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Electron lucky-drift impact ionization coefficients of ZnS : Mn

F M ABOU EL-ELA
Department of Physics, Faculty of Girls, Ain Shams University, Heliopolis, Cairo, Egypt
E-mail: fadlaeg@yahoo.com

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Abstract. Fit of the experimental data of ZnS : Mn by a modified lucky-drift formula has been performed using the least square algorithm. The fit agrees well with the experimental data only at high field. The best fitting parameters at high field are the mean free path of order 102.74 Å and Keldysh factor, $p_0 = 0.0138$. A generalized Keldysh formula has been used, due to introduction of a soft threshold factor. The soft lucky-drift theory can also be used to calculate the impact ionization coefficients of high electron energy of ZnS : Mn without losing its physical significance compared to full band-structure Monte Carlo calculation with a remarkably reduced amount of computer resources.

The curvature on semi-log plot of experimental impact ionization coefficient against the inverse of electric field is different from what is observed for other materials at low electric fields due to impact ionization of deep level impurities.

Keywords. Impact ionization in semiconductors; high field transport; electroluminescent devices; zinc sulphide.

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1. Introduction

Impact ionization across the forbidden gap of the semiconductors usually marks the practical limit of high field effects. Further increase of electric field often leads to the destruction of the sample. Impact excitation is used in electroluminescent display system such as the films of ZnS : Mn. Excitation of the manganese atom has the threshold energy of about 2.2 eV, which requires very hot electrons indeed. Spontaneous de-excitation results in the emission of light.

Electroluminescent devices (ZnS : Mn) recently are of great interest in industry as well as in information technology [1–4]. Understanding the high-field transport of ZnS : Mn semiconductor is useful for the design and operation of alternating current thin-film devices (ACTEFL). The electroluminescent thin-film technology offers means of achieving a high resolution and compact video display panel for both computer terminals and television screens. Also it is a step towards the design of

large area flat screen display for commercial purposes and for the industrial field of entertainment.

There are two main approaches to treat the transport properties at very high electric fields. The first one, which depends on the mean free path for hot carriers, does not contain any indication of the material band structure except the carrier effective mass [5–13]. These theories are analytical studies that depend on the calculation of scattering rates of impact ionization. The second approach relies on Monte Carlo simulation method [1–3, 14–17].

Experimental measurement of ionization coefficient is difficult. Therefore simple theoretical calculations are used. The most prominent analytic theory is Shockley's lucky-electron model [6]. However, it has been found to underestimate ionization coefficients greatly. Numerical calculations, particularly those of Baraff [7], Chwang and Crowell [18] and various Monte Carlo calculations [1,3,14–17] have been more successful. Due to a large amount of computer power required in the Monte Carlo calculation there is a need for a simple analytical model. This may be achieved by the lucky-drift model of impact ionization, which was first proposed by Ridley [8] and has been developed by Burt and McKenzie [9,10]. There was a growing conviction that impact ionization threshold was soft. The argument for soft ionization presented by Ridley [11,12] and Marsland [13] using the Burt version of lucky drift fitted the experimental results. The excellent fit of the experiment obtained, confirms that the threshold was soft. The non-local nature of impact ionization was modeled using the lucky drift [12].

The purpose of the present paper is to describe an application of soft lucky-drift theory of Ridley according to a generalized Keldysh formula [19–21] to fit the experimental data of ZnS : Mn and then to compare with the MC calculations carried by Reigrotzki *et al* [17].

2. The soft lucky-drift formula

A major weakness in the hard lucky-drift approach due to Ridley and Burt [8–10] is the assumption that carriers impact ionize immediately upon attaining the threshold. In this section a lucky-drift model, which does not make this assumption is described. This is the soft threshold energy lucky-drift model.

In order to include soft threshold energy effect, we considered the lucky-drift approach. If $P(E)$ is the probability of an electron starting from zero energy and reaching energy E, then

$$P(E) = \exp\left(-\int_0^t \frac{\mathrm{d}t}{\tau_i(E)}\right) = \exp\left(-\int_0^E \frac{\mathrm{d}E'}{e\varepsilon v\tau_i}\right) \quad (\varepsilon > 0), \tag{1}$$

where v is the velocity (group velocity for ballistic carriers and drift velocity for lucky-drift carriers) and $\tau_i = W_{\mathrm{I}}^{-1}$.

Keldysh [20] defined the energy dependence of impact ionization scattering rate W_{I} to be

$$W_{\mathrm{I}} = W_{\mathrm{ph}}(E_{\mathrm{I}})P\left(\frac{E - E_{\mathrm{I}}}{E_{\mathrm{I}}}\right)^2 \quad (E > E_{\mathrm{I}}), \tag{2}$$

where $W_{\rm ph}(E_{\rm I})$ represents the scattering rate at threshold, usually determined by phonons, and P is a numerical factor, that measures the hardness of the threshold.

In this study, we have used the ionization relaxation rate $\tau_i = W_{\rm I}^{-1}$ to be

$$W_{\rm I} = W_{\rm ph}(E_{\rm I})P\left(\frac{E-E_{\rm I}}{E_{\rm I}}\right)^m \quad (E > E_{\rm I}). \tag{3}$$

Equation (3) is reduced to Keldysh formula (2) for $m = 2$. This approximation is valid only in energy range for $E > E_{\rm I}$. Thus, eq. (3) is defined as a generalization of Keldysh formula [19,22].

The probability for impact ionization becomes

$$P_{\rm I} = \int_{E_{\rm I}}^{\infty} P(E)\exp\left[-\int_{E_{\rm I}}^{E}\frac{{\rm d}E'}{e\varepsilon v\tau_i}\right]\frac{{\rm d}E}{e\varepsilon v\tau_i}. \tag{4}$$

The ionization coefficient is then written as

$$\alpha = \int_{E_{\rm I}}^{\infty}\frac{e\varepsilon}{E}P(E)\exp\left[-\int_{E_{\rm I}}^{E}\frac{{\rm d}E'}{e\varepsilon v\tau_i}\right]\frac{{\rm d}E}{e\varepsilon v\tau_i}. \tag{5}$$

The ionization coefficient depends on a factor p, which is defined as

$$p = \frac{\tau_E}{\tau_i}. \tag{6}$$

Equation (6) can be written as

$$p = p_0\sqrt{\frac{E}{E_{\rm I}}}\left(\frac{E-E_{\rm I}}{E_{\rm I}}\right)^m. \tag{7}$$

A better parameter to measure hardness (p_0), known as Keldysh factor, is defined as

$$p_0 = W_{\rm ph}(E_{\rm I})\tau_E(E_{\rm I})P = \frac{E_{\rm I}(2n(w)+1)}{\hbar w}P, \tag{8}$$

where $\tau_E(E_{\rm I})$ is equal to the energy-relaxation time at threshold energy ($E_{\rm I}$).

3. Results and discussion

Our calculation depended on the best fit of the soft lucky drift to the experimental data in the case of electron in ZnS from two sources, which were reported by Thompson and Allen [23]. One was melt-grown material and the other was vapour-grown. It is the only experimental data available for impact ionization coefficients in ZnS.

Fit of soft threshold lucky-drift theory according to the generalized Keldysh formula to experimental data has made use of the least squares algorithm E04FDF

Table 1. Summary of our initial data parameters of electron in ZnS at 300 K [12].

	E_i (eV)	ρ (g cm^{-3})	$\lambda(0)$ (Å)	$\hbar\omega$ (meV)
ZnS	4.0	4.08	55.5	33

(Nag library). The calculated mean free path length, according to ref. [12], is $\lambda(0) = 55.53$ Å at $T = 0$ K, which corresponds to $\lambda(300) = 31.3$ Å at 300 K.

We, now, choose the mean free path according to eq. (9)

$$\lambda = v_s \tau_m, \tag{9}$$

where v_s and τ_m are the saturated drift velocity and the relaxation time respectively. In ZnS, $v_s = 0.7 \times 10^8$ cm s^{-1} and $\tau_m = 0.5 \times 10^{-14}$ s were estimated, according to [2,24]. Note that the relaxation time (τ_m) is taken for the electron energy of 2.0 eV.

The mean free path calculated by eq. (9) is $\lambda(300) = 35$ Å (or $\lambda(0) = 63$ Å approximately). This value is consistent with the available mean free path of lucky-drift theory [12].

The initial parameters and the corresponding data parameters for fitting programs such as the mean free path at 0 K ($\lambda(0)$), the phonon energy ($\hbar\omega$), the threshold energy (E_I), and the temperature have been summarized in table 1.

Reigrotzki *et al* [17] calculated the impact ionization rate for ZnS using the non-local empirical pseudopotential method. The calculated average impact ionization rate is well-fitted to an analytical formula by

$$W_I = 10^{14} \left(\frac{E - 4.0}{4.0} \right)^{4.556} \quad (E > E_I). \tag{10}$$

The deviation in the calculation from the measured experimental results should be minimized for the impact ionization coefficient (S_α), which is defined as follows:

$$S_\alpha = \sqrt{\frac{1}{n-1} \sum_{i=1}^{n} (\ln \alpha_i(\varepsilon)^{\text{calc}} - \ln \alpha_i(\varepsilon)^{\text{exp}})}, \tag{11}$$

where n represents the number of experimental data.

Plots of S_α, $\lambda(0)$ and p_0 vs. parameter m for the electron in ZnS at 300 K are presented in figures 1a–c, where the threshold electron energy was fixed at 4.0 eV. It is difficult to notice an optimal value of m; therefore we selected $m = 4.556$ as was given by eq. (10). The parameters corresponding to minimum S_α at $m = 4.556$ are: $p_0 = 0.0138$, $\lambda(0) = 102.74$ Å and $S_\alpha = 1.15 \times 10^{-3}$.

We fixed the value of free path length $\lambda(0)$ to be 102.74 Å in figure 2 and varied the value of p_0 between 0.02 and 0.05, while in figure 3 the value of p_0 was fixed at 0.0138 and $\lambda(0)$ varied between 95 and 110 Å. It is important to note that, at high field, the values of $\lambda(0) = 102.74$ Å and $p_0 = 0.0138$ give remarkably well best fitting to both the melt-grown and the vapour-grown experimental data of Thompson and

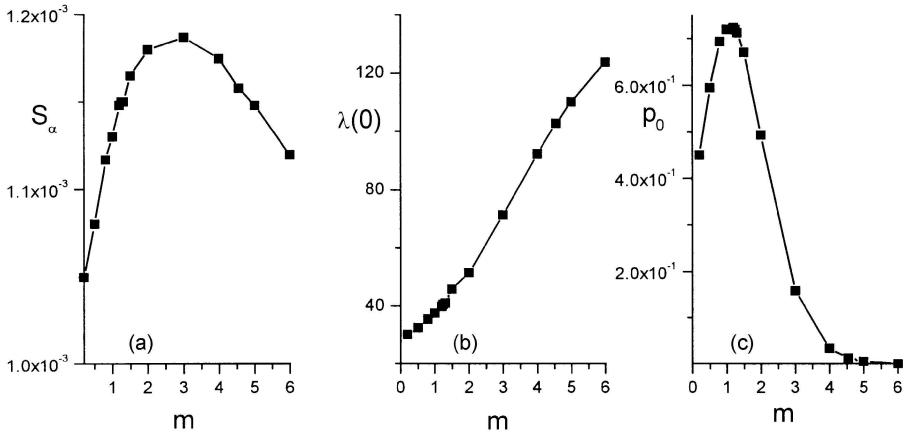

Figure 1(a–c). Deviation function S_α, optimal mean free path $\lambda(0)$, and parameter p_0 vs. parameter m in ionization relaxation of electron for ZnS.

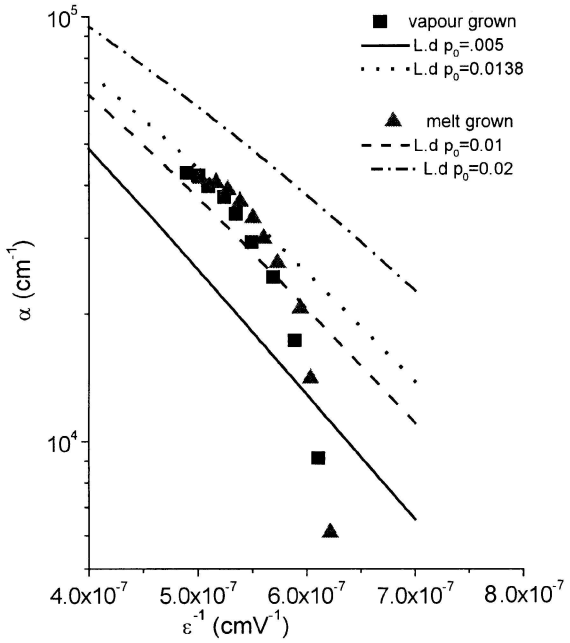

Figure 2. Measured and calculated results for impact ionization coefficient vs. reciprocal electric field strength. $\lambda(0)$ was fixed at 102.74 Å and p_0 varied between 0.02 and 0.05.

Allen. However, the overall fit is very poor. If we choose the best-fit values of Keldysh factor and mean free path at $T = 0\,\mathrm{K}$ to fit the experimental data, we obtain figure 4 which is not an entirely convincing fit. Moreover, the magnitude of the mean free path at $T = 0\,\mathrm{K}$ must be chosen as 47.85 Å and $p_0 = 0.51$. The mean

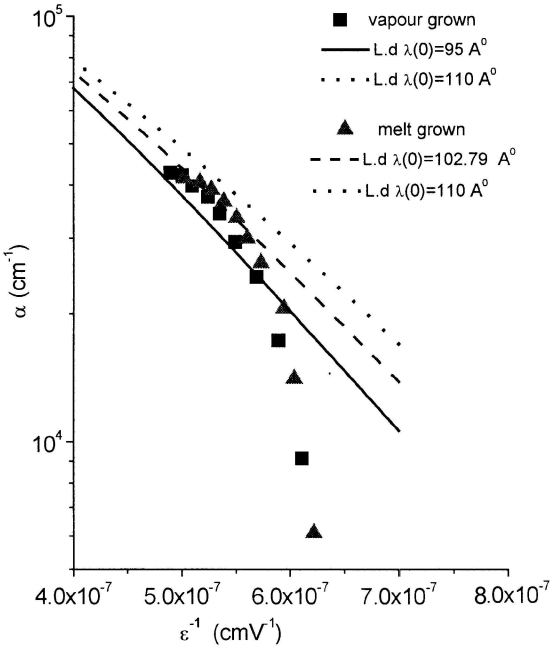

Figure 3. Measured and calculated results for impact ionization coefficient vs. reciprocal electric field strength. p_0 was fixed at 0.0138 and $\lambda(0)$ varied between 95 and 110 Å.

free path is too small at 300 K, the temperature at which the experiments were carried out, the mean free path would be only 26 Å. This is so small that the render transport is virtually impossible. The lack of agreement with the experimental data at lower field may relate to the method of deducing the raw data, which certainly would appear to be more accurate at high field. However, distinct difference in the curvature of the experimental ionization coefficient indicates further effect such as deep level ionization, which must be accounted for in order to obtain a more accurate picture.

As shown in figures 2–4 the curvature in the semi-log plot of α vs. ε^{-1} is different from what is observed for other materials such as Si, Ge, GaAs, InP and GaP to allow an accurate fit to the experimental data. It is interesting to note that the same idea was also deduced from the Monte Carlo calculation of impact ionization rate in ZnS using a non-local empirical pseudopotential band structure [17] as shown in figure 5. A reasonable agreement between the experimental and calculated impact ionization rate is obtained only at high field. The experimental impact ionization data of Thompson and Allen (melt-grown) was fitted by taking deformation potential as adjustable parameter. Two adjustable parameters are used in figure 5; one represents the deformation potential in the lowest conduction band whereas the other is the deformation potential in the upper band. These deformation potentials are included as a pair of numbers in figure 5, which represents the fitting attempt to melt-grown experimental data carried by Reigrotzki *et al* [17]. To bring our soft

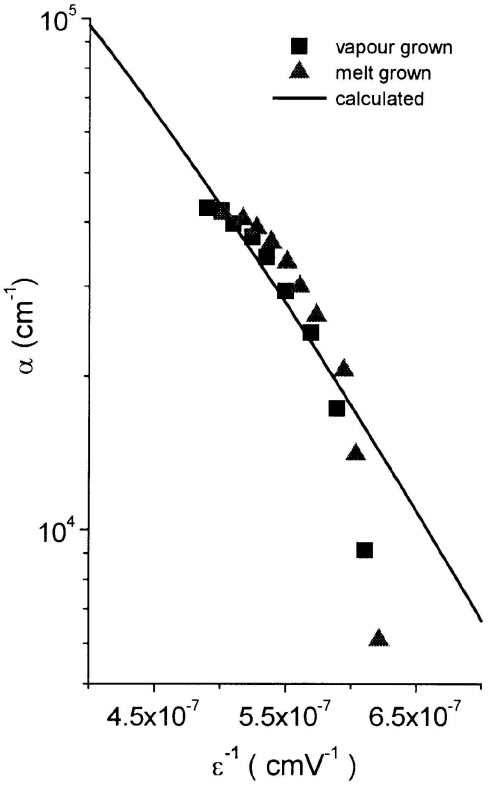

Figure 4. Measured and calculated results for impact ionization coefficient vs. reciprocal electric field strength. The overall fitting is displayed here.

lucky-drift ionization coefficient into agreement with both full-band Monte Carlo calculation of impact ionization coefficient and experimental melt-grown data, we have to fix the mean free path length $\lambda(0)$ to be 102.74 Å as in figure 1 and changed the value of p_0 between 0.05 and 0.02. Figure 5 shows that the agreement is reasonably good over the whole range of applied electric field between Monte Calro calculation of ionization coefficient and soft lucky-drift ionization rate.

4. Conclusion

The present study has attempted to calculate the electron impact ionization coefficient by using the lucky-drift impact ionization theory. We have shown the mean free path length of ZnS to be 102.74 Å at $T = 0$ K, which differed with the lucky-drift estimation of 55.5 Å and Monte Carlo transport calculation of 63 Å. The soft lucky-drift theory can also be used to calculate the impact ionization coefficients of high electron energy of ZnS without losing its physical significance compared to full band-structure Monte Carlo calculation with a remarkably reduced amount of computer resources.

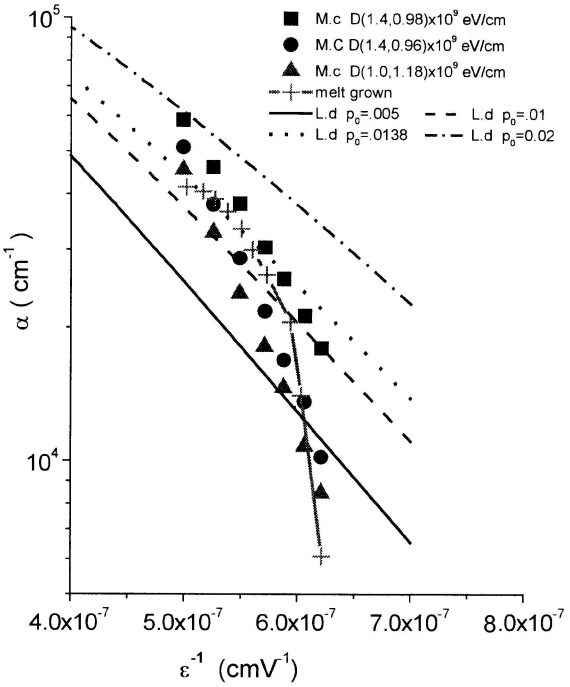

Figure 5. Measured and calculated results for impact ionization coefficient vs. reciprocal electric field strength. Here our results at different p_0 are compared to the Monte Carlo calculations of Reigrotzki *et al* at different deformation potentials.

The impact ionization process in ZnS at relatively low applied electric field occurs mostly from the deep impurity level excitation. As the electric field increases, more impact ionization occurs btween the valence and the conduction band.

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