Analytic Expressions for the Energy Dependent Electron Temperature and Effective Mass for a Realistic Band Structure Energy Transport Model

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It has been shown that energy transport and Monte Carlo calculations of hot carrier transport in MOSFET's seldom yield the same results [1]. The reason for this discrepancy is that the assumptions made in deriving the energy balance equations are too restrictive. In recent years, less restrictive energy balance equations have been developed [2,3,4] These equations have been shown to predict hot carrier characteristics that match Monte Carlo calculations to a greater extent [3]. Here, we investigate the Monte Carlo calculation of the electron temperatures and effective mass as used in the general hydrodynamic model and present relations for the simple incorporation of these parameters into present energy transport device simulators.

Making no assumptions on the band structure of silicon, two electron temperatures are obtained in the derivation of the conservation equations. One, $\overline{\overline{T}}_v$, is found in the momentum equation and the other, $\overline{\overline{T}}_w$, is found in the energy conservation equation. They are defined as:

$$\overline{\overline{T}}_v \equiv \frac{m_o^*}{n(\mathbf{r},t)k_B}\int_{-\infty}^{+\infty}(\overline{\mathbf{v}}(\mathbf{k})-\overline{\mathbf{v}}(\mathbf{r},t))^2 f(\mathbf{r},\mathbf{k},t)d^3\mathbf{k} \qquad \overline{\overline{T}}_w \equiv \frac{1}{n(\mathbf{r},t)k_B}\int_{-\infty}^{+\infty} m^*(\mathbf{k})(\overline{\mathbf{v}}(\mathbf{k})-\overline{\mathbf{v}}(\mathbf{r},t))^2 f(\mathbf{r},\mathbf{k},t)d^3\mathbf{k}$$

$\overline{\overline{T}}_v$ and $\overline{\overline{T}}_w$ were calculated using Monte Carlo techniques. The Monte Carlo parameters and models used are those described in [5]. A simple non−parabolic band was assumed of the form $w(1+\alpha w) = \hbar^2\mathbf{k}\cdot\mathbf{k}/2m_o^*$. Figure 1 shows a comparison between $k_B\mathrm{Tr}(\overline{\overline{T}}_v)/2$ and $k_B\mathrm{Tr}(\overline{\overline{T}}_w)/2$ as a function of average carrier energy for electrons in silicon. It is seen that $\overline{\overline{T}}_w$ can be simplified to an analytical form: $w = (1/2)m^*(w)v(w)^2 + (k_B/2)\mathrm{Tr}(\overline{\overline{T}}_w)$. By normalizing w to w' using the expression $w' = w(1+\alpha w)/(1+2\alpha w)^2$, $\overline{\overline{T}}_v$ can be cast into a similar form, that is, $w' = (1/2)m^*(w')v(w')^2 + (k_B/2)\mathrm{Tr}(\overline{\overline{T}}_v)$. Figure 2 shows this relationship. By ignoring the kinetic energy term introduces less than 15% error for the $\overline{\overline{T}}_v$ energy relation and less than 7% error for the $\overline{\overline{T}}_w$ energy relation.

Continuing to use the same energy-wavevector relationship as shown above, the components of the effective mass tensor as used in the equation of momentum conservation are defined as:

$$\frac{1}{M_{i,j}^*} \equiv \frac{1}{n(\mathbf{r},t)}\int_{-\infty}^{+\infty}\left(\frac{1}{m_o^*\sqrt{1+2\alpha\dfrac{\hbar^2\mathbf{k}^2}{m_o^*}}} - \frac{\hbar^2 k_i k_j(2\alpha)}{m_o^{*2}\left(1+2\alpha\dfrac{\hbar^2\mathbf{k}^2}{m_o^*}\right)^{\frac{3}{2}}}\right) f(\mathbf{r},\mathbf{k},t)d^3\mathbf{k} \quad , \qquad \text{for } i = j$$

The off diagonal elements will be ignored here since their values were found to be negligibly small. Figure 3 shows results of Monte Carlo calculations of $\mathrm{Tr}\left[1/\overline{\overline{M^*}}\right]/3$ as a function of energy. We can see that the expression $m^*(w) = m_o^*(1+2\alpha w)/\left[1-\dfrac{2\alpha w(1+\alpha w)}{3(1+2\alpha w)^2}\right]$, directly derived from the differentiation of the energy-wavevector relation is a very reasonable representation of the Monte Carlo calculation.

We have shown Monte Carlo calculations of electron temperatures and effective mass. Relations were shown that approximate the Monte Carlo data to reasonable accuracies. We believe that these relations can be used in present energy transport simulators to more accurately calculate hot carrier transport.

References:

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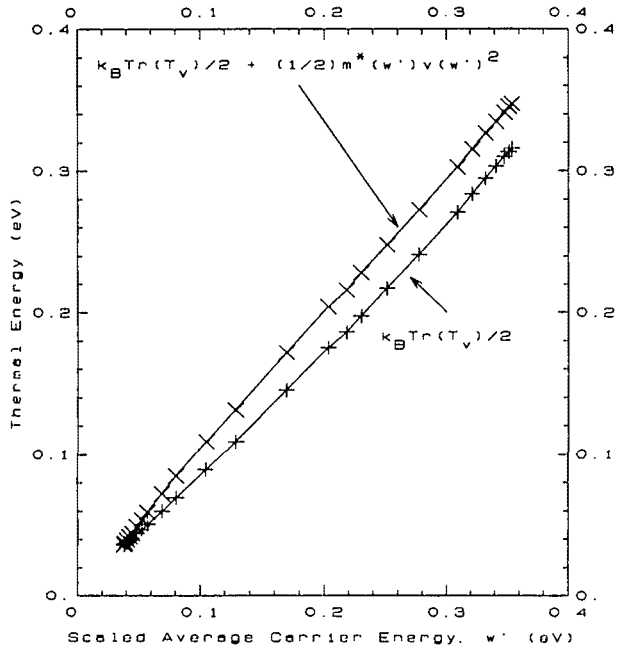

Figure 2. Monte Carlo generated temperature $\overline{T}_v$ for electrons in silicon. By scaling the average carrier energy we see that a simple relationship between $\overline{T}_v$ and average scaled carrier energy can be formed.

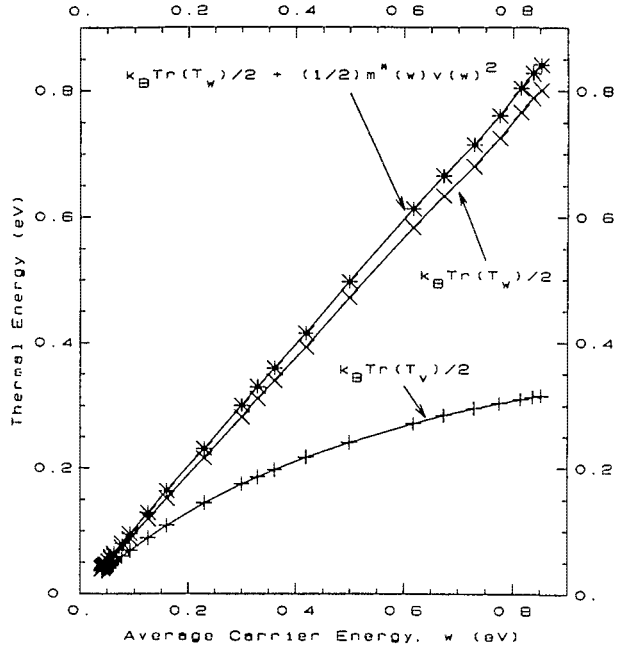

Figure 1. Monte Carlo generated temperatures for electrons in silicon. The calculation of $\overline{T}_v$ assumes a constant effective mass whereas the calculation of $\overline{T}_w$ assumes that the effective mass is dependent on the wavevector. By adding the kinetic energy to $\overline{T}_w$ we find a simple relationship between $\overline{T}_w$ and average carrier energy. The symbols indicate Monte Carlo data and the lines are drawn through the data for ease of visualization.

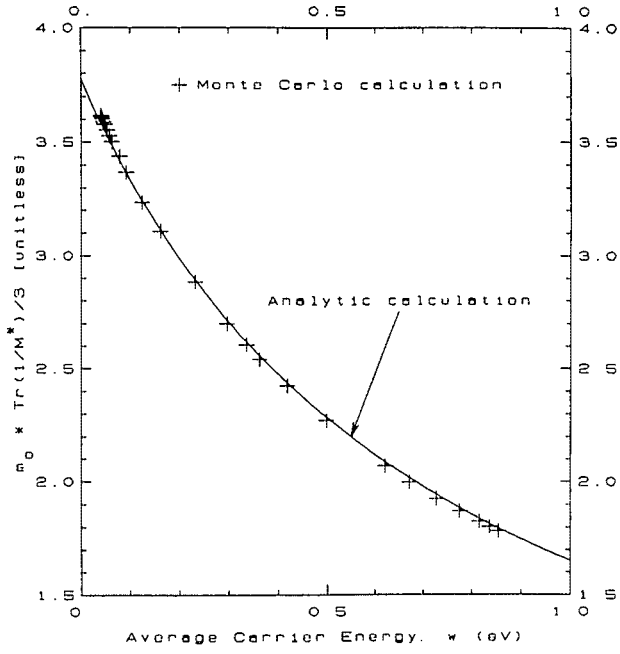

Figure 3. Comparison of Monte Carlo generated effective mass and an analytic expression for the effective mass as a function of average carrier energy for electrons in silicon. We can see a very good fit between the expression and the data.