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Theoretical investigation of a current in the direction of B in p-type silicon in $E \perp B$ fields

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Abstract. In this article we present a theoretical study on Hall transport of hot holes in the anisotropic valence band of Si at low temperatures ($T = 20$ K) in crossed $\boldsymbol{E}$- and $\boldsymbol{B}$-fields. A current in the direction of $\boldsymbol{B}$ is found, which may lead to a Hall field in the direction of $\boldsymbol{B}$ of the order of 5% of the applied electric field.

We used a $\boldsymbol{k} \cdot \boldsymbol{p}$ valence band model including non-parabolicity and anisotropy. The scattering models employed in the Monte Carlo simulation are acoustic and optical phonon scattering.

1. Introduction

In this article we discuss Hall effects in strong crossed electric and magnetic fields in p-type Si at low temperatures. In particular we predict the emergence of a Hall current parallel to the magnetic field. A similar effect has been predicted for p-type Ge [1]. It is expected to occur when the hole distribution is non-thermal (i.e. 'hot holes') and anisotropic due to the crystal anisotropy and the applied fields. Depending on the strengths E and B of the applied electric and magnetic fields $\boldsymbol{E}$ and $\boldsymbol{B}$ we distinguish two regimes for hole transport. When the electric field is relatively strong and the magnetic field weak the hot holes undergo a so-called streaming motion in which they are repeatedly accelerated towards the optical phonon energy ε_{op}, where they emit a phonon relaxing them back to a region in $\boldsymbol{k}$-space near $\boldsymbol{k} = 0$. The second regime requires strong magnetic fields. Then the holes may be caught in cyclotron orbits, such that their energy always remains smaller than ε_{op}. Thus, the holes accumulate in a region in $\boldsymbol{k}$-space where they have a long lifetime because they cannot emit optical phonons.

In the past a lot of research has been done on hot carriers in semiconductors. An overview is given by Komiyama [2]. Most of the attention was focused on hot-electron transport in silver halides because streaming motion is very clear in these polar materials due to the strong polar optical phonon scattering.

Normally, for transport in weak fields in p-Si and p-Ge the anisotropy of the valence band is averaged out by the isotropic (in $\boldsymbol{k}$-space) distribution function. However, applying strong fields makes the distribution function anisotropic and together with the anisotropy of the crystal this results in anisotropic transport properties. This is demonstrated by the dependence of the saturated hole drift velocity in Si and Ge on the direction of the applied electric field with respect to crystallographic axes [3]. Another example is the effect studied by Sasaki *et al* [4] and Gibbs [5]. They found a deviation of the direction of the current density from the applied electric field when this field is applied along a non-symmetry direction.

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Hall measurements on p-type Ge under hot-hole conditions were made, showing features in the Hall voltage which can be explained by accumulation of light and heavy holes [6]. For p-type Si, Hall experiments [7, 8] were done which showed a negative Hall voltage that is caused by the strong anisotropy of the Si valence band. Also, magnetotransport was studied experimentally and explained using a Monte Carlo model [9].

While all of these studies of p-type Si investigate the hole transport in the plane perpendicular to $\boldsymbol{B}$, our present work focuses on transport parallel to $\boldsymbol{B}$. It was shown theoretically [1] that in Ge in crossed fields the current transported by hot holes can have a component in the direction of $\boldsymbol{B}$, when the plane perpendicular to $\boldsymbol{B}$ is not a mirror plane (e.g. $\boldsymbol{B} \parallel [111]$). The similarity of the valence bands in Si and Ge leads one to expect the same current in Si. Indeed our calculations show such a current but it differs from the current in Ge because of the more pronounced anisotropy in Si.

In a sample with finite dimensions such a current induces a compensating electric field along $\boldsymbol{B}$. This field changes the direction of the total electric field causing it to be no longer perpendicular to $\boldsymbol{B}$. This may have dramatic consequences for effects which depend critically on the perpendicularity of the fields, e.g. a hot-hole laser [10].

2. Hot-hole transport in crossed fields

In low-doped Si at low temperatures, the rates for ionized impurity scattering and acoustic phonon scattering are much lower than the rate for optical phonon emission. Then $\boldsymbol{k}$-space can be divided into a region with a low scattering rate and another region with a high scattering rate corresponding to hole states with energy below or above the optical phonon energy respectively. As a result two types of motion can be distinguished for the transport of hot holes in crossed $\boldsymbol{E}$- and $\boldsymbol{B}$-fields.

The first type dominates when B/E is small and is called 'streaming motion'. During this motion, holes will be accelerated by the electric field until they have gained enough energy to emit an optical phonon. Under emission of a phonon they will relax to a low-energy state and subsequently will be accelerated again. Repetition of this cycle results in an anisotropic hole distribution directed along the electric field.

The second type dominates when B/E is large and is called 'accumulation'. Now the magnetic field is so strong that holes are captured in cyclotron orbits, where their energy will never reach ε_{op}. Holes are accumulated in a region in $\boldsymbol{k}$-space with low scattering rate, where they have a long lifetime.

In this latter case a study of the shape and volume of the accumulation regions yields an understanding of the dominating direction of $\boldsymbol{k}$ and hence of the current. Therefore we shall first discuss the distribution of the accumulated states in $\boldsymbol{k}$-space. In a later section we will use a Monte Carlo simulation to investigate the transition from streaming motion to accumulation and the distribution of the holes between streaming and accumulated states.

We use the dimensionless parameter $\zeta_h = (B/E)v_{op}$ for characterization of the transport motion. The velocity v_{op} (2.2×10^5 m s^{-1} in Si) is the average velocity of the heavy holes on the equi-energy surface at $\varepsilon = \varepsilon_{op}$.

3. The valence band model

We use a $\boldsymbol{k} \cdot \boldsymbol{p}$ valence band model [11] for the heavy-hole (h.h.), light-hole (l.h.) and split-off (s.o.) bands with the parameters given in reference [12]. Heavy holes determine the transport of holes because the density of states in the h.h. band is much bigger than

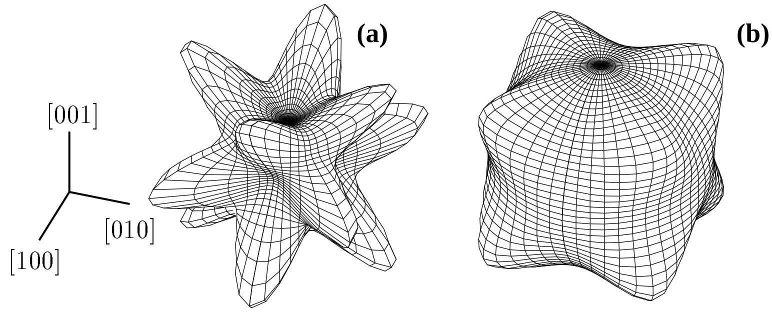

Figure 1. The normed equi-energy ($\varepsilon_{op} = \varepsilon$) surfaces of the heavy (a) and light (b) holes in Si.

in the l.h. or s.o. bands. In figure 1 the equi-energy surfaces of the heavy- and light-hole bands of Si are shown for the energy $\varepsilon = \varepsilon_{op}$ (63 meV in Si). Accumulated holes reside within this surface, while streaming holes are accelerated to this surface, where they emit an optical phonon and fall back to a state with low energy. The shape of such equi-energy surfaces depends strongly on the spin–orbit splitting Δ_{so}. In Si, Δ_{so} is small ($\Delta_{so} = 44$ meV) which results in a heavy-hole band of Si that is highly non-parabolic already at low energies which are relevant to transport. For $\varepsilon \ll \Delta_{so}$ the surface is only slightly warped, while when $\varepsilon \gg \Delta_{so}$ the warping is much more pronounced and the equi-energy surface shows peaks in the [110] directions. The light-hole band is not very anisotropic, it resembles the shape of the heavy-hole band in Ge.

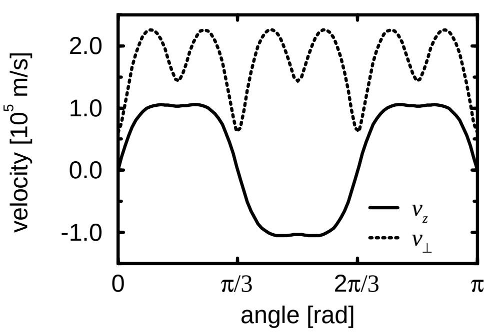

Figure 2. The velocity components v_z and $v_\perp$, parallel and perpendicular to [111] respectively, of a heavy hole with energy ε_{op} and wave vector $\boldsymbol{k}$ that is rotated in the $\langle 111 \rangle$ plane. The zero angle is in the $[1\bar{1}0]$ direction.

We recall that the velocity of the hole

$$\boldsymbol{v} = \frac{1}{\hbar} \boldsymbol{\nabla}_{\boldsymbol{k}} \varepsilon(\boldsymbol{k}) \tag{1}$$

is always perpendicular to the equi-energy surface. Hence $\boldsymbol{v}$ is not parallel to $\boldsymbol{k}$ for non-symmetry directions of $\boldsymbol{k}$. Then the Sasaki–Shibuya effect [4, 5] is observed, i.e. the current direction deviates from the direction of the $\boldsymbol{k}$-vector. Due to the strong anisotropy of the valence band in Si the magnitude of this effect can be quite large. This is demonstrated in figure 2 where equation (1) is evaluated for heavy holes with energy ε_{op}. The figure shows the component v_z of the velocity in the [111] direction and $v_\perp$, the velocity component in the ⟨111⟩ plane, as a function of the direction of $\boldsymbol{k}$ which is rotated in the ⟨111⟩ plane. Only when $\boldsymbol{k}$ is along $[1\bar{1}0]$ or an equivalent axis are $\boldsymbol{v}$ and $\boldsymbol{k}$ parallel.

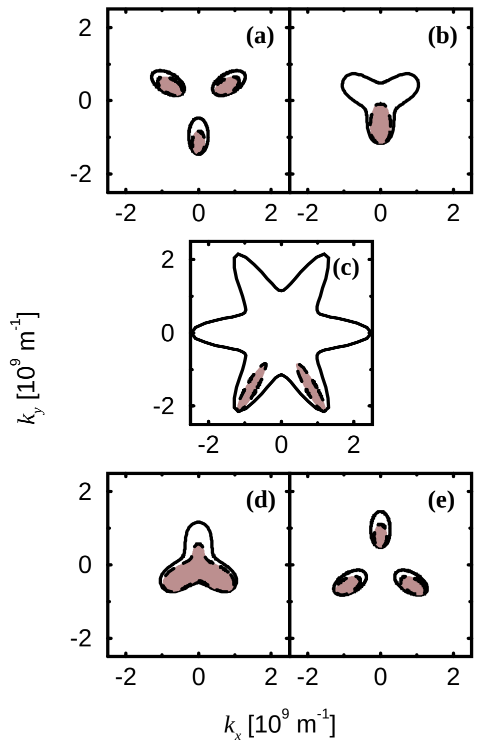

Figure 3. The equi-energy ($\varepsilon = \varepsilon_{op}$) lines (solid) and lines of equal total energy (dashed) in Si in planes perpendicular to the [111] direction. k_x, k_y and k_z are in the $[1\bar{1}0]$, $[11\bar{2}]$ and [111] directions respectively. For panels (a)–(e) k_z has the values -1.5, -0.75, 0, 0.75, 1.5×10^9 m^{-1}. The electric field and the magnetic field are along the positive-k_x and positive-k_z directions respectively and $\zeta_h = 4.4$. The dashed regions are accumulation regions.

3.1. Calculation of the number of accumulated states

In crossed fields, holes in the accumulation region move along parts of cyclotron orbits. In these orbits the total energy [13]

$$\varepsilon'(\boldsymbol{k}) = \varepsilon(\boldsymbol{k}) + eV \tag{2}$$

of those holes is conserved. Here $\varepsilon(\boldsymbol{k})$ is the band energy as a function of the crystal momentum $\hbar\boldsymbol{k}$ and eV the potential energy in the electric field $\boldsymbol{E}$. In crossed $\boldsymbol{E}$- and $\boldsymbol{B}$-fields the potential energy can written as $eV = \hbar\boldsymbol{k} \cdot (\boldsymbol{B} \times \boldsymbol{E})/B^2$. Then, also k_z, the component of $\boldsymbol{k}$ parallel to $\boldsymbol{B}$, is constant. In figure 3 the equi-energy lines of the heavy holes with $\varepsilon(\boldsymbol{k}) = \varepsilon_{op}$ are drawn. This figure also shows contour lines of the total energy enclosing regions with hole states for which the total energy $\varepsilon'(\boldsymbol{k})$ is smaller than ε_{op}. Holes in these states are not scattered by optical phonons and thus will have a long lifetime. Due to anisotropy, several unconnected regions may exist for a hole.

We have calculated the number of heavy-hole states $n_{ac}(k_z)$ in these accumulation regions. For a given band structure and given directions of $\boldsymbol{E}$ and $\boldsymbol{B}$ this number only

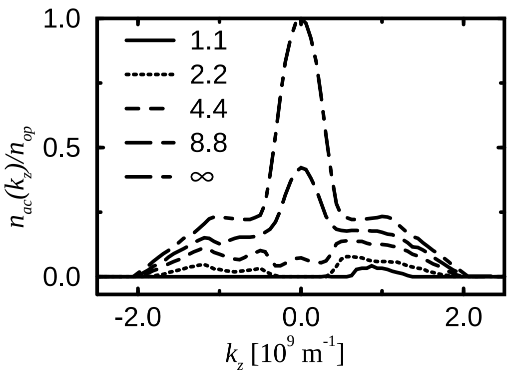

Figure 4. The ratio $n_{ac}(k_z)/n_{op}$ of the number of accumulated states $n_{ac}(k_z)$ and the number of states n_{op} with $\varepsilon \leqslant \varepsilon_{op}$ for $k_z = 0$ is shown. The labelling of the curves is with values of ζ_h. The curve for $\zeta_h = 1.1$ is multiplied by a factor of 5.

depends on ζ_h. In figure 4 the number of accumulated states $n_{ac}(k_z)$ divided by n_{op}, as a function of k_z, is depicted for several values of ζ_h. Here $\boldsymbol{E}$ and $\boldsymbol{B}$ are applied along the [1$\bar{1}$0] and [111] axes, respectively, while n_{op} is the number of states below the optical phonon energy in the $k_z = 0$ plane. The accumulation starts at $\zeta_h \approx 1.1$ for $k_z = 1 \times 10^9$ m^{-1}. For small ζ_h the distribution of accumulated states is asymmetric with respect to $k_z = 0$ because $\boldsymbol{B} \times \boldsymbol{E}$ is parallel to the [11$\bar{2}$] direction which is not a twofold axis. The asymmetry of the accumulated states is demonstrated clearly by the different shapes of the dashed regions in figures 3(b) and 3(d). Although $n_{ac}(k_z)/n_{op}$ is small, these states are important for transport, as will be shown by the Monte Carlo results. As ζ_h increases, the number of accumulated states increases and the asymmetry decreases. In the limit $\zeta_h \to \infty$ (i.e. $E = 0$) the cyclotron orbits coincide with equi-energy lines and all states within the surface shown in figure 1 are accumulated. This means that the number of accumulated states is equal for $k_z < 0$ and $k_z > 0$. Then the accumulation regions for $k_z < 0$ and $k_z > 0$ have the same shape, though they are oriented differently with respect to the [11$\bar{2}$] axis.

We conclude that the heavy holes start to accumulate when $\zeta_h \approx 1.1$ and that the accumulation differs for $k_z > 0$ and $k_z < 0$. Whether this asymmetry leads to k_z- and v_z-components during transport will be investigated using a Monte Carlo simulation.

4. Monte Carlo results

The transition from the streaming transport regime to the accumulation regime is studied using a Monte Carlo program described elsewhere [14]. It is similar to the one developed by Hinckley and Singh [15]. In our M.C. program we use the valence band model as described before. The major scattering processes in pure Si are acoustic and optical phonon scattering. These processes are modelled using deformation potential theory taking into account all anisotropies and non-parabolicities following from a six-band $\boldsymbol{k} \cdot \boldsymbol{p}$ treatment of the valence band. All of the simulations were done for 20 K and magnetic and electric fields along the [111] and [1$\bar{1}$0] direction respectively. We only present the results for $E = 5$ kV cm^{-1}, as for other electric field strengths similar curves are found as functions of ζ_h.

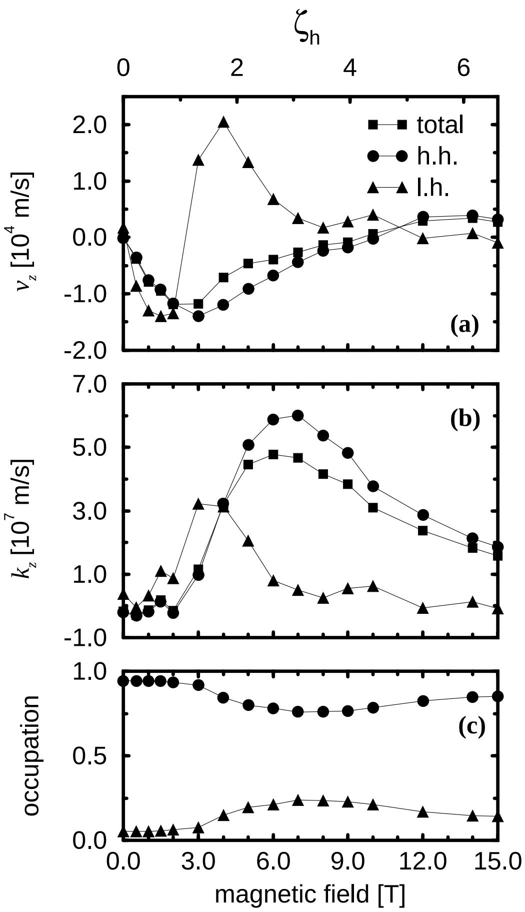

Figure 5. The result of the M.C. calculation: the component v_z of the drift velocity (a) and the component k_z of the wave vector (b) of heavy holes and light holes and the appropriate average over light-hole, heavy-hole and spin–orbit bands against the magnetic field B for $E = 5$ kV cm^{-1}. In part (c) the occupation of the light- and heavy-hole bands is shown.

4.1. Streaming motion

In figures 5(a) and 5(b) the component v_z of the drift velocity and k_z of the wave vector in the [111] direction of the heavy and light holes together with the appropriate average over all three types of carrier as a function of the magnetic field are shown for an applied electric field of 5 kV cm^{-1}. Note that the average curve is determined mainly by the heavy holes. From the results in the previous section we know that the heavy holes start to accumulate at $\zeta_h \approx 1.1$ or $B = 2.5$ T in this case. Up to this field strength, $\boldsymbol{k}$ is rotated by the Lorentz force but remains in the $\langle 111 \rangle$ plane, though, due to the Sasaki–Shibuya effect the velocity has a component v_z perpendicular to this plane. This effect reaches its maximum at $\zeta_h = 1.1$ ($B = 2.5$ T), where the current is directed ten degrees out of the $\langle 111 \rangle$ plane. The same effects are observed for light holes but shifted to lower magnetic fields. The occupation of the light- and heavy-hole bands is shown in figure 5(c). The occupation depends on the density of states and on the scattering times in both bands. During the streaming motion both the density of states and the scattering time remain approximately the same, so the occupation of both bands is fairly constant. The spin–orbit band is not shown because the density of states is so small that only ≈0.1% of the holes are in this band.

4.2. Accumulation

The accumulation of the heavy holes starts at $\zeta_h \approx 1.1$ and leads to the emergence of a component k_z parallel to $\boldsymbol{B}$ with the sign expected from the asymmetry in figure 4. From simulation results (not shown here) we know that $|k| \approx 4 \times 10^8\ \mathrm{m}^{-1}$, so the maximum magnitude of $k_z/|\boldsymbol{k}|$ is about 0.12 and reached at 7.5 T. As discussed in the previous section the decrease of k_z for still higher magnetic field strengths occurs because the asymmetry of the accumulation regions decreases. On the other hand at $B > 2.5$ T the velocity component $\boldsymbol{v}_z$ of the heavy holes remains in the opposite direction to $\boldsymbol{k}_z$. Two reasons have to be considered to explain this. Due to the strong anisotropy in silicon, only very few accumulated states exist at low magnetic field strengths. Hence hole transport remains dominated by streaming holes. Also, because of the anisotropy, accumulated states exist for which $k_z > 0$ but $v_z < 0$. Therefore the accumulated holes just cause a decrease of $|v_z|$ for $B > 2.5$ T instead of a change of sign of v_z as is seen for heavy holes in germanium.

For light holes the results are quite different. First of all, the effects are shifted towards lower magnetic field strength, so at $B = 3$ T most light holes are accumulated. Moreover due to the smaller anisotropy the fraction of light holes accumulated rapidly increases as a function of B and the directions of $\boldsymbol{v}$ and $\boldsymbol{k}$ are more parallel. This results in an abrupt transition from streaming motion to accumulation which is shown by the very clear change of sign of v_z at $B = 2.5$ T. A curve of the same shape is found for the heavy-hole band in Ge under these conditions [1].

In figure 5(c) we see that the occupation of the light-hole band increases as the light holes accumulate and thus their scattering time decreases, while the majority of heavy holes are still streaming. This effect is responsible for the population inversion between the light- and heavy-hole bands in a hot-hole laser. At higher magnetic fields when more heavy holes are accumulated the occupation of the heavy-hole band increases again.

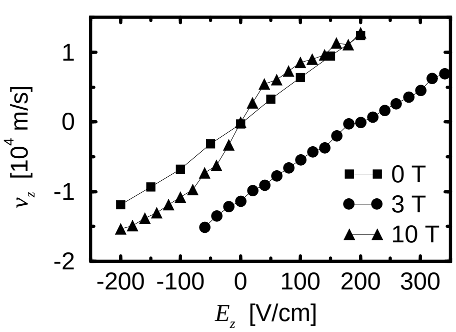

Figure 6. The drift velocity component v_z as a function of the applied electric field E_z.

4.3. Applying an $\boldsymbol{E}$-field along $\boldsymbol{B}$

Due to the drift velocity component v_z a current will flow in the direction of $\boldsymbol{B}$. In an experimental situation a sample will have finite dimensions and thus a compensating electric field will build up in the direction of $\boldsymbol{B}$ to make $v_z = 0$. We calculated this compensating electric field by doing a Monte Carlo simulation not only with the electric and magnetic field applied along the $[1\bar{1}0]$ and [111] directions respectively but also applying a varying electric field E_z along [111]. Figure 6 shows the velocity component v_z as a function of E_z for several magnetic field strengths and an electric field of 5 kV cm^{-1} in the [1$\bar{1}$0] direction. We can read the strength of the compensating electric field from these curves. For $B = 0$ and 10 T, E_z is approximately 0 V cm^{-1}, which is the expected value because $v_z = 0$ for these field strengths. At $B = 3$ T we need an electric field $E_z = 200$ V cm^{-1} to make $v_z = 0$ (see figure 5). This value can be compared with a normal Hall field $E_H = v_\perp B \approx 1500$ V cm^{-1} under these circumstances, where we used $v_\perp = 5 \times 10^4$ m s^{-1} obtained from the simulation results.

The slopes of the curves for $B = 0$ and 3 T are determined by the motion of streaming carriers which give a linear response because E_z is so weak that we are in the ohmic transport regime. For $B = 10$ T the response is non-linear due to contribution of the accumulated light holes. For very small values of E_z these holes have a high mobility because of their low scattering rate. At higher fields, since their motion in the direction of E_z is not hindered by the magnetic field, the holes are easily accelerated until they have enough energy to emit an optical phonon. This results in streaming motion and saturation of the drift velocity. The asymmetry with respect to $E_z = 0$ of the curve for $B = 10$ T is a result of the asymmetry of the accumulation regions.

5. Conclusions

The asymmetric accumulation regions of the heavy holes do not result in a change of the sign of the current component in the direction of $\boldsymbol{B}$ when transport changes from streaming motion to accumulation. Although the light holes show an effect similar to the effect for heavy holes in Ge, the effect of accumulation of the heavy holes in Si is smeared out due to the strong anisotropy of the heavy-hole band. The calculations show that in crossed $\boldsymbol{E}$- and $\boldsymbol{B}$-fields an electric field will build up in the direction of $\boldsymbol{B}$ with a magnitude of ≈5% of the applied electric field.

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