

Spectral resolution of X-ray CCDs

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1 X-ray spectroscopy with CCDs

Photon counting CCDs can be used for X-ray spectroscopy in the absence of any dispersive elements such as a grism or grating. When a high energy (keV) photon is incident on a semiconductor device with a small bandgap (\approx eV), a high energy “primary” photoelectron is ejected. This primary electron ejects multiple other secondary photoelectrons through branching processes such as collisions and lattice-interactions. The number of photoelectrons generated (“yield”) can be used as a proxy for the energy of the incident photon. As the branching processes involved are probabilistic, the yield follows a distribution. The variance of the yield sets the energy-resolution of the detector. It is worth noting that lower energy (\sim eV) optical photons produce only a single photoelectron.

2 Simplified statistical model

This model was originally worked out by [Fano \(1947\)](#). Assume a photon of energy V_0 is incident on a semiconductor. This liberates a photoelectron with energy V_0 (approximately). The problem at hand is to compute the distribution of the number of ionisations this particle generates while losing the fixed amount of energy V_0 . The mean number of ionisations generated in this process is $J_0 = V_0/\epsilon$, where ϵ is defined as the average energy lost in generating a single ionisation pair.

Assume this particle loses energy V generating J ionisations in the process as it travels a distance l . Then, in the next Δl distance, it generates $\Delta J = (V_0 - V)/\epsilon$ ionisations. The total fluctuations in J are given by $J + \Delta J - J_0 = J - V/\epsilon$.

We can assume that the photoelectrons are produced in a group of N successive impacts (collisions). If n_p and E_p are the number of ionizations and the energy loss at the p -th impact, we can write $J = \sum_{p=1}^N n_p$, $V = \sum_{p=1}^N E_p$. Assuming all impacts are independent of each other, n_p and E_p are random independent variables with mean values \bar{n} and \bar{E} respectively. The average ionisation energy is then $\epsilon = \bar{E}/\bar{n}$.

The variance in J is given by $\langle (J - V/\epsilon)^2 \rangle = N \langle (n - E/\epsilon)^2 \rangle$. The number of impacts $N = V_0/\bar{E} = J_0/\bar{n}$. This gives

$$\langle (J - J_0)^2 \rangle = \langle (J - V/\epsilon)^2 \rangle = F J_0 \tag{1}$$

where

$$F = \frac{\langle (n - E/\epsilon)^2 \rangle}{\bar{n}} \quad (2)$$

is the Fano factor. If the number of ionisations at each impact were governed by a Poisson distribution, then $\langle (n - E/\epsilon)^2 \rangle = \bar{n}$ i.e $F = 1$ and $\langle (J - J_0)^2 \rangle = J_0$. However, collision processes that give rise to each ionisation are not purely independent. For example, a single collision could excite an electron into a higher atomic energy level rather than ionising it. This can be followed by a different collision of lower energy that is now capable of generating an ionised pair. This makes the variance lower than what we would expect in the purely Poisson case.

Eq. 2 does not make any assumptions about the processes that occur on molecular scales. Actual physical constants such as the relevant collisional cross-sections are required to calculate the Fano factor using Eq. 2.

3 The Fano factor in semiconductors

Three important physical processes are modeled to calculate the Fano factor in semiconductors

- Photon absorption - The probability that the incident photon is absorbed by an atom depends on its energy. For instance, in Silicon there is a 92% probability of absorption of radiation > 1.84 keV by K-shell electrons.
- Atomic relaxation - The excited atom loses its energy through a series of Auger and fluorescence “cascade” processes.
- Electron energy loss - The ejected photoelectrons (primary and secondary) can lose their energy by one or more of the following mechanisms
 - Electron-phonon interaction
 - Valence band ionisation
 - Excitation of plasmons
 - core L-shell ionisation
 - core K-shell ionisation

These processes are probabilistic and best modeled using a Monte Carlo simulation such as in [Fraser et al. \(1994\)](#). This enables the calculation of the Fano factor (F) and the average ionisation energy (ϵ). Figure 1, taken from [Fraser et al. \(1994\)](#) shows the theoretically calculated values for ϵ and F. Both these quantities depend on the incident photon energy, ϵ ranges from 3.6-4.3 eV and F ranges from 0.14-0.18. These quantities also depend on the detector temperature. Experimentally measured values of ϵ range from 3.6 - 3.8 eV and those of F range from 0.08-0.17.

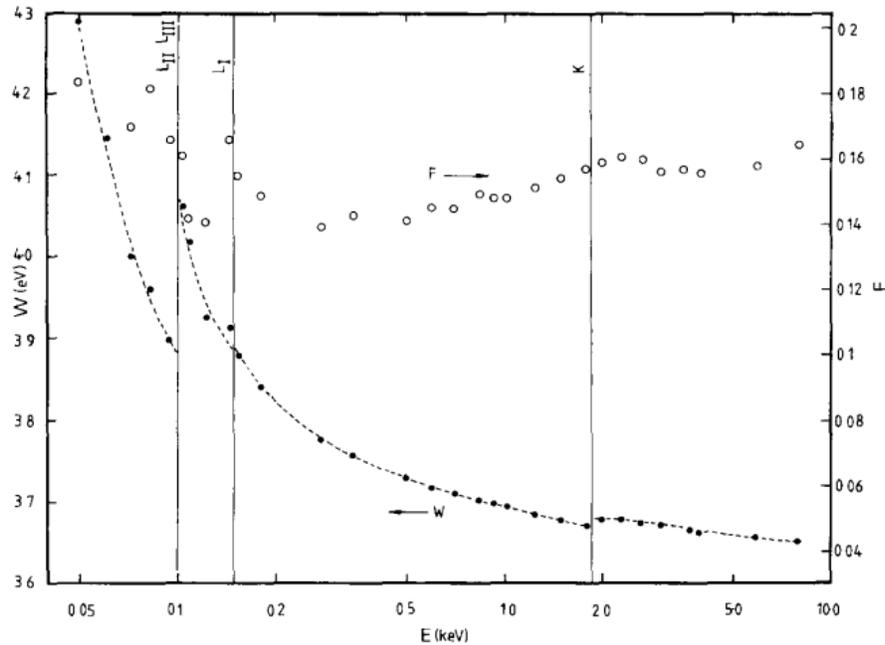


Figure 1: Variation of ionisation energy ϵ (W) and the Fano factor (F) as a function of energy. The breaks in the ionisation energy are caused due to resonant transitions of K and L band electrons. Image taken from (Fraser et al., 1994)

Alternatively, we can estimate the Fano factor by using the following approximate argument ¹. Given an incident energy is E_0 , assume there are N_x lattice interactions (producing phonons) and N_i ionisations (producing electrons). On average,

$$E_0 = E_i N_i + E_x N_x \quad (3)$$

where E_i is the energy required for a single ionisation and E_x is the energy required for a single lattice-phonon excitation. Assuming $E_x \ll E_i$, we can treat the phonon energy levels almost as a “continuum” compared to the electronic/atomic energy levels. The lattice excitations will obey an approximately Poisson distribution. The variance on N_x , $\sigma_x = \sqrt{N_x}$. As the total available energy is constant, $E_x \Delta N_x + E_i \Delta N_i = 0$. This means any fluctuations in energy deposition in one of the processes is balanced out by the fluctuations in the other. Thus, the variance in the energy allocated to the two processes on average will be equal i.e

$$\sigma_i E_i = \sigma_x E_x \quad (4)$$

Substituting from Eq. 3, we obtain

$$\sigma_i = \sqrt{\frac{E_0}{\epsilon}} \sqrt{\frac{E_x}{E_i} \left(\frac{\epsilon}{E_i} - 1 \right)} \quad (5)$$

where ϵ is the average total energy loss required to produce a single charge pair. It is important to understand the difference between ϵ and E_i . E_i is the energy required to create

¹Helmuth Spieler’s lecture on Introduction to Radiation Detectors and Electronics, 18-Mar-1999

a single electron-hole pair, and is equal to the semiconductor bandgap. ϵ is the total energy lost in the creation of a single charge pair, and can exceed E_i as some energy is also lost to lattice vibrations. As the total energy available is E_0 , the number of ionisations $N_i = E_0/\epsilon$. This gives

$$\sigma_i = \sqrt{FN_i} \quad (6)$$

where the Fano factor is

$$F = \frac{E_x}{E_i} \left(\frac{\epsilon}{E_i} - 1 \right) \quad (7)$$

For Silicon, using $E_x = 0.037$ eV, $E_i = 1.1$ eV and $\epsilon = 3.6$ eV, we get $F = 0.08$. The Fano factor for Germanium is also ≈ 0.1 .

4 Spectral Energy resolution of CCDs²

If an X-ray photon of energy E_γ is incident on a detector, the average number of photoelectrons generated is $N = E_\gamma/\epsilon$. The variance is $\sigma^2 = FN = F\frac{E_\gamma}{\epsilon}$. If the detector readout noise is σ_r , the total number of photoelectrons generated has a variance of $\sqrt{\sigma_r^2 + F\frac{E_\gamma}{\epsilon}}$. As the average energy per photoionisation is ϵ , the energy resolution is

$$\Delta E = 2.35\epsilon\sqrt{\sigma_r^2 + F\frac{E_\gamma}{\epsilon}} \quad (8)$$

The spectral resolution of the X-ray CCD is then $E/\Delta E$. The Fano-factor term depends solely on the detector material and temperature. The other term is the system readout noise. The readout noise depends on the readout frequency. Typical X-ray detectors have $\sigma_r = 3-5$ electrons (eg. 4.5 electrons RMS for XMM Newton). Figure 2 shows the dependence of the spectral resolution on incident photon energy, assuming a Si detector with $F = 0.115$ and $\epsilon = 3.65$ eV. These numbers are consistent with that of moderate spectral resolution instruments on missions like NICER, eROSITA and EPIC-MOS on XMM Newton. It is evident that the spectral resolution of photon counting CCDs is limited to $R < 100$. This resolution is enough to resolve elemental lines of Oxygen, Mg, Ti, Fe, etc. CCDs in the X-ray photon counting mode can thus be used as moderate resolution spectrographs.

In order to reach higher resolutions, the ‘‘dispersed X-ray spectroscopy’’ method is used. In this method, an energy-dispersive medium such as a diffraction grating is used. The resolution is then set by this grating, and the dispersed light is read out by an array of CCDs. Examples include the RGS instrument on XMM Newton (R200-800), HETG and LETG (R 30-2000) on Chandra.

References

U. Fano. Ionization Yield of Radiations. II. The Fluctuations of the Number of Ions. *Physical Review*, 72(1):26–29, July 1947. doi: 10.1103/PhysRev.72.26.

²A useful reference is the review on X-ray CCDs by Andrew Holland

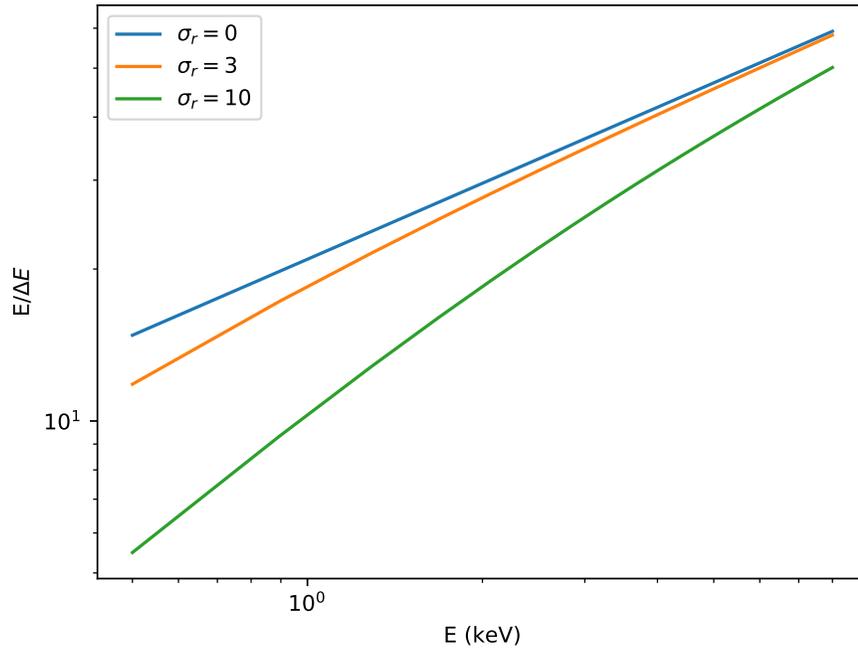


Figure 2: Spectral resolution of photon counting CCDs, for 3 different values of readout noise. This figure indicates that CCDs can be good moderate resolution spectrographs.

G. W. Fraser, A. F. Abbey, A. Holland, K. McCarthy, A. Owens, and A. Wells. The X-ray energy response of silicon Part A. Theory. *Nuclear Instruments and Methods in Physics Research A*, 350(1-2):368–378, Oct. 1994. doi: 10.1016/0168-9002(94)91185-1.