Electron Drift Velocity and Mobility calculation in Bulk Silicon using an Analytical Model for the Phonon Dispersions

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Abstract: We present simulation results for the drift velocity and mobility in silicon at various temperatures using analytical model which incorporates analytical expressions for the acoustic and optical phonon dispersions. Our simulation results for the field-dependent average drift velocity and mobility are in excellent agreement with the results that utilize the rejection technique and the experimental data for silicon for [100] crystallographic direction at different temperatures.

Keywords: silicon electron drift velocity, silicon electron mobility, bulk Monte Carlo method, phonon dispersion.

I. INTRODUCTION

It is well known that crystalline silicon is the material of choice for fabrication of integrated circuits because silicon wafers are cheap and silicon dioxide is abundant in nature. Properties of the crystalline silicon have been explored extensively both experimentally [1] and theoretically [2]. In the theoretical calculations non-parabolic bands [3] and full-band bulk Monte Carlo [4] calculations have been used. Phonons have been treated either using the Debye approximation [5] for the acoustic modes and the Einstein relation [6] for the optical modes or full phonon dispersions have been calculated using the rigid ion approximation [7]. In a recent work by Pop and co-workers [8] analytical model for the phonon dispersion has been used in conjuncture with non-parabolic model which is quite accurate for current state of the art devices because the supply voltages are on the order of 1 V or smaller. The choice of the scattering processes was determined using a rejection algorithm [9], which sometimes tends to be time consuming. To overcome this and obtain results faster, in this work an analytical model for the scattering rates has been used that utilizes the full analytical phonon dispersion.

The paper is organized as follows: in Section 2 the analytical expressions that we have derived are presented. In Section 3 we discuss the drift velocity and mobility results for Si at various temperatures to validate our model. Conclusions related to this research are given in Section 4.

II. ANALYTICAL MODEL

The phonon dispersion relations in the reduced zone representation are shown in Figure 1. It is assumed that the phonon dispersions are almost spherically symmetric. A quadratic fit to the phonon dispersions is performed for both the acoustic and optical branches with parameters summarized in Table 1.

Table 1. Quadratic Fit to the Phonon Dispersions Coefficients [8].

	ω_o (10^{13} rad/s)	υ_s (10^5 cm/s)	c 10^{-3} cm^2/s
LA	0.00	9.01	-2.00
TA	0.00	5.23	-2.26
LO	9.88	0.00	-1.60
TO	10.20	-2.57	1.11

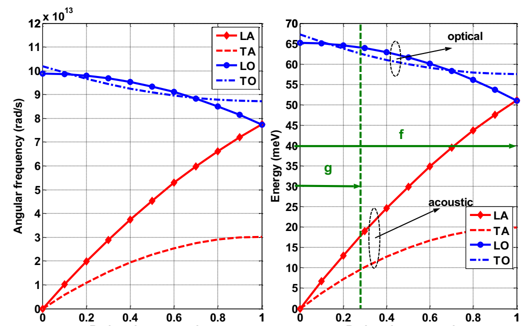

Figure 1. Graphical representation of the quadratic fit to the phonon dispersions in [100] direction [8].

The acoustic and optical phonon scattering rates, in their most general case, are calculated in the following manner [10]:

$$\frac{1}{\tau\,(\mathrm{k})} = \frac{1}{2\pi\hbar}\int_0^\infty \mathrm{k'}^2\,\mathrm{dk'}\int_0^\pi \sin\theta\ \mathrm{d}\theta\ |\mathrm{M(q)}|^2 * \\ \delta\left(\mathrm{E_{k'}} - \mathrm{E_k} \mp \hbar\omega_\mathrm{q}\right)\left(\mathrm{N_q} + \frac{1}{2} \mp \frac{1}{2}\right) \tag{1}$$

The non-parabolic band model is of the form,

$$\frac{\hbar^2 k'^2}{2m} = E_{k'}\,(1 + \alpha E_{k'}) = E_{k'} + \alpha E_{k'}^2 \tag{2}$$

where α is the non-parabolicity parameter and α=0.47 for silicon. On differentiating the above equation and multiplication with k' one obtains

$$k'^2 dk' = \frac{m}{\hbar^2}\,(1 + 2\alpha E_{k'}) \tag{3}$$

$$\sqrt{\frac{2m}{\hbar^2}\,E_{k'}\,(1 + \alpha E_{k'})}\;dE_{k'} = A(E_{k'})dE_{k'} \tag{4}$$

where the auxiliary functional is

$$A\,(E_{k'}) = \frac{m}{\hbar^2}\,(1 + 2\alpha E_{k'})\sqrt{\frac{2m}{\hbar^2}\,E_{k'}\,(1 + \alpha E_{k'})}\;dE_{k'} \tag{5}$$

Integration over the final energy results in

$$\frac{1}{\tau\,(\mathrm{k})} = \frac{1}{2\pi\hbar}\int_0^\pi \sin\theta\ \mathrm{d}\theta\,.\,|\mathrm{M(q)}|^2 * \\ A\left(E_k \pm \hbar\omega_q\right)\left(\mathrm{N_q} + \frac{1}{2} \mp \frac{1}{2}\right) \tag{6}$$

Where

$$N_q = \frac{1}{\exp\left(\frac{\hbar\omega_q}{k_B T}\right) - 1} \tag{7}$$

is the phonon occupancy factor. The q-vectors that satisfy the laws of both energy and momentum conservation are involved in the integral. These q-vectors are calculated using

$k' = k \pm q$ and $E_{k'} = E_k \pm \hbar\omega_q$.

Therefore,

$$\frac{\hbar^2 k'^2}{2m} = \frac{\hbar^2 k^2}{2m} + \frac{\hbar^2 q^2}{2m} \pm \frac{\hbar^2 kq\cos\theta}{m} \tag{8}$$

which leads to

$$E_{k'}(1 + \alpha E_{k'}) = E_k(1 + \alpha E_k) + \frac{\hbar^2 q^2}{2m} \\ \pm \frac{\hbar^2 kq\cos\theta}{m} \tag{9}$$

On substituting $E_{k'} = E_k \pm \hbar\omega_q$, we get

$$\pm\omega_q\,(1 + 2\alpha E_k) + \alpha\hbar\omega_q^2 = \frac{\hbar q^2}{2m} \pm \frac{\hbar kq}{m}\cos\theta \tag{10}$$

In the quadratic form ($Aq^2 + Bq + C = 0$), we have,

$$\frac{\hbar q^2}{2m} \pm \frac{\hbar kq}{m}\cos\theta \mp \omega_q\,(1 + 2\alpha E_k) - \alpha\hbar\omega_q^2 = 0 \tag{11}$$

The dispersion relation for acoustic phonons is of the form: $\omega_q = v_s q + cq^2$. When substituted back into Eq. (10) and ignoring cubic terms (the coefficients in front of these terms are small) we arrive at the following coefficients

$$A = 2\alpha\hbar v_s c \tag{12.1}$$

$$B = \pm c\,(1 + 2\alpha E_k) + \alpha\hbar v_s^2 - \frac{\hbar}{2m} \tag{12.2}$$

$$C = \pm v_s\,(1 + 2\alpha E_k) \mp \frac{\hbar k\cos\theta}{m} \tag{12.3}$$

For Optical Phonons, the phonon dispersion is of the form: $\omega_q = cq^2 + v_s q + \omega_o$, which when substituted back in Eq. (10) and ignoring third and fourth order terms gives,

$$A = \pm c\,(1 + 2\alpha E_k) + \alpha\hbar v_s^2 + 2\alpha\hbar\omega_o c - \frac{\hbar}{2m} \tag{13.1}$$

$$B = \pm v_s\,(1 + 2\alpha E_k) + 2\alpha\hbar\omega_o v_s \mp \frac{\hbar k}{m}\cos\theta \tag{13.2}$$

$$C = \pm\omega_o\,(1 + 2\,\alpha E_k) + \alpha\hbar\omega_o^2 \tag{13.3}$$

Thus, $q = \frac{-B \pm \sqrt{B2 - 4AC}}{2A}$. Here, **q** is limited within the *first Brillouin Zone.*

The next step of the procedure is the calculation of the final polar angle. For that purpose we use well known expression, where r is a random number uniformly distributed between 0 and 1,

$$r = \frac{\int_0^\theta \sin\theta\,\int_0^\infty k'^2\,dk' S\,(k\,,k')}{\int_0^\pi \sin\theta\,\int_0^\infty k'^2\,dk' S\,(k\,,k')} \tag{14}$$

.Since the probability has to be conserved and P(r) = 1, we have

(7b)

$$P(r)dr = P(\theta)d\theta \Rightarrow P(\theta) = P(r)\frac{dr}{d\theta} = \frac{dr}{d\theta} \tag{15}$$

Thus,

$$P\,(\theta) = \frac{\sin\theta\int_0^\infty k'^2\,dk' S\,(k\,,k')}{\int_0^\pi \sin\theta\,\int_0^\infty k'^2\,dk' S\,(k\,,k')} \\ = \frac{\sin\theta\,A\left(E_k + \hbar\omega_q\right)|M(q)|^2\,(N_q + \frac{1}{2} \mp \frac{1}{2})}{\int_0^\pi \sin\theta\,A\left(E_k + \hbar\omega_q\right)|M(q)|^2\,(N_q + \frac{1}{2} \mp \frac{1}{2})} \tag{16}$$

This summarizes our analytical model. The actual implementation goes as follows:

1. Fix the value of E_k.
2. Vary θ from 0 to π in increments dθ. For each dθ, check (B^2-4AC). If (B^2-4AC) < 0, that value of θ does not contribute to the scattering rate or

the calculation of the probability density function for the polar angle.

3. Calculate q using $q = \frac{-B \pm \sqrt{B2-4AC}}{2A}$.
4. Determine ω_q.
5. Calculate the expressions given by the Eqs. (6) and (16).
6. Increment the energy E_k and go to step 2.
7. Repeat the above procedure till $E_{max} = 2$ eV.

For some special cases and under certain approximations closed form analytical expression for the acoustic and intervalley phonon scattering rates can be obtained [11].

Simulation results for the Drift Velocity in Silicon

The optical phonons involved in *g*- and *f*-type of intervalley scattering processes used in this work and the corresponding coupling constants are summarized in Table 2. The longitudinal acoustic (LA) and the transverse acoustic (TA) deformation potential constants are assumed to be 2.75 eV.

Table 2. Intervalley Phonon Energies and Deformation Potentials [8] .

	Type	T (K)	E (meV)	Deformation Potential used (10^8 eV/cm)
f_2	LO	550	47.4	3.5
f_3	TO	685	59.0	1.5
g_3	LO	720	62.0	6.0

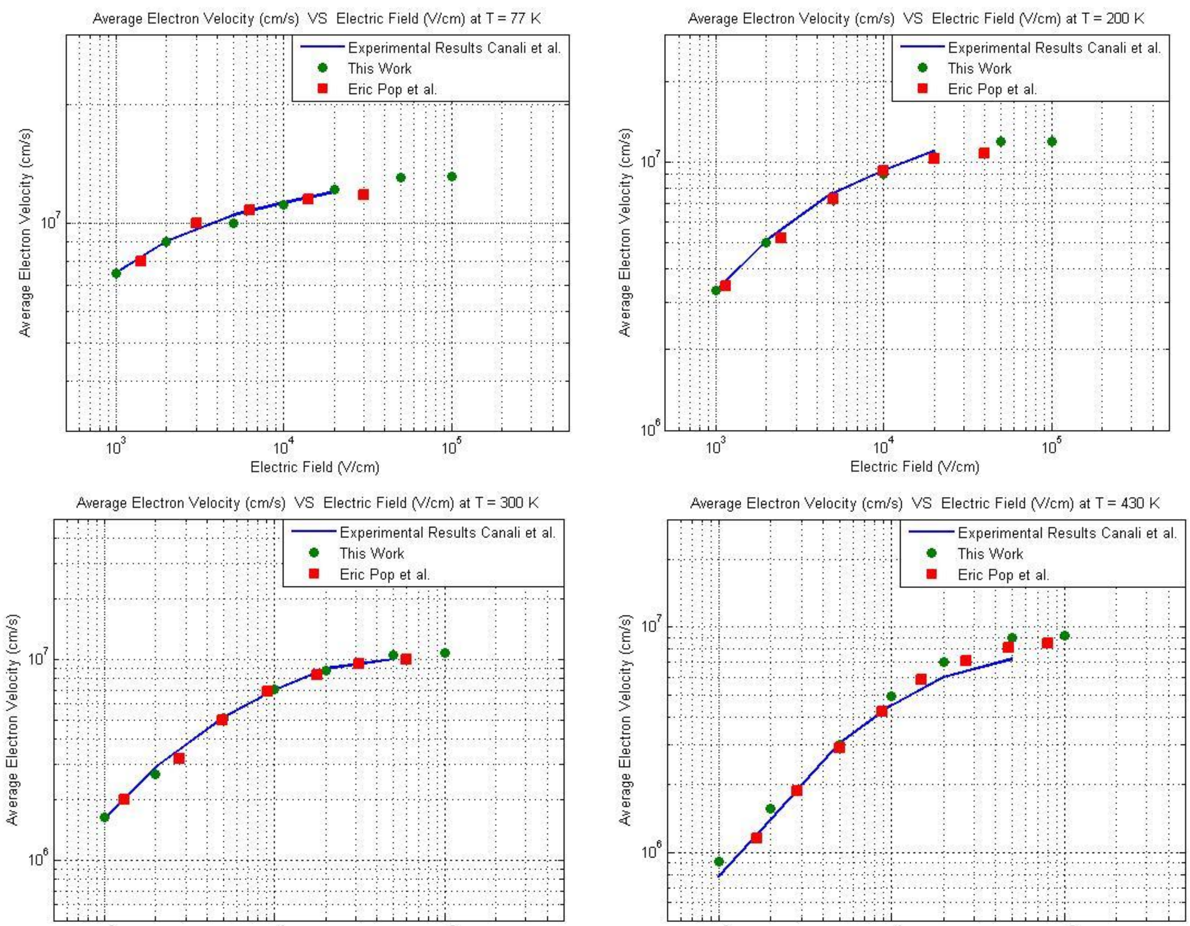

Figure 2. Average electron velocities in bulk silicon as a function of the electric field.

The average electron velocities for T=77K, 200K, 300K and 430K as a function of the electric field are shown in Figure 2. Also shown here are the Pop *et al.* [8] simulation data and experimental data from the literature. Excellent agreement between the three sets of data is being observed for the temperature range considered in this study. The accuracy of the scheme is further justified by the electron mobility plots vs. electric field for T=77K, 200K, 300K and 430K. Again, excellent agreement is observed when compared to Eric Pop *et al*. simulation data [8] and experimental data [1].

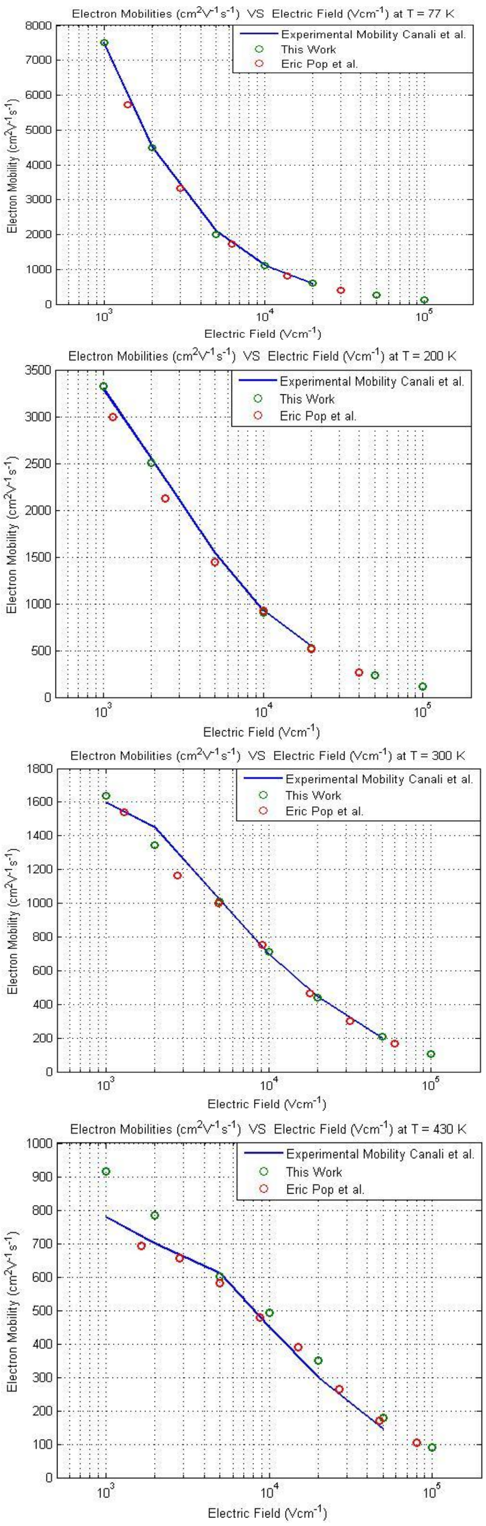

Figure 3. Low-field electron mobility in bulk silicon as a function of the electric field.

III. CONCLUSIONS

A semi-analytical model is presented and implemented that accounts for the phonon dispersions when calculating the acoustic and *f*- and *g*-intervalley scattering rates in bulk silicon. The validity of the model is justified with comparison of the average drift velocity and low field electron mobility with available experimental data. The very good agreement between the theoretical and experimental values justifies the validity of our approach.

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