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An analysis of 'dead space' in semiconductors

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Abstract. An analytic expression is derived for the field dependence of 'dead space' in semiconductors in terms of optical phonon energy and mean free path. The basis for the analysis is the energy distribution function of electrons derived by Keldysh. The result is applicable to a range of devices, such as avalanche photodetectors and MOSFETs, where dead space can occupy a significant fraction of the active region.

1. Introduction

'Dead space' occurs in semiconductors because an electron/hole must travel a finite distance in an electric field before it can acquire the threshold energy of a process such as impact ionization. It is important in devices such as avalanche photodetectors where it can affect noise and multiplication rates. The concept of dead space is not, however, restricted to the process of impact ionization. For instance an electron or hole injected into the gate oxide of a MOSFET must travel a minimum distance or 'dead space' before acquiring sufficient energy to overcome the potential barrier to the oxide. The threshold energy for this process is much greater than that of impact ionization and the dead space is correspondingly larger. Evaluation of dead space within a device is not simple as the electron/hole will, in general, suffer many inelastic collisions with phonons before reaching the threshold energy. Furthermore, in small-geometry devices such as MOSFETs the electric field may vary significantly over the dead space. A knowledge of dead space and its field dependence is therefore important in the study of devices where the spatial dependence of the hot-carrier distribution is significant.

In this paper we derive an analytic expression for the field dependence of dead space in terms of optical phonon energy and mean free path. The result is applicable to semiconductors where at high energies it is reasonable to assume that non-polar scattering dominates. Before proceeding with the analysis we must first establish an unambiguous definition of dead space. Two difficulties arise in defining dead space. The first because the magnitude of the dead space is determined by the upper energy limit of the process under consideration which in the case of impact ionization is uncertain due to the characteristic 'soft-threshold' nature of the process. Since in this work we are seeking a general expression for dead space we remove the need to define an upper energy limit by normalizing to its ballistic value. That is we determine the dead space relative to the distance travelled by an electron in reaching the same energy without colliding with phonons. The theory can always be extended to include 'soft-threshold effects'. The

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second difficulty is to determine the number of collisions an electron will make in traversing the dead space. This is the crux of the problem. Clearly an electron can travel through the electric field without making collisions by Baraff [1] has shown that this process is improbable and such electrons play no part in determining the energy distribution. In solving the Boltzmann transport equation, Keldysh [2] has shown that transport to high energies is dominated by those electrons that fortuitously travel for a larger than average time between collisions. The problem of determining dead space therefore reduces to finding the average energy gained by these electrons between collisions.

The basis for our analysis is the electron energy distribution function derived by Keldysh. He showed that the dominant exponential term in the distribution function can be characterized by a parameter s which is uniquely determined by the field, optical phonon energy and mean free path. In this work we derive an analytic expression for the mean energy gained between collisions in terms of the parameter s. Since the energy lost/gained between collisions is known it is straightforward to determine the dead space.

2. Theory

Keldysh has shown that in the region of large energies $\varepsilon \gg \hbar\omega$ the distribution function of the electrons interacting with the acoustic and optical phonons in a covalent crystal is of the form

$$f_0(\varepsilon) = \text{constant} \times \varepsilon^{\nu} \exp(-(\varepsilon/qEl)s_0(E, T)) \tag{1}$$

where ε is the electron energy, the parameter $s_0(E, T)$ is determined as the positive root of the transcendental equation

$$\frac{(1+\lambda)\cosh(\hbar\omega/2kT)}{\lambda\cosh(\hbar\omega/2kT) + \cosh(\hbar\omega/kT - s_0(\hbar\omega/qEl))} + \frac{1}{2s_0}\ln\frac{1-s_0}{1+s_0} = 0 \tag{2}$$

and the exponent ν is a slowly varying function of s_0. Here $\hbar\omega$ is the optical phonon energy and E is the electric field in the case of a semiconductor with a scalar effective mass. The dimensionless parameter λ determines the relative contribution of acoustic and optical phonon scattering to the total mean free path.

$$\lambda = l_{op}/l_{ac} \qquad 1/l = 1/l_{op} + 1/l_{ac} = (1+\lambda)/l_{op}. \tag{3}$$

Equations (1) and (2) were obtained by solving the Boltzmann transport equation

$$qE\,\nabla_p f(p) + S_p^- f(p) = S_p^+\{f\} \tag{4}$$

to obtain a distribution function $f(p)$ in the form

$$f(p) = \int_{-\infty}^{0} S^+_{p+qEt}\{f\} \exp\left(\int_0^t S^-_{p+qEt'}\,dt'\right) dt \tag{5}$$

where p is the electron momentum, S_p^- the probability of collision with a phonon and S_p^+ is the number of electrons arriving per unit time in the state with momentum p from all other states as a result of emission or absorption of phonons.

By integrating (5) over a surface of constant energy and expanding in powers of $\hbar\omega/\varepsilon_p$ up to first order, Keldysh obtains

$$S_p^- \approx \frac{1}{\tau(p)}\left(1 - \frac{\hbar\omega}{1+\lambda}\frac{\mathrm{d}\ln\Omega(\varepsilon_p)}{\mathrm{d}\varepsilon_p}\tanh\beta\right) \tag{6}$$

$$S_p^+ \approx \frac{1}{(1+\lambda)\tau(p)}\left(\lambda + \frac{\cosh(\beta + \hbar\omega\,\mathrm{d}/\mathrm{d}\varepsilon_p)}{\cosh\beta} + \hbar\omega\frac{\mathrm{d}\ln\Omega(\varepsilon_p)}{\mathrm{d}\varepsilon_p}\frac{\sinh(\beta+\hbar\omega\,\mathrm{d}/\mathrm{d}\varepsilon_p)}{\cosh\beta}\right)f_0(\varepsilon_p) \tag{7}$$

where

$$\beta = \hbar\omega/2kT \qquad \Omega(\varepsilon) = \int \delta(\varepsilon - \varepsilon_p)\frac{\mathrm{d}^3p}{(2\pi\hbar)^3}$$

and the operators $\cosh(\beta + \hbar\omega\ \mathrm{d}/\mathrm{d}\varepsilon_p)$ and $\sinh(\beta + \hbar\omega\,\mathrm{d}/\mathrm{d}\varepsilon_p)$ are defined by the relations $\exp(\pm\hbar\omega\,\mathrm{d}/\mathrm{d}\varepsilon_p)f_0(\varepsilon_p) \equiv f_0(\varepsilon_p \pm \hbar\omega)$. The mean free time $\tau(p)$ is connected with the mean free times for acoustic and optical phonon scattering, τ_{ac} and τ_{op}, via

$$\tau^{-1}(p) = \tau_{ac}^{-1}(p) + \tau_{op}^{-1}(p) = (1+\lambda)\tau_{op}^{-1}(p). \tag{8}$$

Since we are only interested in the dominant exponential term in the distribution function we simplify the derivation at this point by neglecting all terms of order $\hbar\omega/\varepsilon$ in (6) and (7). Hence

$$S_p^- \approx \tau^{-1}(p) \tag{9}$$

$$S_p^+ \approx \frac{1}{(1+\lambda)\tau(p)}\left(\lambda + \frac{\cosh(\beta+\hbar\omega\,\mathrm{d}/\mathrm{d}\varepsilon_p)}{\cosh\beta}\right)f_0(\varepsilon_p). \tag{10}$$

In equation (5) the term

$$\exp\left(-\int_0^t S_{p+qEt'}^-\,\mathrm{d}t'\right)$$

represents the probability of an electron travelling for a time t without collision.

Hence for an electron with momentum p the mean energy gained between collisions is given by

$$\langle\varepsilon_p - \varepsilon_{p+qEt}\rangle = \frac{1}{f(p)}\int_{-\infty}^0 (\varepsilon_p - \varepsilon_{p+qEt})S_{p+qEt}^+\{f\}\exp\left(\int_0^t S_{p+qEt'}^-\,\mathrm{d}t'\right)\mathrm{d}t. \tag{11}$$

Substituting (9) and (10) into (11) and integrating by parts yields

$$\langle\varepsilon_p - \varepsilon_{p+qEt}\rangle = \frac{1}{f(p)}\int_{-\infty}^0 \frac{\mathrm{d}\varepsilon_{p+qEt}}{\mathrm{d}t}\exp\left(\int_0^t \frac{\mathrm{d}t'}{\tau(p+qEt')}\right)\left(\lambda + \frac{\cosh(\beta+\hbar\omega\,\mathrm{d}/\mathrm{d}\varepsilon_{p+qEt})}{\cosh\beta}\right) \times \left(f_0(\varepsilon_{p+qEt}) - (\varepsilon_p - \varepsilon_{p+qEt})\frac{\mathrm{d}f_0(\varepsilon_{p+qEt})}{\mathrm{d}\varepsilon_{p+qEt}}\right)\mathrm{d}t. \tag{12}$$

Following Keldysh we introduce the effective mean free path defined by

$$l = (2\varepsilon_p/m)^{1/2}\tau_p \tag{13}$$

where m is the density-of-states effective mass. Changing variables we have

$$u = \cos\{\boldsymbol{E}, \boldsymbol{p}\} \qquad v = \cos\{\boldsymbol{E}, \boldsymbol{p} + q\boldsymbol{E}t\}. \tag{14}$$

In the case of parabolic energy bands the quantities $\varepsilon = \varepsilon_p$, $\varepsilon' = \varepsilon_{p+qEt}$, u and v are connected by the relation

$$\varepsilon(1 - u^2) = \varepsilon'(1 - v^2) \tag{15}$$

such that

$$1/v = [1 - (\varepsilon/\varepsilon')(1 - u^2)]^{1/2}. \tag{16}$$

Introducing the new variables into (12) and averaging over angles we obtain

$$\langle \varepsilon - \varepsilon' \rangle = \frac{1}{f(\varepsilon)} \int_{-1}^{1} \mathrm{d}u \int_{\Gamma}^{\varepsilon} \exp\left[- \int_{\varepsilon'} \left(1 - \frac{\varepsilon}{\varepsilon''}(1 - u^2)\right)^{1/2} \frac{\mathrm{d}\varepsilon''}{qEl} \right)$$
$$\times \left(\lambda + \frac{\cosh(\beta + \hbar\omega \, \mathrm{d}/\mathrm{d}\varepsilon')}{\cosh \beta}\right) \left(f_0(\varepsilon') - (\varepsilon - \varepsilon') \frac{\mathrm{d}f_0(\varepsilon')}{\mathrm{d}\varepsilon'}\right) \frac{\mathrm{d}\varepsilon'}{1 + \lambda} \tag{17}$$

where Γ is the contour of integration. Since the distribution function depends weakly on the pre-exponential term, equation (17) can be easily solved by assuming a distribution of the form

$$f_0(\varepsilon) = \text{constant} \times \exp\left(- \int_0^{\varepsilon} \frac{s_0 \, \mathrm{d}\varepsilon'}{qEl} \right). \tag{18}$$

In this case the exponent in (17) can be expanded into powers of $\varepsilon - \varepsilon'$ up to first order:

$$\int_{\varepsilon''}^{\varepsilon} \left[\left(1 - \frac{\varepsilon}{\varepsilon''}(1 - u^2)\right)^{-1/2} - s_0 \right] \frac{\mathrm{d}\varepsilon''}{qEl} \approx \left(\frac{1}{u} - s_0\right) \frac{\varepsilon - \varepsilon'}{qEl}. \tag{19}$$

Carrying out all integrations, equation (17) reduces to the form

$$\langle \varepsilon - \varepsilon' \rangle = qEl \left(\frac{2}{(1 - s_0^2)} - \frac{1}{s_0} \ln \frac{1 + s_0}{1 - s_0} \right) \Big/ \ln \frac{1 + s_0}{1 - s_0}. \tag{20}$$

Equation (20) gives the mean energy gained by an electron between collisions. The average energy lost per collision is $[\hbar\omega/(1 + \lambda)] \tanh(\hbar\omega/2kT)$. Hence if we normalize to its ballistic value, the dead space is given by

$$D = \left(1 - \frac{\hbar\omega}{\langle \varepsilon - \varepsilon' \rangle} \frac{\tanh(\hbar\omega/2kT)}{1 + \lambda}\right)^{-1}. \tag{21}$$

The field and temperature dependence of dead space are completely defined by equations (2), (20) and (21).

3. Discussion

We will demonstrate the use of this analysis by determining the normalized dead space in silicon. The optical phonon energy is taken as 63 meV and the mean free path between collisions is assumed to be 7.5 nm. In low fields and at room temperature s is close to 1 and the dead space tends to a value approximately 3/2 of the ballistic value showing that the electron travels relatively long distances between collisions. Only when the temperature is reduced does equation (21) tend to 1 indicating ballistic or lucky electron transport. In high fields $s \approx 0.3$ and the dead space tends to a value approximately twice the ballistic value. This implies that electrons make frequent collisions with optical phonons and effectively 'diffuse' to high energies, confirming the process described by Wolff [3]. Obviously the magnitude of the dead space decreases with increasing field because although collisions with phonons are more frequent the mean energy gained per unit distance is greatly increased. In application the magnitude of dead space will depend upon the threshold energy of the process under consideration and on the number of electrons reaching that energy. In the analysis we have presented the dead space is determined by those electrons with the highest probability of reaching the threshold energy.

In this paper we have derived an analytic expression for the field and temperature dependence of dead space in semiconductors. The theory should be useful in applications where the hot-carrier distribution function is sensitive to dead space.

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