Transverse-velocity-fluctuation autocorrelation function of holes in silicon: The effect of valence-band anisotropy

J. M. Hinckley and J. Singh
Department of Electrical Engineering and Computer Science, The University of Michigan, Ann Arbor, Michigan 48109-2122
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Qualitative behavior is reported for the transverse-velocity-fluctuation autocorrelation function C_t for holes in silicon. Results of high-field Monte Carlo transport calculations show a negative minimum, or "undershoot" in C_t. Previously considered to occur only for the longitudinal-velocity-fluctuation autocorrelation function C_l, the undershooting is shown to depend upon both the orientation of the electric field and the degree of anisotropy of the valence band. This potentially holds consequences for the nature of the very-high-frequency transverse noise and diffusion characteristics of holes in any material with a warped band structure.

I. INTRODUCTION

The velocity-fluctuation autocorrelation function C_v of charge carriers in semiconductors shows the rate at which the motion of those carriers is randomized through scattering. From this autocorrelation function may be determined both the thermal noise spectrum and the diffusivity of the charge carriers.[1-5] The velocity-fluctuation autocorrelation function exists both when no electric field is applied to the material, and when a field is applied and driving a current. In the former case, the temporal behavior of the correlation function is a decaying exponential, starting at some maximum positive value at $t=0$ and approaching $C_v=0$ asymptotically. The rate of decay is of the order of the charge-carrier scattering rate. In the latter case, with an electric field present, two distinct correlation functions exist. One involves velocity fluctuations aligned with the applied field and is known as the longitudinal-velocity-fluctuation autocorrelation function, denoted C_l. The other involves velocity fluctuations perpendicular to the electric field and is known as the transverse-velocity-fluctuation autocorrelation function, denoted C_t. Although having different values, these two functions approach the same value as the electric field is reduced to zero.

It is generally known that under high electric field, the longitudinal function C_l exhibits undershoot.[1-3] That is, starting from some maximum positive value, C_l decreases rapidly, crosses zero, and reaches a minimum value less than zero, then returns toward zero asymptotically from the negative side. This is attributed to the competing effects of momentum relaxation and energy relaxation. In distinction to this behavior, generally it has been believed that the transverse function C_t, under high field, does not exhibit undershoot, but rather decays monotonically, toward zero, from a maximum positive value at $t=0$, much as in the zero-field case. It is this behavior of C_t which has been reexamined in the present work, using Monte Carlo calculations for the case of holes in silicon.

The velocity-fluctuation autocorrelation function is a function of time, and can most generally be expressed as a second rank tensor:[6]

$$C_{ij}(t)=\langle \delta v_i(t')\delta v_j(t'+t)\rangle \ , \tag{1}$$

where $\delta v_i(t')$ is the fluctuation of the velocity component, in direction i, with respect to its average (drift) value. The brackets denote averaging over all charge carriers; the average is independent of t'. If $\hat{\mathbf{n}}$ and $\hat{\mathbf{m}}$ are unit vectors, respectively parallel and perpendicular to the electric field, then the longitudinal and transverse correlation functions are straightforwardly given by

$$\begin{aligned} C_l(t)&=\langle \hat{\mathbf{n}}\cdot\delta\mathbf{v}(t')\hat{\mathbf{n}}\cdot\delta\mathbf{v}(t'+t)\rangle \ , \\ C_t(t)&=\langle \hat{\mathbf{m}}\cdot\delta\mathbf{v}(t')\hat{\mathbf{m}}\cdot\delta\mathbf{v}(t'+t)\rangle \ , \end{aligned} \tag{2}$$

where $\delta\mathbf{v}$ is the fluctuation of the velocity vector: $\delta\mathbf{v}=\hat{\mathbf{x}}\delta v_x+\hat{\mathbf{y}}\delta v_y+\hat{\mathbf{z}}\delta v_z$. In this work, fields oriented in three different directions were used: [100], [111], and [101]. For the [100] field, $\hat{\mathbf{n}}=\hat{\mathbf{x}}$, and all directions perpendicular to $\hat{\mathbf{n}}$ are equivalent, for example $\hat{\mathbf{m}}=\hat{\mathbf{y}}$. The following relations hold:

$$\begin{aligned} C_l&=C_{xx} \ , \\ C_t&=C_{yy}=C_{zz} \ , \\ C_{xy}&=C_{yz}=C_{zx}=0 \ . \end{aligned} \tag{3}$$

For the [111] field, $\hat{\mathbf{n}}=(\hat{\mathbf{x}}+\hat{\mathbf{y}}+\hat{\mathbf{z}})/\sqrt{3}$, and all directions perpendicular to $\hat{\mathbf{n}}$ are equivalent, for example $\hat{\mathbf{m}}=(\hat{\mathbf{x}}-\hat{\mathbf{z}})/\sqrt{2}$. The following relations hold:

$$\begin{aligned} C_a&\equiv C_{xx}=C_{yy}=C_{zz} \ , \\ C_b&\equiv C_{xy}=C_{yz}=C_{zx} \ , \\ C_l&=C_a+2C_b \ , \\ C_t&=C_a-C_b \ . \end{aligned} \tag{4}$$

For the [101] field, $\hat{\mathbf{n}}=(\hat{\mathbf{x}}+\hat{\mathbf{z}})/\sqrt{2}$. In this case, not all directions perpendicular to $\hat{\mathbf{n}}$ are equivalent. Taking $\hat{\mathbf{m}}_1=\hat{\mathbf{y}}$ and $\hat{\mathbf{m}}_2=(-\hat{\mathbf{x}}+\hat{\mathbf{z}})/\sqrt{2}$ as the symmetrically distinct, perpendicular unit vectors, the following relations hold:

$$
\begin{aligned}
&C_a \equiv C_{xx} = C_{zz} \ , \\
&C_b \equiv C_{zx} \ , \\
&C_{xy} = C_{yz} = 0 \ , \\
&C_l = C_z + C_b \ , \\
&C_{t1} = C_{yy} \ , \\
&C_{t2} = C_a - C_b \ , \\
&C_t = \cos^2\phi C_{t1} + \sin^2\phi C_{t2} \ ,
\end{aligned}
\tag{5}
$$

where ϕ is the angle between the y axis and $\hat{\mathbf{m}}$.

In the course of our theoretical research on high-field hole transport in silicon, we have discovered that, contrary to the general belief that C_t approaches zero monotonically, for holes, C_t exhibits undershoot similar to C_l. This paper presents the results of our systematic investigation of this phenomenon and an explanation for its cause.

The work was carried out by simulating hole dynamics in silicon under both zero electric field and high electric field (up to 50 kV/cm), using a Monte Carlo method which has been thoroughly documented in earlier publications.[7–10] The Monte Carlo calculation simulates transport in all three anisotropic valence bands, in which p-type symmetry is fundamentally incorporated using a $\mathbf{k}\cdot\mathbf{p}$ method, along with spin-orbit splitting. The eigenstates are formed from the six-dimensional basis: $|x\rangle\uparrow \cdots |z\rangle\downarrow$. The band structure is obtained by calculating the eigenvalues of the sum of the Shockley $\mathbf{k}\cdot\mathbf{p}$ Hamiltonian and the spin-orbit perturbation Hamiltonian. The form of the Hamiltonian is given in Ref. 8. Acoustic and nonpolar optical-phonon scattering were used at a lattice temperature of 300 K. The models of these scattering processes, which are more fully described in Ref. 8, use deformation-potential operators which have off-diagonal components. The form of these operators arises from the p-type symmetry of the system, and prevents the usual use of an overlap function as a separable part of the squared scattering matrix element. One consequence of this is that the scattering rate depends on the initial and final trajectories, separately, and not only on the scattering angle between them.

Each calculation consisted of an ensemble simulation of 200 000 holes, each having a 2-ps time of flight. In addition to studying the correlation functions as varying with respect to field magnitude and orientation, we investigated the role of anisotropy of the undershoot of C_t, by varying the band-structure parameters, so as to cover the range from a completely isotropic band structure to one that is more anisotropic than in real silicon.

II. RESULTS

The undershoot in C_t was first noticed for holes under high electric fields oriented in the [100] direction. Data for C_l and C_t are shown in Figs. 1 and 2, respectively, for this field orientation, over the range 0–50 kV/cm. As expected, C_l shows an undershoot which increases with field magnitude. Our finding is that C_t does qualitatively

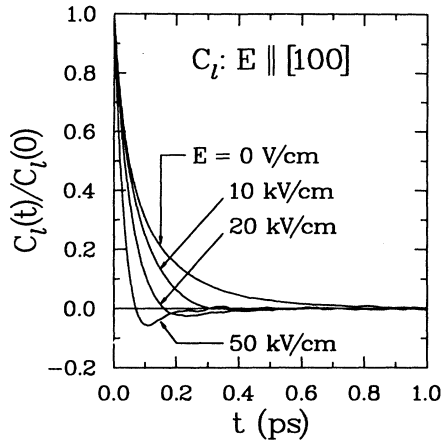

FIG. 1. Longitudinal-velocity-fluctuation autocorrelation function C_l for holes in silicon, $T = 300$ K. The electric field is oriented in the [100] direction.

the same thing. This undershoot in C_l is related to the possibility of the carriers reversing their direction by the influence of the accelerating electric field.[1,2] Previous understanding of the transverse characteristics was that the carriers could not be accelerated transverse to the electric field and therefore would never be reversed by the field between scatterings; thus there would be no undershoot in C_t. The data in Fig. 2 contradict this, and indicate for holes that indeed there can be acceleration perpendicular to the field.

The simulations were repeated for other field orientations ([111] and [101]) over the same range of magnitude (0–50 kV/cm). The data of C_t for all three field orientations are shown in Fig. 3. Along with the undershoot discussed for [100] fields, a somewhat weaker undershoot was found for fields in the [111] direction. As noted above, for fields in the [101] direction, there are two nonequivalent transverse directions: [010], denoted $t1$, and $[\bar{1}01]$, denoted $t2$. For neither of these transverse direc-

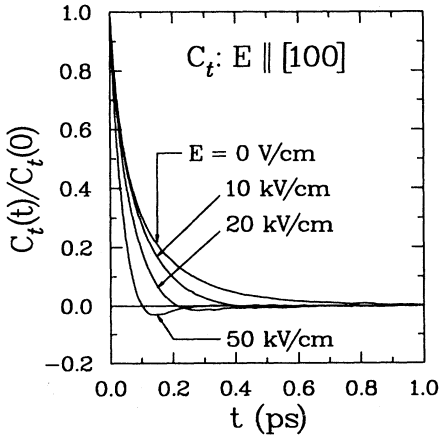

FIG. 2. Transverse-velocity-fluctuation autocorrelation function C_t for holes in silicon, $T = 300$ K. The electric field is oriented in the [100] direction. This shows undershooting of C_t for $E = 20$ and 50 kV/cm.

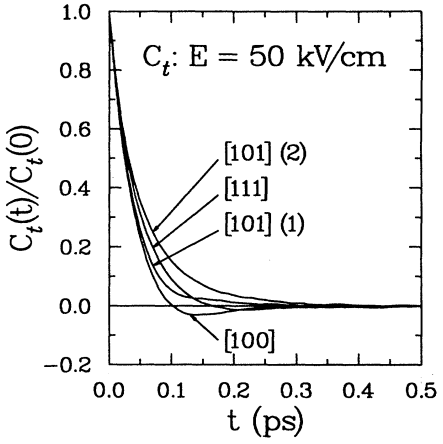

FIG. 3. Transverse-velocity-fluctuation autocorrelation function C_t for holes in silicon, $T=300$ K. The applied electric field is 50 kV/cm, in the following orientations: [100], [111], and [101]. For the [101] orientation, the curve [101] (1) is C_{t1}, pertaining to fluctuations in the [010] direction; and the curve labeled [101] (2) is C_{t2}, pertaining to fluctuations in the $[\bar{1}01]$ direction. C_t is clearly seen to undershoot zero for fields in the [100] and [111] directions, though not for either transverse direction for the field in the [101] direction.

tions was an undershoot found for fields between 0 and 50 kV/cm.

Next we investigated how C_t undershoot is controlled by the anisotropy or warping of the band structure. To do this we compared the result for silicon, with the field in the [100] direction with results for three other fictitious siliconlike materials, referred to as *A*, *B*, and *C*.

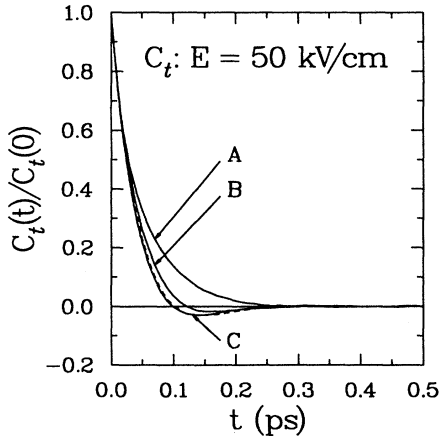

FIG. 4. Dependence of the transverse-hole-velocity-fluctuation autocorrelation function on the band-structure anisotropy. Data are shown with an electric field of 50 kV/cm applied in the [100] direction for silicon (dashed curve) and three fictitious materials (solid curves): *A*, *B*, and *C*. Material *A* is isotropic, material *B* is less anisotropic than silicon, and material *C* is more anisotropic than silicon. No undershooting of C_t is seen for *A*, the isotropic material. Undershooting is seen to increase with the degree of anisotropy.

These fictitious materials had band structures with varying degrees of anisotropy, achieved by varying the Luttinger parameters γ_2 and γ_3 from the silicon values. These parameters were adjusted so that the resulting heavy-hole density of states was as close as possible to that in silicon over the range of 0–10 meV. All other material parameters were kept the same as used for silicon. The Luttinger parameters used were as follows: Si ($\gamma_1=4.22$, $\gamma_2=0.39$, and $\gamma_3=1.44$); *A* ($\gamma_1=4.22$, $\gamma_2=1.67$, and $\gamma_3=1.67$); *B* ($\gamma_1=4.22$, $\gamma_2=1.00$, and $\gamma_3=1.61$); and *C* ($\gamma_1=4.22$, $\gamma_2=0.00$, and $\gamma_3=1.32$). Material *A* is isotropic ($\gamma_2=\gamma_3$). Material *B* is less anisotropic than Si. Material *C* is more anisotropic than Si. The calculations of C_t for these four materials for an electric field of 50 kV/cm, in the [100] direction, are shown in Fig. 4. Consistent with earlier work,[1,2] the isotropic material (*A*) shows no C_t undershoot at all. Examining C_t for Si and materials *B* and *C*, a correlation is evident between the degree of warping of the valence band and the degree of C_t undershooting zero. This implies that while, in an isotropic band (such as for electrons), there is no acceleration perpendicular to the field, in a warped band (such as for holes), at high fields, there is a possibility of perpendicular acceleration.

The longitudinal autocorrelation function C_l exhibits little variation with respect to changes in the degree of anisotropy. Data for materials *A*–*C* are qualitatively like that for Si, as shown in Fig. 1.

III. DISCUSSION

The results of this work show a feature of hole transport which is qualitatively different from that of electron transport by virtue of the warping of the band structure. A very simple calculation can show that this is plausible. The velocity is the crystal momentum gradient of the energy:

$$\mathbf{v}=\frac{1}{\hbar}\nabla_k E \ . \tag{6}$$

Consider, for example, an electric field F applied in the [100] direction and a perpendicular velocity fluctuation in the y direction, $\delta v_\perp=\delta v_y$. The fluctuation occurs during a free flight of duration δt in which the energy changes from E_1 to E_2, and may be expressed as

$$\delta v_\perp=\frac{1}{\hbar}\hat{\mathbf{y}}\cdot[(\nabla_k E)_2-(\nabla_k E)_1] \ . \tag{7}$$

Performing a Taylor expansion on the energy,

$$E_2=E_1+\frac{F}{\hbar}\delta t\hat{\mathbf{x}}\cdot(\nabla_k E)_1 \ . \tag{8}$$

And so the perpendicular velocity fluctuation is given by

$$\delta v_\perp=\frac{1}{\hbar}\hat{\mathbf{y}}\frac{F}{\hbar}\delta t[\nabla_k\hat{\mathbf{x}}\cdot(\nabla_k E)_1]$$
$$=\frac{F}{\hbar^2}\delta t\frac{\partial^2 E}{\partial k_y\partial k_x} \ . \tag{9}$$

For an isotropic, parabolic band structure, $E=\hbar^2k^2/2m^*$, $\partial^2E/\partial k_y\partial k_x=0$, so that $\delta v_\perp=0$ for all wave vec-

tors. However, for a warped parabolic band, such as

$$E=\frac{\hbar^2}{2m^*}[Ak^2+\sqrt{B^2k^4+C^2(k_x^2k_y^2+k_y^2k_z^2+k_z^2k_x^2)}]\ ,$$
$$\frac{\partial^2 E}{\partial k_y \partial k_x}=\frac{\hbar^2}{2m^*}\frac{4B^2C^2\sin\phi\cos^3\phi(\sin^2\phi-\cos^2\phi)}{(B^2+C^2\cos^2\phi\sin^2\phi)^{3/2}}\ , \tag{10}$$

where $\cos\phi=k_x/k$, $\sin\phi=k_y/k, k_z=0$. This shows how a transverse acceleration $(\delta v_\perp/\delta t)$ may arise for some wave vectors in the case of a warped parabolic band, but does not occur in the case of an isotropic parabolic band for any wave vectors. The transverse acceleration results from variation of the inverse effective mass tensor, as expressed in Eq. (3), and drives a transverse momentum relaxation. As in the case for C_l, this effect competes with the energy relaxation and causes an undershoot in C_t.

Transverse acceleration may occur, in principle, for both isotropic and warped nonparabolic bands. However, for an isotropic nonparabolic band, with a dispersion relation of the form $E(1+\alpha E)=\hbar^2k^2/2m^*$, we have found that the transverse acceleration is typically at least two orders of magnitude smaller than in the case of the warped band, for a comparable density-of-states effective mass. We carried out Monte Carlo simulations on this type of isotropic nonparabolic band structure, and found no undershoot for fields up to 300 kV/cm, and nonparabolicity factors α up to 5 eV^{-1}.

In summary, we find that the transverse-velocity-fluctuation autocorrelation function for holes in silicon exhibits an undershoot behavior which is qualitatively different than expected on the basis of electron transport. This phenomenon is a consequence of the warped shape of the valence-band energy surfaces. Between scatterings, the hole will experience not only a longitudinal acceleration in the direction of the applied field, but also a transverse acceleration, which varies with wave-vector orientation. This transverse acceleration drives a relaxation of the transverse component of the momentum. The combination of transverse momentum relaxation and energy relaxation results in an undershoot of the transverse-velocity-fluctuation autocorrelation function, in the same way that it occurs for the longitudinal autocorrelation function. This undershooting will cause the transverse noise spectra and diffusion of holes, with fields in selected orientations, to exhibit features previously thought to occur only for the longitudinal characteristics.

Finally, it has been suggested to us that an analogous effect to C_t may occur in nonwarped band structures with the application of a transverse magnetic field. This does seem plausible, although we are not aware of any investigations in this area.

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