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Monte Carlo simulation of high-energy transport of electrons and holes in bulk SiGeC alloys

M Michaillat, D Rideau, F Aniel and H Jaouen

1 STMicroelectronics, 850, rue Jean Monnet, 38926 Crolles, France
2 IEF - CNRS UMR 8622, Bât. 220, Université Paris-Sud, 91045 Orsay, France
E-mail: marc.michaillat@st.com

Abstract. High-energy transport properties of charge carriers in ternary random Si$_{1-x-y}$Ge$_x$C$_y$ alloys are investigated using Full-Band Monte Carlo simulations. Models for scattering mechanisms include phonon scattering, impact ionization and alloy scattering. Phonon scattering rates are wave-vector dependent and calculated consistently with the Full-Band structure. Impact ionization rates are modeled using analytical Keldysh formulas fitted to previously reported ab initio results. We derive a model for alloy scattering rate specific to ternary random alloys. It involves 2 effective alloy potentials which are independently calibrated on experimental mobility measurements. Presented Monte Carlo simulation results are shown to be in very good agreement with a variety of high-energy transport measurements, including drift velocities, impact ionization coefficients and quantum yields. Effects of alloy composition on the electrical characteristics of Si$_{1-x-y}$Ge$_x$C$_y$ alloys are investigated.

1. Introduction
Performance optimization of advanced heterojunction bipolar transistors has led to the introduction of germanium and carbon in the device base, yielding SiGeC base layers biaxially strained on Si. TCAD simulation of the electrical operation of such SiGeC/Si HBTs should include transport parameter models relevant to ternary SiGeC alloys. The aim of this work is to investigate high-energy carrier transport in Si$_{1-x-y}$Ge$_x$C$_y$ materials within the alloy composition domain defined by 0 < x < 100% and 0 < y < 2%, by means of Full-Band Monte Carlo (MC) method. The physical models for scattering mechanisms are described and compared with literature in section 2. In section 3, simulation results for high-field transport properties in Si$_{1-x-y}$Ge$_x$C$_y$ materials are reported.

2. Scattering models
Our MC simulations rely on SiGe band structures calculated with Tight-Binding method [1]. In order to simulate high-energy transport phenomena, it is necessary to accurately describe the dispersion relation up to 5 eV above the band minima, consequently 5 conduction bands and 3 valence bands are accounted for.

Phonon scattering rates are wave-vector dependent and are calculated consistently with the Full-Band structure [2]. Phonon modes in SiGeC alloys are modeled by 4 Si-Si modes and 4 Ge-Ge modes. Alloy modes such as C-C modes or mixed Si-Ge modes are neglected. The probability for a carrier of wave-vector $k$ in band $\nu$ to interact with a phonon mode $\eta$ is given
by:

$$P_{\eta,\nu}(k) = \sum_{\nu',k'} \frac{\pi}{\rho\omega_\eta(q)} \Delta_\eta^2 \times I(k,k')^2 \times \delta \left( E_\nu - E'_\nu \mp \hbar\omega_\eta(q) \right) \left( n_\eta(q) + 1/2 \pm 1/2 \right) \quad (1)$$

where upper and lower signs respectively refer to phonon emission and absorption. In (1), phonon dispersions $\omega_\eta(q)$ are approximated by isotropic quadratic expressions, as in Ref.[3]. Electron overlap integrals $I(k,k')$ are modeled within the Nordheim approximation [4]. Hole overlap integrals are described by Wiley’s angular expressions [5]. Deformation potentials $\Delta_\eta$ are treated as empirical parameters. As such they are assumed to depend on the square root of the initial carrier energy, in a similar way as in Ref.[6]. The total carrier-phonon scattering rates in bulk Si and Ge are plotted in Fig.1. In the case of Si, it can be seen that our calibrated rates are in excellent agreement with the consensus established by the modeling community. However in the case of Ge, although several studies have applied Full-Band techniques to the simulation of charge carrier transport [7, 8, 9, 4, 10], only the early work of Fischetti was found to have reported the total electron-phonon scattering rate magnitude. It appears that our results are in strong disagreement with Fischetti’s, however it must be stressed that our scattering rate was calibrated together with a realistic impact ionization rate derived from ab initio calculations, whereas the early work of [7] relied on an arbitrary Keldysh formula. In SiGeC alloys, the total phonon rate is expressed as a weighted sum of the scattering rates due to Si-Si and Ge-Ge modes [11]:

$$P_{\eta,\nu}(x,y,k) = (1-x) \cdot P_{\eta,\nu}^{Si}(k) + x \cdot P_{\eta,\nu}^{Ge}(k) \quad (2)$$

Impact ionization rates in bulk Si and Ge are modeled with analytical energy-dependent Keldysh formulas:

$$P_{\text{II}}(E) = P_0 \times (E - E_0)^{\alpha} \quad (3)$$

Figure 1: Electron- and hole-phonon scattering rates as a function of carrier energy in bulk Si and Ge at 300 K. Our results are compared with Full-Band results exposed in Refs.[12, 6] and [7] for Si and Ge, respectively.
Table 1: Keldysh formula parameters for the impact ionization rate in bulk Si and Ge.

<table>
<thead>
<tr>
<th>Material</th>
<th>Carrier</th>
<th>( P_0 ) (eV(^{-\alpha_0} ) s(^{-1} ))</th>
<th>( \alpha_0 )</th>
<th>( E_0 ) (eV)</th>
<th>Ref.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Si</td>
<td>e</td>
<td>( 1.0 \times 10^{11} )</td>
<td>4.6</td>
<td>1.1</td>
<td>[13]</td>
</tr>
<tr>
<td></td>
<td>h</td>
<td>( 1.14 \times 10^{12} )</td>
<td>3.4</td>
<td>1.49</td>
<td>[14]</td>
</tr>
<tr>
<td>Ge</td>
<td>e</td>
<td>( 4.0 \times 10^{11} )</td>
<td>4.8</td>
<td>0.8</td>
<td>[8]</td>
</tr>
<tr>
<td></td>
<td>h</td>
<td>( 1.2 \times 10^{12} )</td>
<td>3.8</td>
<td>1.0</td>
<td>[15]</td>
</tr>
</tbody>
</table>

The parameters \( P_0, E_0 \) and \( \alpha_0 \) are adjusted so that the empirical rate in (3) fits \textit{ab initio} calculated ionization rates. Parameter values together with references of the \textit{ab initio} studies from which they were determined are indicated in table 1. In SiGe alloys, Keldysh parameters are linearly interpolated between their respective values in Si and Ge. Since no information was found concerning impact ionization in bulk carbon or in carbon alloys, C mole fraction \( y \) is assumed to have no influence on impact ionization rates.

Once models for phonon scattering and impact ionization have been specified, simulations of carrier transport in pure Si and Ge materials can be carried out. MC results are compared to a variety of experimental data, including drift velocity characteristics (cf. Fig.2a), impact ionization coefficients (cf. Fig.2b), and quantum yield measurements.

Simulation of charge carrier transport in random alloys requires the inclusion of an additional scattering mechanism, namely alloy scattering. Our model for alloy scattering extends the commonly used model specific to binary random alloys (see e.g. Refs.[11, 16]) to the more general case of ternary random alloys. Alloy scattering rate in ternary \( \text{Si}_{1-x-y}\text{Ge}_x\text{C}_y \) is expressed as:

\[
P_{\text{alloy}}(x,y,E) = \frac{2\pi}{h} \Omega_c \cdot D(E) \cdot \left[ x(1-x) \cdot U_{\text{Si-Ge}}^2 + y(1-y) \cdot U_{\text{Si-C}}^2 - 2xy \cdot U_{\text{Si-Ge}} \cdot U_{\text{Si-C}} \right]
\]

where \( D(E) \) is the density of states per spin. In (4), \( U_{\text{Si-Ge}} \) and \( U_{\text{Si-C}} \) are effective alloy potential parameters, which are independently calibrated to reproduce low-field mobility measurements in binary \( \text{Si}_{1-x}\text{Ge}_x \) [17] and \( \text{Si}_{1-y}\text{C}_y \) [18] alloys. When the particle undergoes an alloy scattering event, the MC particle post-scattering state \((k',\nu')\) is randomized on the energy-conserving surface.

![Figure 2: Comparison between MC simulations and measurements for the drift velocity and impact ionization coefficient of holes in bulk Si and Ge.](image-url)
Figure 3: Electron drift velocity as a function of electric field in bulk binary SiGe and SiC alloys. MC simulation results are shown for several alloy compositions.

3. Simulation results
Based on the bandstructure and scattering models exposed in section 2, high-field properties of Si$_{1-x}$Ge$_x$C$_y$ alloys can be investigated by constant-field single-particle MC simulation. In order to study how the substitutional Ge and C concentrations affect SiGeC electrical properties, we plot in figures 3a and 3b the electron velocity-field characteristics as obtained from MC simulations of binary SiGe and SiC alloys, respectively. It can be seen that both Ge- and C-alloying result in a strong degradation of the electron mobility and saturation velocity. However equivalent results are obtained with 10% Ge and 0.2% C, emphasizing the higher scattering strength of substitutional C atoms as compared to Ge atoms.

4. Conclusion
In this paper, the Monte Carlo technique has been applied to the simulation of high-field properties of ternary SiGeC materials. All the relevant scattering mechanisms have been physically accounted for, and specifically addressed to both electrons and holes. Results for high-energy transport in bulk Si and Ge have been extensively compared to measurements. The models should yield a robust basis for the study of charge carrier transport in SiGeC alloys.

References