Average energy expended per e-h pair for germanium-based dark matter experiments

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ABSTRACT: We report a new method, which allows us to derive the temperature dependence of the average energy expended per electron-hole (e-h) pair, $\varepsilon$, for germanium detectors. Applying energy partition mechanism in ionization for a given energy deposition, the Fano factor and the value of $\varepsilon$ can be determined separately. Subsequently, we illustrate the variation of $\varepsilon$ as a function of temperature. The impact of $\varepsilon$ on the energy threshold for germanium detectors at a given temperature is evaluated.

KEYWORDS: Cryogenic detectors; Dark Matter detectors (WIMPs, axions, etc.); Detector modelling and simulations I (interaction of radiation with matter, interaction of photons with matter, interaction of hadrons with matter, etc); Ionization and excitation processes

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1 Introduction

Many galactic observations indicate a large fraction (∼85%) of the total matter in the Universe is dark matter [1–4]. The most compelling candidate for dark matter particles is the WIMP (Weakly Interacting Massive Particle), which is believed to interact through the weak force and gravity. Therefore, the interaction cross section with ordinary matter is extremely small. One of the ways to detect WIMPs is to measure the recoil energy of a nucleus from a WIMP-nucleus collision in a detector, either directly or indirectly, which will give an estimate of the mass of the incoming WIMPs [5].

In the direct detection of WIMPs, the value of the average energy expended per electron-hole (e-h) pair, $\varepsilon$, is critical to the determination of both energy threshold and energy scale for a germanium (Ge) detector. The charge collected by a Ge detector, $Q_c$, is proportional to the number of e-h pairs, $N_i$, generated by an incident particle [6], 

$$Q_c = aeN_i = ae\varepsilon,$$

where $a$ is the charge collection efficiency, $e$ is the elementary charge, $E$ is the energy deposition, and $\varepsilon = 2.2E_g + rE_R$ [6, 7] with $E_g$ the band gap energy, $E_R$ the Raman energy (the highest optical phonon energy in Raman vibration) and $r = \frac{L_i}{L_x}$ ($L_i$ and $L_x$ are mean free path between ionizing collisions and between phonon collisions, respectively). Since there is temperature dependence in $E_g$ [6, 8–10] and $r$ [6], $\varepsilon$ is dependent on temperature as well. The temperature-dependent $\varepsilon$ has been widely studied in the literature [6, 7, 11–14], from which $\varepsilon$ was accurately measured to be ∼3 eV at 77 Kelvin. However, there are no direct measurements for the value of $\varepsilon$ when the temperature decreases to the milli-Kelvin range, which is the operating temperature for a bolometer-type detector. Therefore, measuring $\varepsilon$ at the milli-Kelvin range is needed for a bolometer-type detector since its nuclear recoil energy threshold is directly determined by a given value of $\varepsilon$ [15]. It is quite difficult for a bolometer-type detector to measure the value of $\varepsilon$ without knowing the collection efficiencies.
of charge and three types of phonons (primary, recombination and Luke) in the energy deposition process in the detector [16]. This necessitates an independent way to evaluate the value of $\varepsilon$ at the milli-Kelvin range. As described in our previous work [17], $\varepsilon$ is related to the Fano factor through $F = \sqrt{\frac{E_x}{E_g} \left( \frac{E_g}{E_x} - 1 \right)}$ with $E_x$ the average energy of primary phonons. The Fano factor ($F$) is also related to the detector energy resolution contributed by the intrinsic statistical variation ($\sigma_{\text{stat}}$) through $\sigma_{\text{stat}} = \sqrt{FN_i} = \sqrt{FE_x} \sigma_{\text{stat}}$ with $N_i = \frac{E_x}{E_g}$. Thus, the value of $\varepsilon$ can be determined using the Fano factor ($F$) formula, the detector energy resolution due to the statistical variation ($\sigma_{\text{stat}}$), and the average primary phonon energy ($E_x$).

In this paper, we investigate the value of $\varepsilon$ at 10’s milli-Kelvin and derive the temperature dependence of $\varepsilon$, based on the existing experimental data, in section 2, followed by the impact of $\varepsilon$ on the energy threshold of a bolometer-type detector in section 3. Finally, we summarize our conclusions in section 4.

2 Average energy expended per e-h pair, $\varepsilon$

The temperature effects on $\varepsilon$ have been investigated for many years. Figure 1 shows the temperature dependence in $\varepsilon$ from existing data and theoretical models. The data were obtained by Emery and Rabson [6], Pehl et al. [11], and Antman et al. [19]. To explain the data, based on the theory from Shockley [7] ($\varepsilon = 2.2E_g + rE_R$), Emery and Rabson [6] developed a model (model 1 in figure 1):

$$\varepsilon = 2.2 \cdot E_g(T) + 1.99 \cdot E_g(T)^{3/2} \cdot \exp\left(\frac{4.75 \cdot E_g(T)}{T}\right),$$

where, 1.99 and 4.75 are two fitting parameters, the band gap data, $E_g(T)$, are from Smith [9]. Later on, also on the basis of Shockley theory [7], Klein [12, 13] proposed another model:

$$\varepsilon = \frac{14}{5}E_g + r\hbar\omega_R,$$

where, $r\hbar\omega_R$ is the fraction of energy attributed to phonons, with $r$ the mean-free-path ratio for ionizing collisions and phonon emission and $\omega_R$ the frequency of Raman phonon, which is the highest frequency among all optical phonons in the vibration. Model 2 and 3 in figure 1 are the model in eq. (2.2) with parameters provided by Varshni [8] and Thurmond [10], respectively.

As can be seen in figure 1, none of the theoretical models is capable of explaining all existing data. To have a good interpretation of the variation of $\varepsilon$ as a function of temperature down to the milli-Kelvin range, it is necessary to evaluate the value of $\varepsilon$ at the milli-Kelvin range first and then find a model which can fit all data.

2.1 Estimation of $\varepsilon$ at 10’s milli-Kelvin

For a bolometer-type detector, the operating temperature is at 10’s milli-Kelvin [20, 21]. The total measured phonon energy ($E_p$) of a bolometer-type detector is the sum of energies from three types of phonons [16, 22]: primary phonons, recombination phonons and Neganov-Trofimov-Luke phonons (often also called “Luke phonons” for simplicity) [23, 24]. Primary phonons are produced due to displacements of nuclei and electrons. Recombination phonons are created at the electrodes
due to the recombination of electrons and holes. The Luke phonons are generated due to the charge carriers drifting across the detector by the external applied electric field. Taking into account the detection efficiencies for charge carriers and each type of phonon, the total phonon energy ($E_p$) can be expressed as [25]:

$$E_p = \eta_{pri} \left( E_r - \frac{E_Q}{\epsilon} E_g \right) + \eta_{rec} \left( f_Q E_Q \right) E_g + \eta_{Luke} \left( f_Q \frac{E_Q}{\epsilon} eV_b \right),$$

(2.3)

where, $\eta_{pri}$, $\eta_{rec}$ and $\eta_{Luke}$ represent the detection efficiency for primary phonons, recombination phonons and Luke phonons, respectively, $f_Q$ is the fraction of the total charge observed, $E_r$ is the recoil energy, $E_Q$ is the ionization energy, $\epsilon$ is the elementary charge, and $V_b$ is the bias voltage.

From eq. (2.3), we can see that the mean energy expended per e-h pair, $\epsilon$, cannot be determined if the four efficiencies $\eta_{pri}$, $\eta_{rec}$, $\eta_{Luke}$ and $f_Q$ are not known. Thus, an alternative way to estimate the value of $\epsilon$ is needed.

Utilizing the energy partition process for an energy deposition in a Ge detector, we developed a theoretical model that relates $\epsilon$ to the Fano factor ($F$), energy resolution ($\sigma_{stat}$) and average primary phonon energy ($E_x$) in our earlier work [17]:

$$F = \sqrt{\frac{E_x}{E_g} \left( \frac{\epsilon}{E_g} - 1 \right)},$$

(2.4)

and

$$\sigma_{stat} = \sqrt{\frac{F E_x}{E_g}},$$

(2.5)

where, the variation of $E_g$ with temperature can be evaluated by the following model [8, 10] based on the assumption that $E_g$ is proportional to $T$ at high temperatures and proportional to $T^2$ at low temperatures.

![Figure 1](image-url) Figure 1. All existing data [6, 11, 19] and theoretical models [6, 12, 13] for the variation of $\epsilon$ with temperature.
temperatures:
\[
E_g(T) = 0.7437 - \frac{4.774 \times 10^{-4} \cdot T^2}{T + 235},
\]
where, \(E_g\) is in eV and \(T\) is in Kelvin. 0.7437 is the value of \(E_g\) at 0 Kelvin. This model is valid for all temperatures from 0 Kelvin to the melting point of Ge, \(\sim 1211\) Kelvin.

To solve eq. (2.4) and eq. (2.5) for \(\epsilon\) and \(F\), we need to investigate the average primary phonon energy, \(E_x\), and the energy resolution due to the intrinsic statistical variation, \(\sigma_{stat}\).

### 2.1.1 Determination of \(E_x\)

The average primary phonon energy, \(E_x\), has no temperature dependence since it mainly depends on the lattice type and spacing [6]. This indicates that we can use the value of \(E_x\) at 77 Kelvin for the case of 10’s milli-Kelvin.

At 77 Kelvin, \(\epsilon\) is almost a constant, \(\sim 3\) eV [6, 7, 11–14], \(E_g = 0.73\) eV from eq. (2.6), and \(F = 0.13\) [12]. Substituting these values into eq. (2.4), we can obtain \(E_x = 0.00414\) eV, which corresponds to \(\sim 1\) THz in terms of average frequency for the primary phonon.

It is worth mentioning that the Raman phonon energy (\(E_R = 0.037\) eV) in Shockley’s model [7] \((\epsilon = 2.2E_g + rE_R)\) and the average energy of primary phonon, \(E_x\), determined using the measured Fano factor at 77 Kelvin, is different by a factor of \(\sim 10\). This is because \(E_R\) and \(E_x\) represent different types of phonons from the emission of primary phonons. Right after the primary phonons are generated by the recoiling particle, the primary phonons are very energetic and they down convert from the high-energy optical branch to the low-energy (\(\sim 1\) THz) acoustic branch [16, 22]. Due to this decay process, it is the acoustic branch instead of optical branch of primary phonons that are the final state of phonons in the energy partition between ionization and lattice excitation, which determines the statistical variation (the Fano factor), for a given energy deposition. Furthermore, \(E_R\) (Raman phonon energy) is the energy of optical phonons in the Raman vibration, which scatters the charge carriers capable of secondary ionizations during the thermalization process. While \(E_x\) is the energy of the acoustic primary phonons in the final state of the energy partition between ionization and lattice excitation, i.e. \(E_0 = E_iN_i + E_xN_x\), where \(E_0\) is the energy deposition of an incoming particle in the target, \(E_i\) is the energy of e-h pairs per ionization, \(N_i\) is the number of ionizations, and \(N_x\) is the number of excitations. Note that each ionization leads to an e-h pair production accompanied by the generation of phonons. Therefore, \(N_i\) is the number of e-h pairs and \(N_x\) is the number of phonons per energy deposit. Correspondingly, \(E_i\) is the minimum energy (the indirect band gap energy) required for the production of a charge pair and \(E_x\) is the average energy of phonons accompanying the production of an e-h pair. Since the initial primary phonons, Raman phonons with energy \(E_R (0.037\) eV), are energetic optical phonons, they decay into acoustic phonons with an average energy of \(0.00414\) eV in the final state to participate in the energy partition between ionization and excitation for a given energy deposition, the values of \(E_R\) and \(E_x\) are different by a factor of \(\sim 10\).

### 2.1.2 Determination of \(\sigma_{stat}\)

There are three main contributions to the total measured energy resolution, \(\sigma_{tot}\), for a gamma-ray [26]:
\[
(\sigma_{tot})^2 = (\sigma_{noise})^2 + (\sigma_{stat})^2 + (\sigma_{in-ch})^2,
\]
where, $\sigma_{\text{noise}}$, $\sigma_{\text{stat}}$ and $\sigma_{\text{in-ch}}$ are the energy resolution contributed by electronic noise, intrinsic statistical variation, and incomplete charge collection, respectively.

SuperCDMS reported the measured Ge detector energy resolution in two papers [15, 27]. One was reported in 2010 [27], which showed that the average detector energy resolution (ionization signal only) for energy below 10 keV is:

$$\sigma(E) = \sqrt{(0.293)^2 + (0.056)^2 E},$$  \hspace{1cm} (2.8)

where, the energy resolution, $\sigma(E)$, and the energy $E$ are both in keV. As discussed in our work [17], the term, $(0.056)^2 E$, is the contribution mostly from the intrinsic statistical variation. According to eq. (2.7), we then have, $(\sigma_{\text{stat}})^2 = (0.056)^2 E$. If one sets $\sigma_{\text{stat}}$ in this equation and eq. (2.5) to be equal to each other, then we obtain, $\epsilon F \times 10^{-3} = (0.056)^2$, where $\epsilon$ is in eV and the factor of $10^{-3}$ is due to the unit conversion of $\epsilon$ from eV to keV.

The other energy resolution was reported in 2015 [15]. According to ref. [15], the relative energy resolution ($\epsilon/E$, $\mu$ is the peak energy) for three energy peaks from $^{71}$Ge electron-capture, 0.16 keV, 1.30 keV and 10.37 keV, are $(11.4 \pm 2.8\% )$, $(2.36 \pm 0.15\% )$ and $(0.974 \pm 0.009\% )$, respectively. This allows us to generate $(\sigma_{\text{tot}})^2$ versus energy as presented in figure 2. The best-fit function with reduced $\chi^2 = 0$ for data points in figure 2 is:

$$(\sigma_{\text{tot}})^2 = (2.57 \pm 1.90) \times 10^{-4} + (4.64 \pm 2.04) \times 10^{-4} E + (4.77 \pm 1.83) \times 10^{-5} E^2, \hspace{1cm} (2.9)$$

where, $E$ is the energy in keV. The constant, linear and quadratic terms in eq. (2.9) correspond to $(\sigma_{\text{noise}})^2$, $(\sigma_{\text{stat}})^2$ and $(\sigma_{\text{in-ch}})^2$ in eq. (2.7), respectively. This is because the electronic noise has no energy dependence. The intrinsic statistical variation $(\sigma_{\text{stat}})^2$ is proportional to the number of e-h pairs created in the detector, and is thus proportional to the deposited energy. The energy dependence of the incomplete charge collection is a bit complex since it is dependent on the detector and determined by data. It is customary to assume that $(\sigma_{\text{in-ch}})^2$ is proportional to $E^2$. Hence, we have, $(\sigma_{\text{stat}})^2 = (4.64 \pm 2.04) \times 10^{-4} E$, where $E$ is the energy in keV. Similarly, we set $\sigma_{\text{stat}}$ in this equation and eq. (2.5) to be equal to each other and we obtain, $\epsilon F = 0.464 \pm 0.204$, where $\epsilon$ is in eV. Note that there are systematic uncertainties associated with the value of $\epsilon F$. Since the calculation of the $\epsilon F$ product in this work is related to the measured energy resolution, which is dependent on the systematic uncertainties during the measurements, the systematic uncertainties on $\epsilon F$ eventually arise from the processes of source positioning, energy calibration, fitting, etc.

### 2.1.3 Determination of $\epsilon$

Using eq. (2.4) and substituting $E_g$ and $E_x$ with their value, 0.74 eV (eq. (2.6)) and 0.00414 eV, respectively, we obtain, $F = \sqrt{5.59 \times 10^{-3} \cdot \left( \frac{\epsilon}{0.74} - 1 \right)}$, where $\epsilon$ is in eV. If one combines this equation with $\epsilon F \times 10^{-3} = (0.056)^2$ and solves for $F$ and $\epsilon$, we have $F = 0.28$ and $\epsilon = 11.3$ eV. However, if one combines this equation and $\epsilon F = 0.464 \pm 0.204$ together, we have $F = 0.14^{+0.02}_{-0.03}$ and $\epsilon = 3.35^{+0.84}_{-0.97}$ eV. Two different sets of values indicate that the determination of $\epsilon$ and Fano factor ($F$) using this method depends strongly on the measured energy resolution in which the noise contribution must be largely separated from statistical variation. Note that the value of $\epsilon = 11.3$ eV is not reasonable since the statistical variation is probably overestimated by assuming the linear term in the measured energy resolution shown in eq. (2.8) is totally contributed by the statistical
variation [28]. Other broadening effects such as time variance, position variance, charge collection on the detector resolution could also contribute to the linear term in eq. (2.8) [28]. The value of \( \varepsilon = 3.32^{+0.84}_{-0.97} \) eV is more reasonable since the energy resolution was optimized [28].

2.1.4 Comparison with measured \( \varepsilon \) at 10’s milli-Kelvin

The value of \( \varepsilon \) at 20 milli-Kelvin was measured by the EDELWEISS dark matter experiment [29] using the relationship, \( E_p = E_Q(1 + \frac{eV_b}{\varepsilon}) \) (for electronic recoils), since the ratio of total phonon energy (\( E_p \)) to ionization energy (\( E_Q \)) can be measured for a given bias voltage (\( V_b \)) as shown in figure 3. The detailed work about how to obtain the above relationship (\( E_p = E_Q(1 + \frac{eV_b}{\varepsilon}) \)) for electronic recoils from eq. (2.3) will be discussed in section 3.

As shown in figure 3, \( \varepsilon = 3.32 \) eV (blue solid line) has a better agreement with data (red points) than \( \varepsilon = 3.0 \) eV (magenta dashed line). The best fit (black dashed line) indicates that \( \varepsilon = (3.37 \pm 0.01) \) eV, which also verifies that \( \varepsilon = 3.32 \) eV measured using the energy resolution from SuperCDMS at 50 milli-Kelvin. The physics meaning of 0.85 in the best fit is the conversion efficiency from primary and recombination phonons to thermal phonons relative to the conversion efficiency from Luke phonons to thermal phonons.

2.2 \( \varepsilon \) as a function of \( T \)

To have a better understanding of the value of \( \varepsilon \) at 10’s milli-Kelvin derived from the previous sections, it is necessary to study the temperature dependence of \( \varepsilon \) and thus to develop a decent model of \( \varepsilon \) as a function of temperature. This model should be able to fit all existing data shown in figure 1 and also to predict the value of \( \varepsilon \) at 10’s milli-Kelvin. Using the theory from Emery and Rabson [6] presented in eq. (2.1), according to the definition of \( \varepsilon \), the first term in eq. (2.1) consists of two components: a) the band gap energy, \( E_g \), and b) the final retained kinetic energy.
Figure 3. The ratio of total phonon energy ($E_p$) to ionization energy ($E_Q$) versus bias voltage ($V_b$). The data (red points) were measured by the EDELWEISS detector [29] at 20 milli-Kelvin.

$(E_I)$ of electrons and holes which cannot further conduct ionization in the detector with assumption that $\sim60\%$ of $E_g$ is retained by both electrons and holes, i.e., $E_I \sim 0.6E_g$. Hence, eq. (2.1) can be rewritten as:

$$\varepsilon = E_g(T) + 2 \cdot 0.6E_g(T) + B \cdot E_g(T)^{3/2} \cdot \exp \left( \frac{C \cdot E_g(T)}{T} \right),$$

(2.10)

where, $B$ and $C$ are constants and needed to be determined from data. There are two issues in this model when fitting all data as shown in figure 1: a) it cannot explain the data in the high temperature range, $T > 80$ Kelvin; b) it will blow up when $T$ is close to zero. The first issue is because the second term in eq. (2.10), the final retained kinetic energy ($E_I$) of charge carriers is dependent on the Auger recombination-impact ionization process which has strong temperature dependence [6, 30]. However, only assuming $E_I \sim 0.6E_g$ cannot provide sufficient temperature effects on $E_I$ to explain data in the high temperature range since the temperature dependence in $E_g(T)$ is too weak as can be seen from eq. (2.6). Thus, an additional temperature factor needs to be added into the second term in eq. (2.10). The second issue is due to no constraint in the denominator of the last term in eq. (2.10), so that $\varepsilon$ will reach infinity when $T$ is approaching zero. Therefore, to resolve these two issues, we made two corrections in eq. (2.10) and then it becomes:

$$\varepsilon = E_g(T) + 1.2 \cdot E_g(T) \cdot T^A + B \cdot E_g(T)^{3/2} \cdot \exp \left( \frac{C \cdot E_g(T)}{T + D} \right),$$

(2.11)

where, both $B$ and $C$ are constants and needed to be determined from data. $A$ and $D$ are chosen values that give the best fit for all data points except points at $3.32^{+0.84}_{-0.97}$ eV and 11.3 eV for 50 milli-Kelvin.

As shown in figure 4, the model in eq. (2.11) fits well all existing data with $E_g$ in the form of eq. (2.6), $A = 0.1 \pm 0.001$ and $D = 5 \sim 15$. $B = 1.23 \pm 0.02$, $C = 14.48 \pm 0.8$ and $\chi^2/\text{ndf} = 4.556/5$ for $D = 5$. $B = 1.17 \pm 0.02$, $C = 22.22 \pm 1.24$ and $\chi^2/\text{ndf} = 6.12/5$ for $D = 15$. Due to the uncertainty of $D$, the model in eq. (2.11) can only predict the range of the value of $\varepsilon$, from 3.55 to 7.95 eV. This range verifies that there is overestimate in the value of $\varepsilon = 11.3$ eV and the value of $\varepsilon = 3.32^{+0.84}_{-0.97}$ eV is close
to the lower value of the allowed range. To more precisely predict the value of $\varepsilon$ at 10’s milli-Kelvin by using the model of eq. (2.11), more measurements of $\varepsilon$ for low temperatures ($T<20$ Kelvin) are needed to decrease the uncertainty in $D$. For example, if $\varepsilon$ is measured to be around 3.32 eV at 50 milli-Kelvin, then the value of $D$ is constrained to be around 15.

3 The impact of $\varepsilon$ on the energy threshold of a bolometer-type detector

The nuclear recoil energy threshold, $E_r$, for experiments using bolometer-type detectors is closely related to $\varepsilon$ according to eq. (2.3). Under the assumption that all phonons and charges are being detected at 100% efficiency by bolometer-type detectors [16], eq. (2.3) reduces to be the ideal case [15, 16]:

$$E_p = E_r + \frac{eV_b}{\varepsilon} E_Q,$$

(3.1)

where, the ionization energy ($E_Q$) is related to the recoil energy ($E_r$) through $E_Q \equiv E_r \cdot \eta$ [16] with $\eta$ the ionization yield or the so-called ionization efficiency. Hence, eq. (3.1) can be rewritten as:

$$E_p = E_r \left( 1 + \frac{eV_b}{\varepsilon} \eta \right),$$

(3.2)

where, $\eta \equiv 1$ for electronic recoils. For nuclear recoils, $\eta$ can be calculated by the Lindhard theory [31] or Barker-Mei model [5, 32]. With $V_b = 69$ Volts and $\varepsilon = 3.0$ eV, the nuclear recoil equivalent energy threshold ($E_r$) reported by SuperCDMS is [33], $E_r = 2$ keV, which corresponds to $E_p = 10.7$ keV according to eq. (3.2).

Nevertheless, with the total phonon energy ($E_p$) measured to be 10.7 keV and $V_b = 69$ Volts, the energy threshold of a bolometer-type detector will be about 7.5% different if the value of $\varepsilon$ varies.

Figure 4. $\varepsilon$ versus temperature with all available data points [6, 11, 19] and calculated value at $T = 50$ milli-Kelvin.
from 3.0 eV to 3.32 eV. This suggests that the value of $\varepsilon$ is an important ingredient in modelling a potential signal and eventually understanding a dark matter recoil spectrum.

4 Conclusion

Traditionally, the product of $\varepsilon F$ is measured using the energy resolution function for a given detector. To determine the value of Fano factor or the value of $\varepsilon$, one has to assume either Fano factor or $\varepsilon$ is a constant. In this paper, we developed a method that allows the average energy expended per e-h pair, $\varepsilon$, and the Fano factor to be measured separately. Using the measured energy resolution functions reported by SuperCDMS experiment, the values of $\varepsilon$ and Fano factor are determined for a detector operated at 50 milli-Kelvin. We demonstrate that our method depends strongly on the energy resolution function in which the statistical term is well defined. Using the existing data, we illustrate the best fit function that predicts the range of $\varepsilon$, which is within the range from the SuperCDMS and EDELWEISS measurements at 50 and 20 milli-Kelvin, respectively.

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