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Solid State Communications 145 (2008) 397–400
solid state communications
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Band structure anisotropy effects on the ultrafast electron transport in 4H-SiC

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Received 9 March 2007; received in revised form 19 August 2007; accepted 13 November 2007 by B. Jusserand
Available online 17 November 2007

Abstract

We study band structure anisotropy effects on the electron transport transient in 4H-SiC subjected to electric fields parallel and perpendicular to the c-axis direction. Coupled Boltzmann-like energy–momentum balance transport equations are solved numerically within a single equivalent isotropic valley picture in the momentum and energy relaxation time approximation. The electron drift velocity is shown to be higher in the direction parallel to the c-axis than that perpendicular to it, due to the electron effective mass being larger in the former direction. The ultrafast transport regime develops on a subpicosecond scale ($\lesssim$0.2 ps) in both directions, during which an overshoot in the electron drift velocity is observed at 300 K for sufficiently high enough electric fields (>60 kV/cm).
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PACS: 72.20.Ht; 72.20i; 73.40.Lq

Keywords: A. Semiconductors; D. Electronic transport

The silicon carbide polytype 4H-SiC is a potential candidate for applications in high-speed devices [1], high temperature power switching, and high-frequency power generation [2]. It has the advantage of having an electron mobility almost two times larger and a much smaller band structure anisotropy than the polytype 6H-SiC, as well as a band energy gap and breakdown field higher than that of the 3C-SiC polytype. The modelling of 4H-SiC-based field effect transistors has highlighted effects of nonstationary carrier transport on high-frequency domain operation [1], but without considering the band structure anisotropy. Electronic effective masses differ significantly for orientations parallel and perpendicular to the c-axis [3], with 4H-SiC having an anisotropy ratio (the ratio between the parallel and perpendicular electron mobilities) of 0.8 [4,5]. Effects of band structure anisotropy on the steady-state electron transport in 4H-SiC have been studied through Monte Carlo simulations [3,6,7] and hydrodynamic balance equations [8]. The calculated electron drift velocity for steady-state transport parallel to the c-axis was shown to be higher than that in the perpendicular direction and, for electric fields of the same intensity, has a stronger negative differential resistivity. This is due to the fact that the electron effective mass is smaller ($0.29m_0$) in the direction parallel to the c-axis than in the perpendicular direction ($0.42m_0$) [9]. m_0 is the free space electron mass.

Due to the trend of reducing the size of transport channels in silicon carbide devices to submicron scales, in particular for high-speed/high-field switching applications, nonstationary physical conditions will often be imposed upon carrier transport mechanisms in silicon carbide polytypes, leading to transients in the carrier drift velocity and in the mean energy occurring mainly at the beginning, for example, of the source–drain length. High-field transport transient of electrons in 6H- and 3C-SiC during the subpicosecond regime has been modeled within parabolic and nonparabolic band schemes, taking into account high lattice temperature effects [10,11]. The transient regime was predicted to be shorter than 0.2 ps, having an overshoot in the electron drift velocity for sufficiently high (>300 kV/cm) electric fields. This effect is more pronounced when band nonparabolicity is considered. An increase in the lattice temperature ΔT was shown to reduce the electron

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0038-1098/$ - see front matter © 2007 Elsevier Ltd. All rights reserved.
doi:10.1016/j.ssc.2007.11.005

drift velocity, and was even able to eliminate the overshoot effect in the electron drift velocity in 4H- and 3C-SiC, when $\Delta T \sim 400$ K, depending on the applied electric field strength. Recently, high lattice temperature effects on the ultrafast electron transport parallel to the c-axis direction in 4H-SiC has been studied [12]. It was demonstrated that the ultrafast transport regime follows a subpicosecond scale ($\lesssim$0.5 ps), during which an overshoot in the electron drift velocity occurs for high electric fields ($\gtrsim$60 kV/cm), depending on the lattice temperature. When the electric field strength is sufficient, an increase in the lattice temperature cannot eliminate the electron drift overshoot effect, although it can reduce it considerably due to the stronger electron–phonon scattering, while at the same time shifting the overshoot peak of the electron drift velocity to earlier times. However, band structure anisotropy effects on the electron transport transient properties in 4H-SiC have not been investigated.

The purpose of this work is to present results on how the band structure anisotropy in 4H-SiC changes the electron transport during the ultrafast transient regime. A partially compensated n-type material with $N_A = 10^{16}$ cm^{-3} and $N_D = 6 \times 10^{16}$ cm^{-3} is assumed in the calculations, and numerical solutions were obtained considering electric fields applied in directions parallel and perpendicular to the c-axis; $m_{e\parallel c} = 0.29 m_0$ and $m_{e\perp c} = 0.42 m_0$ [9]; the band nonparabolicity factor is 0.323 ev^{-1}; the other 4H-SiC parameters are taken from Ref. [6]. All the calculations were performed for a lattice temperature of 300 K. The evolution of the mean electron drift velocity $v(t)$ and mean energy $\epsilon(t)$ towards the steady state is studied by solving numerically the following coupled Boltzmann-like energy–momentum balance transport equations, within the single equivalent valley picture of Tsukioka, Vasileska, and Ferry [13], and considering the momentum (τ_p) and energy (τ_ε) relaxation time approximation:

$$\frac{\mathrm{d}v(t)}{\mathrm{d}t} = \frac{qE}{m_c} - \frac{v(t)}{\tau_p(\epsilon)}; \tag{1}$$

$$\frac{\mathrm{d}\epsilon(t)}{\mathrm{d}t} = qv(t)E - \frac{\epsilon(t) - \epsilon_L}{\tau_\epsilon(\epsilon)}, \tag{2}$$

where $\epsilon_L = 3k_\mathrm{B}T_L/2$ is the average electron thermal energy at the lattice temperature T_L; $\tau_p(\epsilon)$ and $\tau_\epsilon(\epsilon)$ are the momentum and energy relaxation times, respectively; k_B is the Boltzmann constant, q is the electric charge of the electron, and m_c is the electron effective mass in the band. The relaxation times τ_p and τ_ε are estimated taking full advantage of the stationary state data of Quan, Weng, and Cui [8], *i.e.* acoustic deformation potential scattering, polar-optical phonon scattering, and ionized impurity processes are taken into account. However, nonpolar optical phonon, alloy and impact ionization scattering, and band-to-band tunneling are not considered [7], which is a drawback of our work. These mechanisms seem to contribute strongly to the existence of a negative differential resistance (NDR) in 4H-SiC for electric fields higher than 3 kV/cm [7]. However, the recent transport measurements of Ardaravičius et al. [14] in 4H-SiC at 293 K indicate the absence of NDR for electric fields up to 280 kV/cm.

The momentum and energy relaxation time strategy follows the scheme originally proposed by Shur [15], Rolland et al. [16], Carnez et al. [17], and Nougier et al. [18]. This approach was used by Alencar et al. [19] to investigate the high-field transport transient of minority carriers in p-GaAs, and by Caetano et al. [20] to study high magnetic field effects on the terahertz mobility of hot electrons in n-type InSb. Recently, Foutz et al. [21] compared transient electron transport results in wurtzite GaN, InN, and AlN calculated using Monte Carlo simulations and using the energy–momentum balance approach, finding a quite reasonable overall agreement. The great advantage of the approach used in this work is that it requires a shorter computation time when compared with the full Monte Carlo method. It is important to remark that a possible way of taking into account nonpolar optical phonon, alloy and impact ionization scattering, as well as band-to-band tunneling indirectly, in order to study their influence on the 4H-SiC transient transport regime, is to use the steady state $v \times E$ and $\epsilon \times E$ obtained by Hjelm et al. [7] for the calculation of the momentum and energy relaxation times to be used in the coupled Boltzmann-like energy–momentum balance transport equations.

Fig. 1 presents the ultrafast transient behavior of the electron drift velocity $v(t)$ in the parallel (solid lines) and perpendicular (dashed lines) directions with respect to the c-axis in 4H-SiC subjected to electric field intensities of (a) 66 kV/cm, (b) 360 kV/cm, (c) 660 kV/cm, and (d) 960 kV/cm. For a given electric field, $v_{e\parallel c}(t)$ is always higher than $v_{e\perp c}(t)$ at any instant in time t, due to the fact that $m_{e\parallel c} < m_{e\perp c}$. For electric field intensities smaller than 100 kV/cm, the transient regime of the electron drift is longer than 0.2 ps; however, when electric field strength increases, the ultrafast electron drift velocity transient becomes faster, arriving in less than 0.08 ps for electric fields stronger than 660 kV/cm. The onset of the drift velocity overshoot effect is weakly dependent on the band structure anisotropy, as can be observed in Fig. 1(a): a weaker electric field is necessary for the overshoot effect to occur in the direction parallel to the c-axis than that perpendicular to it. From Fig. 1(b)–(d), the overshoot effect is slightly stronger and occurs earlier in the direction parallel to the c-axis than in the perpendicular direction. The electric field dependence of the instant $t_{\mathrm{peak},v_{e\parallel c}}$ ($t_{\mathrm{peak},v_{e\perp c}}$) at which the peak of the electron velocity $v_{\max,e\parallel c}$ ($v_{\max,e\perp c}$) occurs is plotted in Fig. 2, showing that $t_{\mathrm{peak},v_{e\parallel c}} < t_{\mathrm{peak},v_{e\perp c}}$ for a given electric field. The difference between them becomes smaller when the electric field strength increases.

The evolution towards the steady state of the energy of the electron accelerated in the parallel (solid lines) and perpendicular (dashed lines) directions with respect 4H-SiC c-axis is depicted in Fig. 3. The transient regime of the electron energy is always shorter and reaches higher-steady state values in the former direction than in the latter, due to the fact that the overall electron scattering mechanisms are weaker in the parallel than in the perpendicular direction. In a similar way to that which occurs in the case of the transient regime of the electron drift velocity, the transient regime of the electron energy is longer than 0.2 ps for electric field intensities smaller

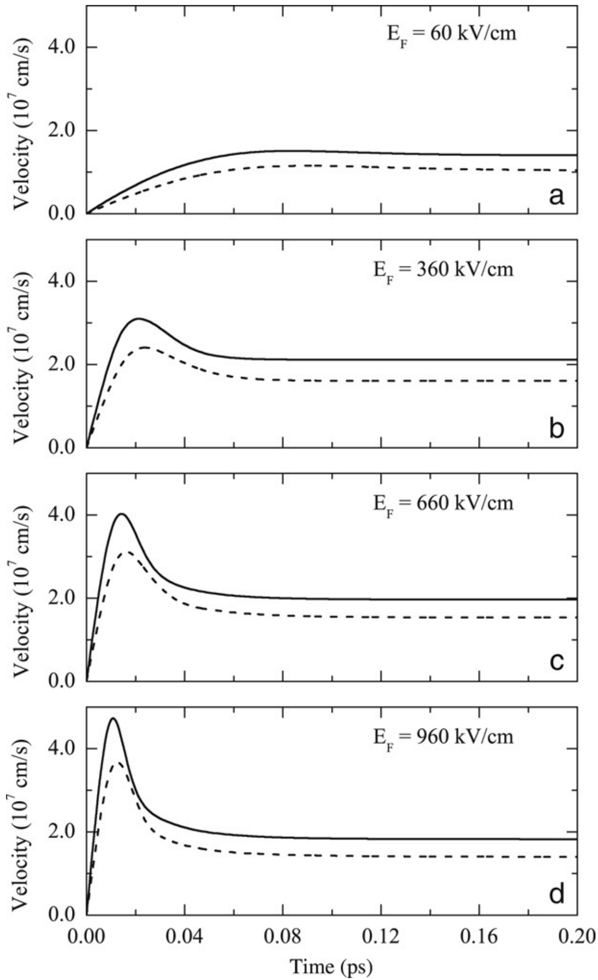

Fig. 1. Time evolution of the electron drift velocity in 4H-SiC at 300 K for electric fields applied in the directions parallel (solid line) and perpendicular (dashed line) to the c-axis with intensities: (a) 60 kV/cm; (b) 360 kV/cm; (c) 660 kV/cm; and (d) 960 kV/cm.

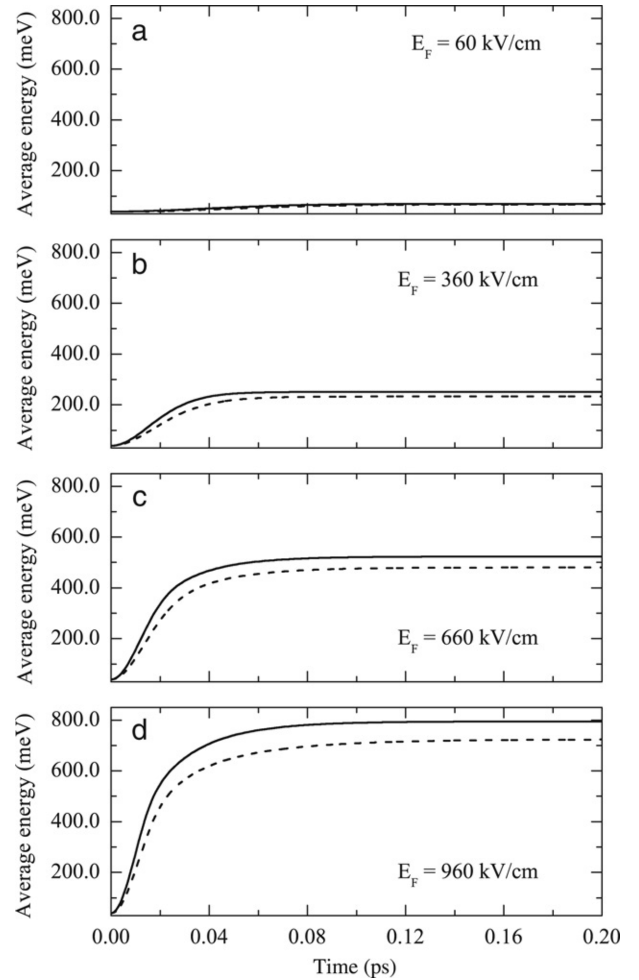

Fig. 3. Time evolution of the electron energy in 4H-SiC at 300 K for electric fields applied in the directions parallel (solid line) and perpendicular (dashed line) to the c-axis with intensities: (a) 60 kV/cm; (b) 360 kV/cm; (c) 660 kV/cm; and (d) 960 kV/cm.

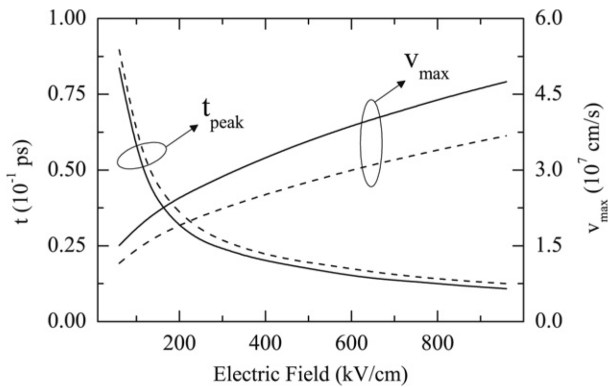

Fig. 2. Electric field behavior of the time in which the electron drift velocity overshoot peak occurs in 4H-SiC at 300 K for electric fields applied in the directions parallel (solid line) and perpendicular (dashed line) to the c-axis for $t_{\mathrm{peak},v_{e\parallel c}}$ and $t_{\mathrm{peak},v_{e\perp c}}$, respectively.

than 100 kV/cm; however, when the electric field strength increases, the ultrafast electron energy transient becomes faster, arriving in less than 0.12 ps for electric fields stronger than 660 kV/cm.

In conclusion, results concerning band structure anisotropy effects on the ultrafast transient properties of electrons in 4H-SiC subjected to electric fields in the directions parallel and perpendicular to the c-axis have been presented. The anisotropy was shown to be able to change the characteristics of the overshoot effect in the electron drift velocity (the strength and instant at which the velocity peak occurs) and to alter the transient regime of the electron energy. Although the theoretical scheme used to describe the electron transport transient regime in 4H-SiC is recognized as very effective computationally, it has the drawback of not taking into account detailed characteristics of the band structure, like mixing and crossing points [7]. A possibility of indirectly taking these scattering mechanisms into account, in order to study their influence on the 4H-SiC transient transport regime, is to use the steady state $v \times E$ and $\epsilon \times E$ calculated by Hjelm et al. [7] to determine the momentum and energy relaxation times. However, improved measurements of the 4H-SiC band structure have not yet been performed, which is a limiting factor for taking into account the detailed band structure in transport calculations. The theoretical methods used at present for band structure calculations also

have their own problems if a detailed description is sought (the problems related to the calculation of the valence band are well known, for example). Despite the drawbacks of the theoretical approach used in this work, it should stimulate state-of-the-art transport calculations based on detailed experimental band structure results in order to confirm the band structure anisotropy effects on the ultrafast electron transport in 4H-SiC presented here. With regard to measurements of the 4H-SiC transient transport properties, this difficult task has not yet been accomplished. However, optical-based techniques have been used recently to measure velocity-field characteristics and transient velocity overshoot in III-nitrides [22–25], overcoming the difficulties of classical transport measurement methods, and show promise for probing transport properties in silicon carbide polytypes.

Acknowledgements

FFM received a fellowship from the Coordenação de Aperfeioamento de Pessoal de Nível Superior (CAPES) at the Physics Department of the Universidade Federal do Ceará during the development of this research. The authors acknowledge the financial support provided by CNPq through the grant from CNPq-Rede NanoBioestruturas (No 555183/2005-0). VNF and JAPC are CNPq Research Fellows.

References

[1] F. Schwierz, M. Kittler, H. Förster, D. Schipanski, Diamond Related Mater. 6 (1997) 1512.
[2] R.R. Siergiej, R.C. Clarke, S. Sriram, A.K. Agarwal, R.J. Bojko, A.W. Morse, V. Balakrishna, M.F. MacMillan, A.A. Burk Jr., C.D. Brandt, Mat. Sci. Eng. B 61–62 (1999) 9.
[3] R.P. Joshi, J. Appl. Phys. 78 (1995) 5518.
[4] W.J. Schaffer, G.H. Negley, K.G. Irvine, J.W. Palmour, Mater. Res. Soc. Symp. Proc. 339 (1994) 595.
[5] M. Schadt, G. Pensl, Appl. Phys. Lett. 65 (1994) 3120.
[6] H.-E. Nilsson, U. Sannemo, C.S. Petersson, Appl. Phys. Lett. 80 (1996) 3365.
[7] M. Hjelm, H.-E. Nilsson, A. Martinez, K.F. Brennan, E. Bellotti, J. Appl. Phys. 93 (2003) 1 and references therein.
[8] H.J. Quan, X.M. Weng, H.L. Cui, Phys. Status Solidi (b) 219 (2000) 339.
[9] N.T. Son, W. Cheng, O. Kordina, A.O. Konstantinov, B. Monemar, E. Janzen, D. Hofman, D. Volm, M. Drechsler, B.K. Meyer, Appl. Phys. Lett. 78 (1995) 5518.
[10] E.F. Bezerra, E.W.S. Caetano, V.N. Freire, E.F. da Silva Jr., J.A.P. da Costa, Semicond. Sci. Technol. 14 (1999) 1007.
[11] E.W.S. Caetano, E.F. Bezerra, V.N. Freire, J.A.P. da Costa, E.F. da Silva Jr., Solid State Commun. 113 (2000) 539.
[12] F.F. Maia Jr., V.N. Freire, J.A.P. da Costa, J. Appl. Phys. 102 (2007) 053710.
[13] K. Tsukioka, D. Vasileska, D.K. Ferry, Physica B 185 (1993) 466.
[14] L. Ardaravičius, A. Matulionis, O. Kiprijanovic, J. Liberis, H.-Y. Cha, L.F. Eastman, M.G. Spencer, Appl. Phys. Lett. 86 (2005) 022107.
[15] M. Shur, Electron. Lett. 12 (1976) 615.
[16] P.A. Roland, E. Constant, G. Salmer, R. Fauquembergue, Electron. Lett. 15 (1979) 373.
[17] B. Carnez, A. Cappy, A. Kaszynski, E. Constant, G. Salmer, J. Appl. Phys. 51 (1980) 784.
[18] J.P. Nougier, J.C. Vaissiere, D. Gasquet, J. Zimmermann, E. Constant, J. Appl. Phys. 52 (1981) 825.
[19] A.M. Alencar, F.A.S. Nobre, A.J.C. Sampaio, V.N. Freire, A.J. Costa Sampaio, Appl. Phys. Lett. 59 (1991) 825.
[20] E.W.S. Caetano, E.A. Mendes, V.N. Freire, J.A.P. da Costa, X.M. Weng, X.L. Lei, Phys. Rev. B 57 (1998) 11872.
[21] B.E. Foutz, S.K. O'Leary, M.S. Shur, L.F. Eastman, J. Appl. Phys. 85 (1998) 7727.
[22] M. Wraback, H. Shen, J.C. Carrano, T. Li, J.C. Campbell, M.J. Schurman, I.T. Ferguson, Appl. Phys. Lett. 76 (2000) 1155.
[23] M. Wraback, H. Shen, J.C. Carrano, C.J. Collins, J.C. Campbell, R.D. Dupuis, M.J. Schurman, I.T. Ferguson, Appl. Phys. Lett. 79 (2001) 1303.
[24] R. Collazo, R. Schlesser, A. Roskowski, R.F. Davis, Z. Sitar, J. Appl. Phys. 88 (2000) 5865.
[25] R. Collazo, R. Schlesser, Z. Sitar, Appl. Phys. Lett. 81 (2002) 5189.