Anisotropic hole drift velocity in 4H-SiC

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1. Introduction

The intrinsic properties of the wide band gap semiconductors, specifically the wide band gap energy that enables higher junction operating temperatures, high saturated electron drift velocity, small dielectric constant, and in the case of SiC a relatively high thermal conductivity, make these materials particularly attractive for high power device applications. The most attractive candidate materials for high power device applications are GaN and some of the various polytypes of SiC [1–5]. In both of these materials, the breakdown electric field strengths are expected to be about four times larger than in either silicon or GaAs. In addition to the similar properties of GaN (large energy band gap, high carrier saturation drift velocity, and relatively small dielectric constant) SiC has a significantly higher thermal conductivity: a high thermal conductivity is necessary in order to overcome device-heating effects which is particularly important in power amplifiers [1–5].

Silicon carbide can form in many distinct crystal structures (know as polytypes), with some of the most common being 3C-SiC (cubic), 4H-SiC (hexagonal) and 6H-SiC (hexagonal) [6]. Hexagonal SiC polytypes, 4H-SiC and 6H-SiC, commonly used for the fabrication of devices, have anisotropic transport properties, but the degree and characteristics anisotropy are different. The anisotropy is associated with the hexagonal symmetry, which causes the hole effective masses to differ significantly between orientations parallel to the c-axis (which we call \( m_{hc} \)), and those along the basal plane perpendicular to the c-axis (which we call \( m_{hb} \)). Among the several polytypes in SiC, 4H-SiC has been recognized as the most attractive material for electronic devices in high-power, high-frequency, and high-temperature operations because of its wider band gap and higher electron mobility than other polytypes [7–12].

The optical and transport properties of semiconductors have been studied by using Nonequilibrium Green’s Functions Techniques, Monte Carlo simulation, balance equation, etc. Here, we use the NESEF (Non Equilibrium Statistical Ensemble Formalism) [13–23]. The NESEF is practical and efficient in the study of the transport and optical properties of semiconductors [24–29]. More specifically, we use a Nonequilibrium Quantum Kinetic Theory derived from NESEF [30].

In this work NESEF has been used for the study of bulk nonlinear transport properties in 4H-SiC when the transport direction is along the c-axis, or when the transport direction is in the plane perpendicular to it. The hole drift velocity and the nonequilibrium temperature in the transient and steady state are obtained, and their dependence on the electric field strength is derived and analyzed.
interaction of the holes with the impurities, the hole-phonon interaction, the anharmonic interaction of the TO-phonons with AC-phonons, the anharmonic interaction of the LO-phonons with AC-phonons, the interaction of the AC-phonons with the thermal bath (external thermal reservoir at temperature $T_0$). In Section III we use the parameters corresponding to the semiconductor 4H-SiC for numerical calculations.

The nonequilibrium thermodynamic state of the system is very well characterized for the set of basic variables:

\[
\{ (E_{ht}), N, (P_{ht}), (E_{LO}), (E_{TO}), (E_{AC}) \}
\]

that is: the energy of the holes $E_{ht}(t)$; the number $N$ of the holes; the linear momentum $P_{ht}(t)$ of the holes; the energy of the LO-phonons $E_{LO}(t)$; the energy of the TO-phonons $E_{TO}(t)$; and the energy of the AC-phonons.

### Table 1

Parameters of the 4H-SiC [6,34,35].

| Parameter                                      | Value     |
|-----------------------------------------------|-----------|
| Hole effective mass for $e_\perp m_0^*_{\perp}$| 0.59 $m_0$ |
| Hole effective mass for $e_\parallel m_0^*_{\parallel}$ | 1.60 $m_0$ |
| Lattice constant $a$                          | 3.073 Å   |
| Lattice constant $c$                          | 10.053 Å  |
| Longitudinal optical phonon energy $h\omega_{LO}$ | 120 meV   |
| Transverse optical phonon energy $h\omega_{TO}$ | 98 meV    |
| Mass density                                 | 3.12 g/cm$^3$ |
| Longitudinal sound velocity $v_{L}$          | 1.355 $\times$ 10$^5$ cm/s |
| Transverse sound velocity $v_{T}$            | 7.5 $\times$ 10$^5$ cm/s  |
| Acoustic deformation potential $D_a$         | 6.5 eV    |
| Optical deformation potential $D_o$          | 3.2 $\times$ 10$^9$ eV/cm |
| Low frequency dielectric constant $\varepsilon_0$ | 10.0     |
| High frequency dielectric constant $\varepsilon_\infty$ | 6.7      |
The nonequilibrium thermodynamic variables associated with variables of set (1), according to the NESEF [16–18,31], are

\[
\{ \beta_n^* (t), -\beta_n^* (t)\mu_n^* (t), -\beta_{n\beta}^* (t)v(t), \beta_{\beta\beta}^* (t), \beta_{\beta\tau}^* (t), \beta_{\beta AC}^* (t) \}.
\]  

where \( v(t) \) is the drift velocity of the holes, \( \mu_n^*(t) \) is the quasi-chemical potential and

\[
\beta_n^* (t) = \frac{1}{k_B T_n^*(t)}, \quad \beta_{LO}^* (t) = \frac{1}{k_B T_{LO}(t)}, \quad \beta_{TO}^* (t) = \frac{1}{k_B T_{TO}(t)}, \quad \beta_{AC}^* (t) = \frac{1}{k_B T_{AC}^*(t)},
\]

where \( k_B \) is Boltzmann constant, \( T_n^*(t) \) is the nonequilibrium temperature of the holes, \( T_{LO}(t) \) is the nonequilibrium temperature of the LO-phonons, \( T_{TO}(t) \) is the nonequilibrium temperature of the TO-phonons and \( T_{AC}(t) \) is the nonequilibrium temperature of the AC-phonons [31–33].

By using the Nonlinear Quantum Kinetic Theory based on the NESEF, we obtain the equations of evolution for the basic macrovariables [30]:

\[
\frac{dP(t)}{dt} = -nVeE + J_{\beta n}(t) + J_{\beta m}(t), \quad \frac{dE_n(t)}{dt} = \frac{e}{m_h} E\cdot P(t) + J_{\beta n}(t),
\]

\[
\frac{dE_{LO}(t)}{dt} = J_{LO}(t) - J_{LO,an}(t), \quad \frac{dE_{TO}(t)}{dt} = J_{TO}(t) - J_{TO,an}(t),
\]

\[
\frac{dE_{AC}(t)}{dt} = J_{AC}(t) + J_{LO,an}(t) + J_{TO,an}(t) - J_{AC,df}(t),
\]

where \( n \) is the concentration of holes fixed by doping (and consequently \( dn/dt = 0)\); \( E_n(t) \) is the energy of the holes; \( P(t) \) is the linear momentum of the holes; \( E_{LO}(t) \) is the energy of the longitudinal optical phonons that interact with the holes via optical deformation potential and Fröhlich potential; \( E_{TO}(t) \) is the energy of the transverse optical phonons that interact with the holes via optical deformation potential; \( E_{AC}(t) \) is the energy of the acoustic phonons that interact with the holes via acoustic deformation potential; \( E \) is the constant electric field applied perpendicular (\( \perp \)) or parallel (\( \parallel \)) to the c-axis direction. Moreover, \( m_h^* = m_n^* \) when the constant electric field is applied perpendicular to the c-axis, or \( m_h^* = m_h^* \) when the constant electric field is applied parallel to the c-axis. These values and other parameters for the study of transport phenomena in 4H-SiC are shown in Table 1.

We notice that in Table 1 \( m_0 \) stands for the free electron mass.

In Eq. (4), the first right hand term (\( -nVeE \)) is the driving force created by the constant electric field applied. The second term, \( J_{\beta n}(t) \), is the rate of hole momentum transfer due to interaction with the LO, TO and AC phonons. The third term, \( J_{\beta m}(t) \), is the rate of hole momentum transfer due to interaction with the ionized impurities [36].

In Eq. (5), the first right hand term (\( -eE\cdot P(t)/m_h^* \)) is the rate of energy transferred from the constant electric field applied to the holes, and the second term, \( J_{\beta n}(t) \), is the transfer of the energy of the holes to the LO, TO and AC phonons.

In Eqs. (6)–(8), the first right hand term accounts for the rate of change of the energy of the LO, TO or AC phonons, respectively, due to interaction with the holes, that is, the gain of energy transferred to the phonons from the hot holes. Like this, the sum of contributions \( J_{LO}(t) + J_{TO}(t) \) and \( J_{AC}(t) \) is equal to the last term in Eq. (5), \( J_{\beta m}(t) \), but with change of sign. The second term in Eq. (6), \( J_{LO,an}(t) \), is the rate of transfer of energy from the LO-phonons to the AC-phonons via anharmonic interaction. We noticed that the term \( J_{TO,an}(t) \) is the same, however with different sign in Eqs. (6) and (8). The second term in Eq.
The hole energy dispersion relation $\varepsilon_h$ (three sub-bands) are highly non-parabolic – due to the small spin-orbit splitting $\gamma$, what implies in effective hole masses becoming strongly $k$-dependent. However, we shall restrict the situation to the conditions of low densities and weak to moderate electric field intensities so that the parabolic band approximation is acceptable, i.e., we take $\varepsilon_h = h^2 k^2 / 2m^*_h$.

3. Results and conclusions

The time evolution of the basic intensive nonequilibrium thermodynamic variables are obtained after numerically solve the set of coupled nonlinear integro-differential equations: Eqs. (4a)-(8). We assumed that the reservoir temperature is $T_0 = 300$ K, that the dopant concentration $n_t$ is equal to the hole concentration $n$, with $n = n_t = 10^{16}$ cm$^{-3}$. Moreover, we noticed that the electric fields applied to 4H-SiC (applied parallel to the $c$-axis or applied perpendicular to the $c$-axis) is restricted to be smaller than 200 kV/cm since inter-valley scattering is not considered in this work. We have used the parameters for 4H-SiC listed in Table 1 to perform the numerical calculations.

The time evolution of the hole drift velocity, $v_h(t)$, and the hole nonequilibrium temperature, $T_h(t)$, towards the steady state, for five values of the electric field intensity, is depicted in Figs. 1 and 2, respectively. In Figs. 1 and 2, the upper figure is for the $c$ applied perpendicular to the $c$-axis and the lower figure is for the $c$ applied parallel to the $c$-axis. It can be noticed that the time for the holes to attain the steady state is in this paper very approximately the same obtained previously by other authors using different descriptions of the transient transport phenomena [34,37]. Figs. 1 and 2 show the existence of an overshoot in both the hole nonequilibrium temperature and the hole drift velocity. The overshoot occurs when the carrier relaxation rate of energy is less than the carrier relaxation rate of momentum during the evolution dynamics of the macroscopic state of the system [38].

Fig. 3 shows the dependence of the hole drift velocity, in the steady state, with the electric field strength, and Fig. 4 shows the dependence on the electric field strength of the nonequilibrium temperatures of holes in the steady state of 4H-SiC. In Figs. 3 and 4, the upper figure is for the $c$ applied perpendicular to the $c$-axis and the lower figure is for the $c$ applied parallel to the $c$-axis. Looking at Fig. 3, it can be noticed that the lower drift velocity corresponds to $c$ applied parallel to the $c$-axis. This is a consequence that the holes have a greater effective mass in the direction parallel to the $c$-axis than in the direction perpendicular to the $c$-axis (see Table 1).

The Fig. 5(a) shows the ratio $\alpha_v = v(\varepsilon_d)/v(\varepsilon_0)$, that is, the ratio between the hole drift velocity with the $c$ applied perpendicular to the $c$-axis ($\varepsilon_d$) and the hole drift velocity with the $c$ applied parallel to the $c$-axis ($\varepsilon_0$). Moreover, the Fig. 5(b) shows the ratio $\alpha_T = T_h^c(\varepsilon_d)/T_h^c(\varepsilon_0)$, that is, the ratio between the hole nonequilibrium temperature with the $c$ applied perpendicular to the $c$-axis ($\varepsilon_d$) and the hole nonequilibrium temperature with the $c$ applied parallel to the $c$-axis ($\varepsilon_0$). Inspection of Figs. 5(a) and 5(b) tells us that the difference between $v(\varepsilon_d)$ and $v(\varepsilon_0)$ decreases with increasing of the electric field intensity, and the difference between $T_h^c(\varepsilon_d)$ and $T_h^c(\varepsilon_0)$ increases with increasing of the electric field intensity.

We emphasize that we take the “Einstein model” dispersionless frequency relation for $LO$ and $TO$ phonons and the “Debye model” dispersionless frequency relation for $AC$ phonons.
properties is required to develop high performance electronic devices. Depending on the particular device, one is interested in the carrier mobility either parallel to the c-axis or perpendicular to it.

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