Band structure anisotropy effects on the hole transport transient in 4H–SiC


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Abstract

We study the role of band structure anisotropy on the hole transport in 4H–SiC during the transient regime. For the same strength of the applied electric field, the drift velocity overshoot of the hole is stronger and reaches steady state later when the field is applied perpendicular to the c-axis, than when the field is in the c-axis direction. In both cases, the time for the hole drift velocity and mean energy to reach steady state is under 50 fs, depending on the electric field strength, and are one order of magnitude shorter than the time for the electron drift velocity and mean energy to attain the steady state.

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Keywords:

1. Introduction

Electronic devices based on silicon carbide polytypes are finding applications in the domain of high-temperatures, high-frequencies and chemically aggressive environments [1,2]. The 4H–SiC polytype has electron mobility almost two times larger than polytype 6H–SiC, and band gap and breakdown field higher than polytype 3C–SiC. However, despite the technological advantages of the 4H–SiC polytype, only a few works have been published concerning its electron [3–5] and hole [6–8] steady state transport properties.

The role of band anisotropy on the hole transport in 4H–SiC was studied through a full Monte Carlo simulation [8]. It was shown that there exists a significant anisotropy in the calculated steady-state hole drift velocities for electric fields applied parallel and perpendicular to the c-axis direction. The calculated drift velocity for transport parallel to the c-axis showed a stronger negative differential resistivity than that for electric fields applied perpendicular to the c-axis. In particular, recently we have investigated the effects of anisotropy and lattice temperature on the ultrafast electron transport transient of 4H–SiC, whose understanding is important for device-down scaling [9].

The purpose of this work is to present results on the effects of the 4H–SiC band anisotropy on the evolution of the hole drift velocity and mean energy towards the steady state. They are calculated by solving balance transport equations within the energy and momentum relaxation times approximation. It is shown that the electric field \( E_p \) applied perpendicular to the c-axis produces an overshoot effect on the transient hole drift velocity, which is considerably longer than that which occurs when the electric field is applied parallel to the c-axis.

2. The calculations procedure

By taking full advantage of the Monte Carlo steady state data of Bellotti et al. [6], the energy and momentum relaxation times are calculated. Consequently, hole–phonon interactions with acoustic, nonpolar, polar optical modes, and ionized impurity scattering are taken into account. Following the scheme proposed originally by Shur [10] and adopted by several authors [11–15], coupled Boltzmann-like equations for the hole drift velocity and mean energy are solved numerically within the relaxation time approximation, and taking the hole effective mass perpendicular (parallel) to the c-axis \( m_{ML} = 0.59m_0 \) (\( m_{ML} = 1.60m_0 \)) [16] when the electric field is applied in this direction. Here, \( m_0 \)
is the free space electron mass. Although Bellotti et al. [6] have considered electric field intensities up to 4 MV/cm, in our calculations we have imposed the field strength to be smaller than 1000 kV/cm, avoiding stronger occupation of the highest energy bands, since in our model only one is considered for each direction of the field. We point out that interband tunneling contributes only indirectly through the calculation of the relaxation times that we have performed with the steady state data of Bellotti et al. [6].

3. The anisotropy effects

The evolution of the hole drift velocity towards steady state for electric fields $E_F = 100$, 400, and 700 kV/cm applied in the directions perpendicular (solid lines) and parallel (dashed lines) to the c-axis is presented in Fig. 1. When the electric field strength is small ($E_F \approx 100$ kV/cm), there is no overshoot in the hole drift velocity in both the perpendicular ($E_{F,\perp}$) and in the parallel direction ($E_{F,\parallel}$) to the c-axis.

The onset of the overshoot occurs at 120 kV/cm for $E_{F,\perp}$, and at 200 kV/cm for $E_{F,\parallel}$. For the same electric field intensity, the overshoot in the hole drift velocity in the direction perpendicular to the c-axis is always considerably stronger than that in the direction parallel to the c-axis. This is due to the fact that $m_{M,\perp}$ is smaller than $m_{M,\parallel}$. However, in both cases the time for the hole to attain steady state is $\sim 50$ fs (1 fs = $10^{-15}$ s) when the overshoot in the hole drift velocity occurs. The transient regime of the hole drift velocity in 4H–SiC is one order of magnitude shorter than that of an electron: in 4H–SiC for both the directions perpendicular and parallel to the c-axis [9]; and the same comparison applies also to wurtzite InN subjected to electric fields applied in the $\Gamma - A$ and $\Gamma - M$ directions [13].

Fig. 2 shows the evolution of the hole energy towards the steady state. One can observe that the transient regime becomes shorter when the electric field intensity increases. For the same electric field strength, the hole energy at a given time $t$ is always higher when the $E_F$ is applied in the perpendicular direction to the c-axis than in the parallel direction, which is due to the fact the hole scattering mechanisms are weaker in the former direction, rather than in the later, and this is a consequence of the energy dependence of the band flattening in those directions. As for the drift velocity, the hole energy transient regime in 4H–SiC is also much shorter than that of an electron: in 4H–SiC for both the directions [9] and that in wurtzite InN subjected to fields applied in the $\Gamma - A$ and $\Gamma - M$ directions [13].

4. Concluding remarks

Although the theoretical scheme used to describe the transport transient regime of holes in 4H–SiC is recognized as very effective computationally, it has the drawback of do not take into account in detail the characteristics of the band structure (mixing and crossing points) and tunneling between bands as in the Monte Carlo simulation approach of Belloti et al. [6]. These effects were indirectly considered through their contribution to the momentum and energy relaxation times that we have calculated using the steady state relations between the hole drift velocity and energy and the applied electric field $E_F$.

On the other hand, since good 4H–SiC samples with small density of defects were not grown yet, detailed measurements of the 4H–SiC band structure were not performed yet—see, however, Refs. [17,18]. Although quiet useful to obtain a full band picture of a crystal structure, even the most improved theoretical method used nowadays (EPM, LAPW, etc.) have their limitations if a detailed description is sought. As a consequence, state of the art points also to the limitations of this work, since its results...
are rooted on the steady state data of Bellotti et al. [6] as mentioned previously. However, they allowed to estimate, for the first time, to the knowledge of the authors, the effects of band anisotropy on the hole transport in 4H–SiC during the transient regime.

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