Drift Velocity and Mobility Calculation in Bulk Silicon Using Analytical Dispersion Models for Acoustic and Optical Phonons

M. L. Gada[1], D. Vasileska[1], K. Raleva[2] and S. M. Goodnick[1].

[1]Arizona State University, Tempe, AZ.
[2]University Sts. Cyril and Methodius, FEIT, Skopje, Republic of Macedonia.
e-mail: mgada@asu.edu, vasileska@asu.edu.

Abstract

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 and theoretically. In the theoretical calculations non-parabolic bands and full-band bulk Monte Carlo calculations have been used. Phonons have been treated either using the Debye approximation for the acoustic modes and the Einstein relation for the optical modes or full phonon dispersions have been calculated using the rigid ion approximation. In a recent work by Pop and co-workers [1] 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, which tends to be time consuming. To obtain results faster, in this work an analytical model for the scattering rates has been used that utilizes the full phonon dispersion.

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 phonons dispersions is performed for both the acoustic and optical branches with parameters summarized in Table 1.

The actual implementation of the scattering rates calculation goes as follows:

1. Fix the value of E_k.
2. Vary θ from 0 to π in increments $d\theta$. Retain only real values of q from the corresponding quadratic equation.
3. Calculate q.
4. Determine ω_q from the dispersion relation.
5. Calculate the probability for the final polar angle of scattering.
6. Increment the energy E_k and go to step 2.
7. Repeat the procedure until E_{max} is reached. (E_{max}=2 eV)

In Figure 2 we show the low-field electron mobility and the drift velocity along the channel for different temperatures (77K and 300K). Excellent agreement between theoretical and experimental data is obtained, which justifies the validity of the analytical model derived.

[1] E. Pop, R. Dutton and K. Goodson, *Analytic band Monte Carlo model for electron transport in Si including acoustic and optical phonon dispersion,* Journal of Applied Physics Volume 96, Number 9, November 2004.

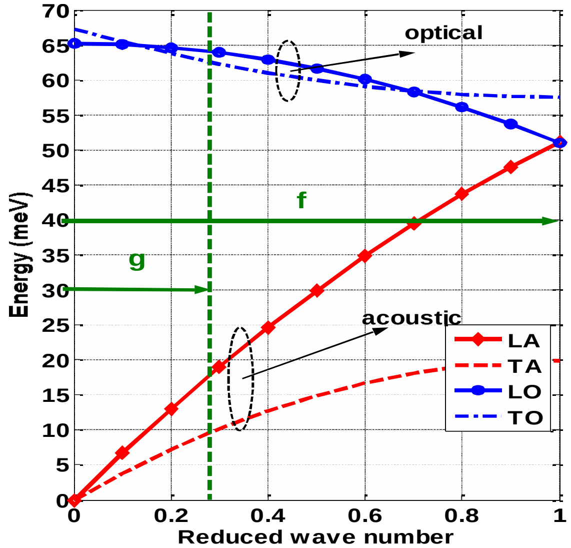

Table. 1 Quadratic Phonon Dispersion Coefficients:

	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. Phonon dispersions along [100] direction used in the model.

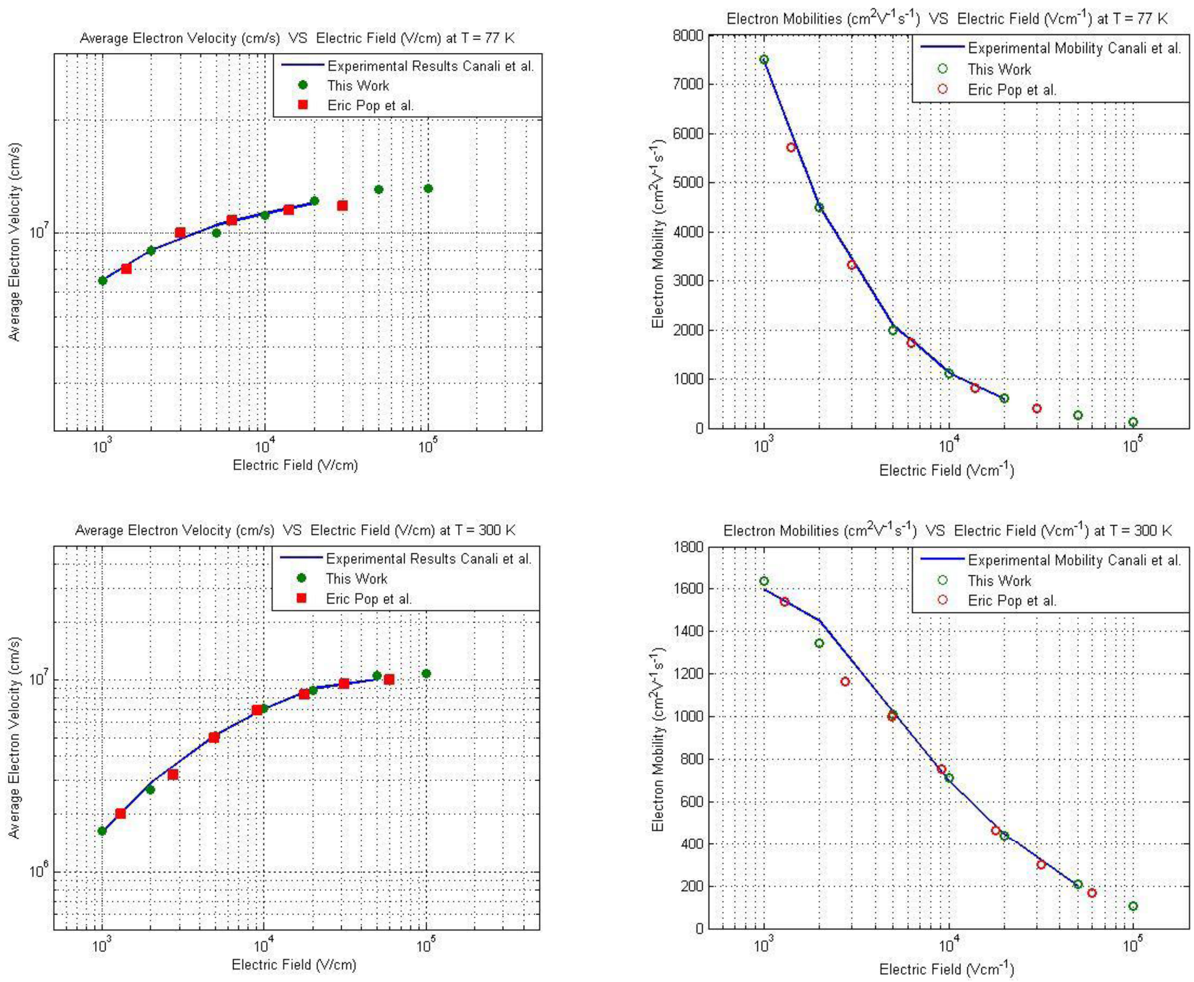

Figure 2. Drift velocity (left column) and mobility (right column) in bulk Si at 77K and 300 K.