Temperature dependence of mean number of of e-h pairs per eV of x-ray energy deposit

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The conversion factor from ADU to e-h pairs in a CCD is commonly obtained using x-rays of known energy from a calibration source such as ^{55}Fe. Absolute quantum efficiency (QE) is obviously dependent upon this number, so its systematic uncertainty is one of the many encountered in trying to make an absolute measurement QE. The factor is usually given as $w = 3.65$ eV/e-h, but this is a room-temperature (300 K) value. It is dependent upon the silicon indirect bandgap energy, which increases significantly as the CCD is cooled. The room-temperature value is obviously not correct for CCD's operated at 130–170 K.

The conversion factor w has been measured for decades, usually at room temperature but sometimes at cryogenic temperatures. Values at 300 K have usually been in the 3.62–3.68 eV/e-h range. ICRU 31 (1979) [1] gives 3.68 ± 0.02 without references. In a recent paper Scholze *et al.* report 3.66 ± 0.03 [2]. Since there is no way to sensibly decide how to weigh the many results, we take these two as the more dependable and somewhat arbitrarily choose 3.67 ± 0.03 eV/e-h.

Measurements of w at cryogenic temperatures are sparse. Ryan [3] reports $w = 3.631$ eV/e-h at 300 K and 3.745 at 100 K. The EG&G Ortec catalog [4] gives 3.62 at room temperature and 3.72 at 80 K.

Both theoretically and experimentally, w can be represented by a linear function of the indirect bandgap energy, [5,6]

$$w = a\,E_g + b\ ,$$

which can conveniently be rewritten as

$$\Delta w\,(T) = w\,(T) - w\,(300\ \text{K}) = a\left[E_g\,(T) - E_g\,(300\ \text{K})\right]\ .$$

Varshi [7] proposed expressing the indirect bandgap energy E_g in silicon as a function of temperature T by *

$$E_g\,(T) = E_g\,(0) - \frac{\beta T^2}{T+\gamma}\ .$$

For silicon,

$$\begin{aligned} E_g\,(0) &= 1.1557\ \text{eV} \\ \beta &= 7.021\times 10^{-4}\ \text{eV/K} \\ \gamma &= 1108\ \text{K}\ . \end{aligned}$$

With these constants, $E_g(300\ \text{K}) = 1.1108$ eV. Many values very close to this, for example 1.12 eV (commonly) and 1.107 eV (Handbook of Chemistry and Physics) can be found.

Different papers—most demonstrating the linear behavior of $w(E_g)$—find surprisingly different values for a. b is of course is highly correlated with a, but since we are only interested in Δw, it doesn't matter much.

* His expression is a little more accessible in Refs. [8] and [9].

Table 1

Paper	Material	a	Plotted?	Δw (130 K)	Δw (170 K)	Comments
Klein 68 [5]	Many	14/5	Yes	0.099	0.081	Theory, fits data shown
Key 71 [10]	Si	2.80	No	0.099	0.081	^{241}Am 5.48 MeV α's
Canali 72 [11]	Si	2.15	No	0.076	0.062	^{241}Am 5.48 MeV α's
Ryan 73 [3]	Si	2.87 ± 0.07	Yes	0.101	0.083	Detector 1, ^{207}Bi γ's
	Si	2.77 ± 0.08	Yes	0.098	0.080	Detector 3, ^{207}Bi γ's
	Si	1.83 ± 0.08	No			Detector 1, ^{241}Am α's
	Si	1.77 ± 0.08	No			Detector 3, ^{241}Am α's
Alig 80 [6]	Many	2.73	No			Claimed from Klein (68) [5]
		1.6	No		1.89	Their calc., text, section III C
		2.12	Yes	0.075	0.061	My fit to data they show

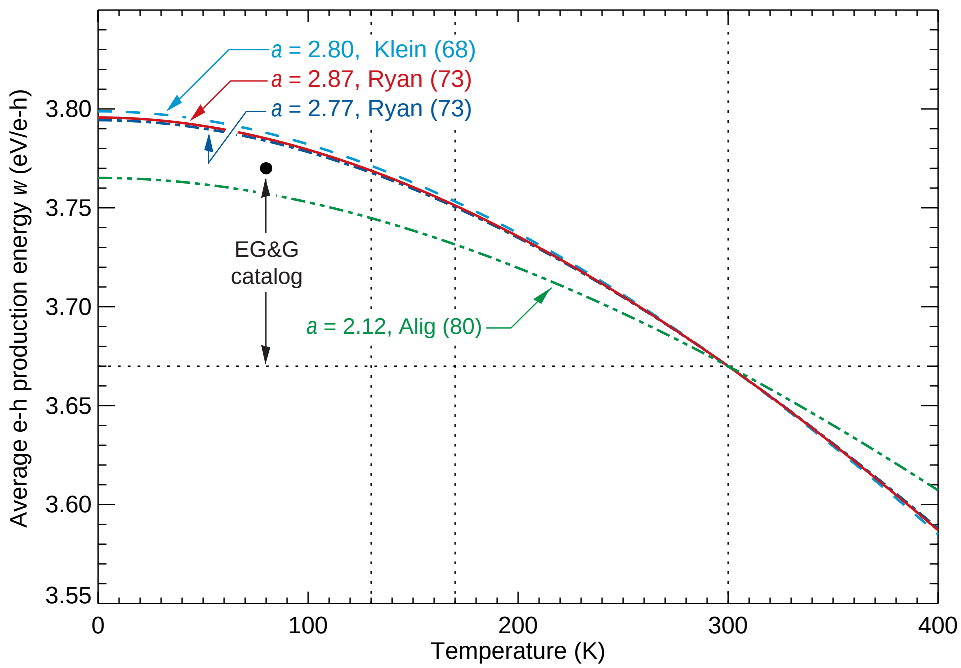

Figure 1. $w(T)$ for selected values of a.

A list of values for the coefficient a is given in Table 1. In some cases [5,6] a survey of room-temperature bandgap energies spanning 0.7–5.5 eV were used. In the case of silicon, data were obtained as a function of temperature for ($T \leq 300$ K). Measurements were obtained by exposing a Si(Li) detector to either a ^{207}Bi γ-ray source or to a ^{241}Am α-particle source. While it was first thought that the detector response should be the same, this is not the case. The mechanism is not understood. Part of it is probably recombination in the relatively long time it takes the very highly ionized column to disperse; to the extent this is true the unreported conductivity of the silicon is at play.

Nor are the results using γ- or α-sources consistent among themselves. As can be seen from the Table, $2.12 \leq a \leq 2.87$ for γ (or, equivalently, electron) irradiation and $1.77 \leq a \leq 2.80$ for α's. Figure 1 shows $w(t)$ for the cases marked as "Plotted" in the Table.

Experiments by Dodge *et al.* (66) [12] showed that w was constant to within about 0.02% for 6–77 K, which is more or less consistent with the slowly varying behavior of E_g in this range.

A 1994 EG&G-Ortec catalog [4] suggests $w(300\ \mathrm{K}) = 3.62$ eV and $w(80\ \mathrm{K}) = 3.72$ eV, or $\Delta w(77\ \mathrm{K} = 0.10$ eV/e-h. References are not given. The value $w(77) = 3.67 + 0.10$ is shown in the Figure.

A curious 1968 paper [13] by a Lawrence Berkeley Lab group presents beautiful data indicating a *linear* dependence of $w(T)$ on temperature. This result is at variance with everything else in the literature, and we have been unable to find the resolution that must have occurred.

The situation is less than satisfactory, but it is probably safe to say $2.12 \leq a \leq 2.80$ for x-rays, γ's, and electrons incident on silicon. This reflect into $\Delta w = 0.075$ to 0.099 eV/e-h at 140 K and $\Delta w = 0.061$ to 0.081 eV/e-h at 170 K, the temperature range appropriate to CCD's used in astronomy. This is about a 2% effect if γ- or x-ray emitting radioactive sources are used, large enough to produce a significant systematic error in absolue quantum efficiency.

In conclusion: Based upon data presently available, I recommend $w = 3.76$ eV/e-h at -140° C and $w = 3.74$ eV/e-h at -100° C.

I thank Chris Bebek for suggesting the method and many of the references.

1. ICRU Report 31, "Average Energy Required to Produce an Ion Pair," (1979).
2. F. Scholze, H. Rabus, & G. Ulm, J. App. Phys. **84**, 2926–2939 (1998); F. Scholze, H. Henneken, P. Kuschnerus, H. Rabus, & G. Ulm, Nucl. Instrum. Methods **A439**, 208–215 (2000);.
3. R. D. Ryan, IEEE Trans. Nucl. Sci. **NS-20**, no. 1, 473–480, Feb. 1973.
4. EG&G Ortec, "Modular Pulse-Processing Electronics and Semiconductor Radiation Detectors," #95 (November 1994).
5. C. A. Klein, J. Appl. Phys. **39**, 2029 (1968).
6. R. C. Alig, S. Bloom, & C. W. Struck, Phys. Rev. **B22**, 5565–5582 (1980).
7. Y. P. Varshni, Physica **34**, 149 (1967).
8. K. Rajkanan, R. Singh, & J. Schewchun, Solid-State Elec. 22, 793–795, (1979).
9. S. M. Sze, *Physics of Semiconductor Devices*, John Wiley & Sons, (1969).
10. J. R. Key & T. A. Rabson, IEEE Trans. Nucl. Sci. **NS-18**, no. 1, 473–480, 1971.
11. G. Canali *et al.*, IEEE Trans. Nucl. Sci. **NS-19**, no. 4, 9–19, Aug. 1972.
12. R. W. Dodge, S. R. Domen, T. F. Leedy, & D. M. Skopik, Phys. Rev. Lett. **17**, 653 (1966).
13. R. H. Pehl, F. S. Goulding, D. A. Landis, & M. Lenzlinger, Nucl. Instrum. Meth. **59** (1968).