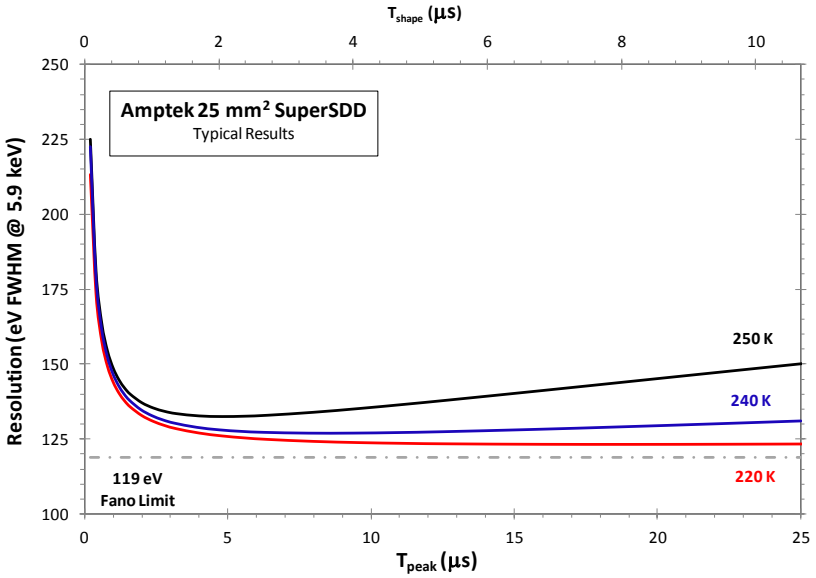


Figure 1. Plot showing the energy resolution, at the 5.9 keV Mn K_α line, for a typical SDD detector versus peaking time at three temperatures.

4) Other factors which may affect the energy resolution

Electromagnetic Interference

Electromagnetic interference commonly degrades the energy resolution. It is not present in a properly configured system but is a very common problem. The electronic noise given in equation [3] is intrinsic noise, irreducible fluctuations in the current through the components in the detector and preamplifier, e.g. shot noise through the detector. Interference or extrinsic noise arises when energy outside the circuit couples into the circuit. It is a common problem in X-ray spectroscopy: the signals, pulses of a few thousand electrons, are quite small, so small ground currents or induced currents can be important. Interference has a few key characteristics which separate it from intrinsic noise:

- The intrinsic noise sources in [3] are all broadband, either white or pink, while interference is usually narrowband. It occurs at a specific frequency, the frequency of the source. If one measures noise vs peaking time, then instead of the curve of **Error! Reference source not found.**, it will peak at a shaping time comparable to the inverse of the frequency. If one observes the pulses on an oscilloscope, the periodicity can be distinguished from the broadband intrinsic noise.

- The peaks are not Gaussian. If the broadening due to interference is larger than the intrinsic noise, one actually measures double peaks. If it is smaller, one may see a flat top or something similar.
- Interference noise goes away when you turn off the source. This may seem obvious but is an important clue in identifying and solving interference problems.

In addition to electromagnetic interference, high frequency acoustic vibrations can into a detector and preamplifier and lead to noise. If your detector has a resolution significantly different from that due to Fano broadening and intrinsic noise, then interference is a likely culprit.

Charge collection, ballistic deficit, and related effects

There are many higher order effects which complicate this simple picture. Some higher order effects add to the spectral background, adding peaks or a continuum. These lead to a complicated detector response function but, if they do not affect the photopeak, are not considered to impact the energy resolution. Some of these higher order effects distort the primary photopeak shape and thus affect the resolution.

For example, in a Si detector, near the detector's surface there will be a region where the field is weak. The carriers move slowly through this region and some are trapped. The trapped carriers do not contribute to the signal, thus *Q* is less than expected, resulting in a pulse height deficit. This causes counts on the lower energy portion of the photopeak, i.e. a non-Gaussian shape, though it rarely affects the FWHM. In a CdTe detector, trapping occurs throughout the volume, also leading to a low energy tail. In CdTe, this tailing is more important at high energies (where the X-rays interact throughout the detector volume) and is significant enough to affect FWHM. This is discussed in a separate application note.

As another example, if the charge collection time is longer than the flat top of the shaped pulse, a pulse height deficit results. This also leads to a low energy tail, i.e. a non-Gaussian photopeak shape and can degrade the FWHM.

As a third example, there can be regions near the boundaries of a detector where charges are trapped or collection is slow. This leads to incomplete charge collection and/or ballistic deficit and thus to a low energy tail. These effects are negligible in a properly configured Amptek Si detector but are not zero.

5) Other factors which may affect the peak width

X-ray characteristic X-ray intrinsic resolution

X-ray emission lines are not monoenergetic. Characteristic X-rays are produced when an atom in an excited state decays to the ground state. Because these states have finite lifetimes, there is a nonzero width to the atomic energy levels and hence a distribution in the energy of the emitted X-rays. The intrinsic width is not important at low energies but can be important for higher Z elements: the Cd $K_{\alpha 2}$ line at 7.45 keV has an intrinsic width of only 2 eV, but the U $K_{\alpha 2}$ line at 94.65 keV has an intrinsic width of 105 eV. Moreover, the energy distribution of the emitted X-rays is not Gaussian but Lorentzian so have a relatively wide tail.

Closely spaced peaks

Closely spaced peaks have caused some users to erroneously report a poor resolution. The K_{α} line is actually the sum of two lines. For Mn, the two K_{α} lines are 12 eV apart, which is negligible. For Pb, the K_{α} lines are 2.16 keV apart so are separately resolved for many detectors. For Ag, they are 22.162 and 21.988 keV, 174 eV apart. The Fano broadening is 232 eV, so the two peaks are not resolvable (one sees a single peak) but they are far enough apart that the resulting peak is wider than 232 eV FWHM and is not Gaussian. The plot belows computed individual $K_{\alpha 1}$ and $K_{\alpha 2}$ peaks (in red and green), the computed sum (in blue), and a measured Ag K_{α} photopeak. The individual peaks have widths described by **Error! Reference**

source not found., but the sum peak is wider than either individual peak. This problem usually occurs when a customer has been using a detector with poor resolution, so that the peak spacing is negligible relative to detector resolution, and then obtains a detector with much better resolution.

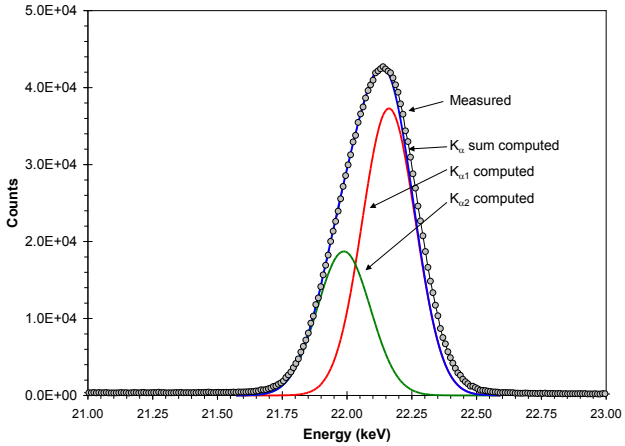
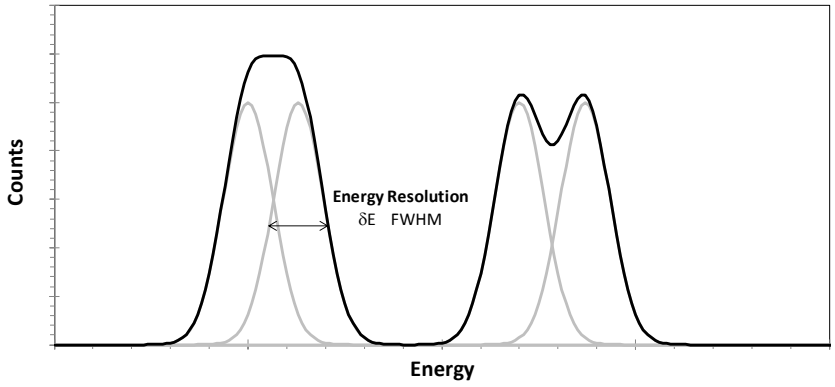


Figure 2. Plot showing an Ag K_α peak. The red and green curves show computed $K_{\alpha1}$ and $K_{\alpha2}$ peak, with resolution from **Error! Reference source not found.**. The blue curve shows the sum, with a resolution worse than either. The black circles show the measured photopeak.

6) What is "energy resolution" and why does it matter?

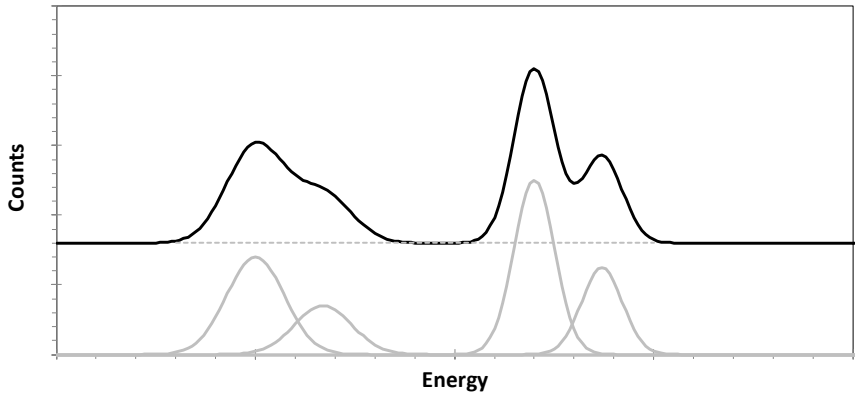
Energy resolution (δE) of a photopeak is generally defined as the full width at half maximum (FWHM) of that peak. It is important because, two peaks which are separated by more than the FWHM will show a small dip between them, i.e. they can be resolved. In the sketch below, two separate peaks (gray) are separated by slightly less than the FWHM on the left and by slightly more on the right. For a Gaussian photopeak, the FWHM equals 2.35 times σ, the rms fluctuation.



Some users think that, when peaks are closer than the FWHM thus forming a single broad peak as shown above, they cannot be analyzed. But this is not the case: one can fit such a peak as the sum of two separate peaks and obtain quantitative analytical results. The precision, accuracy, and detection limits are degraded when peaks are closer than the FWHM but quantitative results can still be obtained.

A system with a good energy resolution has two advantages over a system with poor resolution: (1) the peak to background ratio will be better and (2) closely space peaks overlap less. The plots below sketch show two peaks, with the same total counts and background, measured with poor energy resolution (left) and better (right). On the left, because the peaks are spread over more channels, there are more background counts, and this degrades the precision. On the left, because the peaks overlap more, the

computed intensities depend more strongly on the deconvolution algorithm. This typically degrades both the precision and the accuracy of the analytical result.



All other things being equal, better resolution leads to better precision and accuracy. But all other things are not typically equal: to improve energy resolution usually requires lower count rates, more cooling, or a different detector. In many cases, one can improve the precision and accuracy more by improving count rates than resolution. In some cases, if background and overlap are unimportant, then the resolution is unimportant. Although resolution is often stressed as a goal it is not always the most important factor. Some examples of the trade-offs are discussed in ref [1].