SLAC-PUB-13909

Intrinsic Spin-Hall Effect in n-Doped Bulk GaAs

B. Andrei Bernevig and Shou-Cheng Zhang
Department of Physics, Stanford University, Stanford, CA 94305

We show that the bulk Dresselhauss (k^3) spin-orbit coupling term leads to an intrinsic spin-Hall effect in n-doped bulk GaAs, but without the appearance of uniform magnetization. The spin-Hall effect in strained and unstrained bulk GaAs has been recently observed experimentally by Kato *et. al.* [1]. We show that the experimental result is quantitatively consistent with the intrinsic spin-Hall effect due to the Dresselhauss term, when lifetime broadening is taken into account. On the other hand, extrinsic contribution to the spin-Hall effect is several orders of magnitude smaller than the observed effect.

PACS numbers: 73.43.-f,72.25.Dc,72.25.Hg,85.75.-d

Recent theoretical work predicts dissipationless spin currents induced by an electric field in semiconductors with spin-orbit coupling[2, 3]. The response equation is given by $j_j^i = \sigma_s \epsilon_{ijk} E_k$, where j_j^i is the current of the i-th component of the spin along the direction j and ϵ_{ijk} is the totally antisymmetric tensor in three dimensions. The response equation was derived by Murakami, Nagaosa and Zhang[2] for p-doped semiconductors described by the Luttinger model of the spin-3/2 valence band. In another proposal by Sinova *et al.* [3], the spin current is induced by an in-plane electric field in the 2-dimensional electron gas (2DEG) described by the Rashba model[3]. The intrinsic spin-Hall effect predicted by these recent theoretical works is fundamentally different from the extrinsic spin-Hall effect [4, 5] due to the Mott type of skew scattering by impurities [6]. The intrinsic spin-Hall effect arises from the spin-orbit coupling of the host semiconductor band, and has a finite value in the absence of impurities. On the other hand, the extrinsic spin-Hall effect arises purely from the spin-orbit coupling to the impurity atoms.

Experimental observation of the spin-Hall effect has been recently reported by Kato *et al.* [1] in an electron doped bulk sample and by Wunderlich *et al.* in a two dimensional hole gas (2DHG)[7]. The 2DHG experiment has been analyzed in a previous paper [8] where it was shown that the vertex correction due to potential impurity scattering vanishes for that particular system. The experimental system is also in the regime where lifetime broadening due to impurity scattering is much less than the spin splitting, thus strongly suggesting an intrinsic mechanism of the spin-Hall effect. In the experiment of Ref. [1], spin accumulation due to a spin current is observed even in the unstrained GaAs where no apparent spin splitting is observed. The absence of observed spin splitting seems to show the absence of intrinsic spin-orbit coupling in unstrained n-doped GaAs. This fact prompted the authors of Ref. [1] to interpret the observed spin-Hall effect in terms of the extrinsic mechanism due to impurity scattering only. In this paper we show that, under close scrutiny, the results of [1] are consistent with an intrinsic mechanism. We first show that the unstrained GaAs has a Dresselhauss k^3 spin splitting which escapes detection by the method used in [1, 9]. We then show that this spin splitting leads to a spin-Hall current. This therefore explains the observed spin accumulation on the edges of the unstrained GaAs within the framework of the intrinsic spin-Hall effect. Furthermore, the observed magnitude is consistent with the theory, after lifetime broadening due to impurity scattering is taken into account. We also predict that the bulk Dresselhauss term produces no net uniform magnetization in the sample, this being generated solely by the strain terms. In the case of strained GaAs, we compute the self-energy correction in the weak spin-orbit coupling limit and find a value for the spin-Hall conductivity close (enough) to the measured value. The independence of the spin current on the crystalographic directions can also be explained by the dominance of the k^3 term over the k-linear terms induced by the small strain. We also perform an order-of magnitude estimate and find out that the extrinsic spin-Hall effect is seven orders of magnitude lower than the clean limit of the intrinsic spin-Hall effect, and several orders of magnitude lower than the observed experimental value.

Let us first examine the extrinsic spin-Hall effect. In the extrinsic mechanism[4, 5], there is no spin-orbit coupling in the band structure, and the spin-Hall effect is caused by the scattering of electrons by the spin-orbit interaction with impurities. The Hamiltonian is given by:

$$H = \frac{\hbar^2 k^2}{2m} + \frac{\hbar^2}{2m^2c^2}\vec{\sigma}(\vec{\nabla}V(r) \times \vec{k}), \qquad (1)$$

where $V(r)$ is the impurity potential. The extrinsic spin-Hall effect is basically derived from the atomic Mott scattering [6], and the important length scale is governed by the Compton wave length $\lambda_c = \hbar/mc$. The extrinsic spin-Hall effect has been computed systematically for this Hamiltonian[10], and the order of the magnitude of the effect can be estimated to be:

$$\sigma_{extrinsic} \sim \frac{e^2}{\hbar}(\lambda_c k_F)^2 k_F, \qquad (2)$$

SIMES, SLAC National Accelerator Center, 2575 Sand Hill Road, Menlo Park, CA 94309
Work supported in part by US Department of Energy contract DE-AC02-76SF00515.

where k_F is the fermi wave vector. For the experimental system by Kato *et al.*, with $k_F = 10^8 m^{-1}$ and a conduction band effective mass of $m = 0.0665 m_e$, Eq. (2) gives $\sigma_{extrinsic} = 1.2 \times 10^{-4} \Omega^{-1} m^{-1}$, almost 4 orders of magnitude smaller than the observed spin-Hall conductance. On the other hand, the intrinsic spin-Hall effect is a genuine solid state effect, governed purely by the fermi wave vector k_F, and the order of magnitude of the effect is given by

$$\sigma^{clean}_{intrinsic} \sim \frac{e^2}{\hbar} k_F \tag{3}$$

in the clean limit. Therefore, we see that the ratio of the two effects is given by [11]

$$\frac{\sigma_{extrinsic}}{\sigma^{clean}_{intrinsic}} \sim (\lambda_c k_F)^2 \sim 10^{-7}. \tag{4}$$

Therefore, in distinguishing between the two effects, it is extremely important to keep in mind the smallness of the dimensionless parameter $\lambda_c k_F$. In the literature of the anomalous Hall effect, a so called “enhancement factor” is sometimes introduced in a rather ad-hoc basis[10, 12]. However, this “enhancement factor” is microscopically based on the spin-orbit coupling within the band structure, and would necessarily lead to a spin splitting of the bands. Therefore, we can safely conclude that *if there were no spin splitting due to the intrinsic spin-orbit coupling within the band*, the extrinsic spin-Hall effect is far too small to explain the experiment by Kato *et al.* in the unstrained GaAs.

Let us now turn to the intrinsic spin-orbit coupling within the conduction band. The Hamiltonian of an inversion asymmetric bulk (unstrained) semiconductor contains a Dresselhauss k^3 spin splitting term in the conduction band, which can be written as a momentum dependent magnetic field:

$$H = \frac{\hbar^2}{2m} k^2 + B_i(\mathbf{k})\sigma^i, \quad i = 1, 2, 3 \tag{5}$$

where $B_x = \gamma k_x (k_z^2 - k_y^2)$, $B_y = \gamma k_y (k_x^2 - k_z^2)$, $B_z = \gamma k_z (k_y^2 - k_x^2)$. The coupling constant γ has been determined in a number of independent experiments, and a value of $\gamma \approx 25 eV \mathring{A}^3$ is widely quoted in the literature [13, 14, 15, 16]. We must now reconcile this spin splitting with the fact that the measurement carried out in Ref. [9] does not see any splitting in the unstrained sample. In [9], a spin packet injected at the Fermi momentum is subsequently dragged by an external electric field $\vec{E}$. Experiments are performed along two crystallographic directions $\vec{E}||[110]$ and $\vec{E}||[1\bar{1}0]$. This creates an average nonzero particle momentum $\langle \vec{k} \rangle \sim \frac{e}{\hbar} \vec{E} \tau$ which in turn creates a non-zero average (over the Fermi surface) internal magnetic field $\langle \vec{B} \rangle$. The spin splitting in [9] is obtained as a derivative of the averaged $\langle \vec{B} \rangle$ with respect to the drag momentum $\langle \vec{k} \rangle$. Due to the special symmetry of the Dresselhauss spin-orbit coupling, this procedure turns out to yield a null result, even if γ is finite. Take, for example $\vec{E}||[110]$, then the momentum of a particle injected near the Fermi momentum $\vec{k}^F$ is:

$$\vec{k} = \vec{k}^F + \langle \vec{k} \rangle, \quad \langle \vec{k} \rangle = -\frac{e\tau}{m} \vec{E}||[110], \quad \langle k_x \rangle = \langle k_y \rangle. \tag{6}$$

To first order in $\langle \vec{k} \rangle$, the components (say x) of $\langle \vec{B} \rangle$ averaged over the Fermi surface is:

$$\langle B_x \rangle = \langle k_x \rangle \int \frac{d\Omega}{4\pi} \left[(k_z^F)^2 - (k_y^F)^2 - 2 k_x^F k_y^F \right]. \tag{7}$$

Since the spin-orbit coupling term is much smaller than the kinetic term, the Fermi surface is, to first order in γ, a sphere (there is, of course, a zero order in $\langle k_x \rangle$ term, but this obviously vanishes upon integration over the Fermi surface so we have omitted it). As the integration is carried over a sphere, it is obvious that $\int (k_z^F)^2 = \int (k_y^F)^2 = (k^F)^2/3$ and $\int k_x^F k_y^F = 0$. Therefore $\langle B_x \rangle = 0$, and no spin splitting is expected from this procedure, even though in the Dresselhauss term γ maybe finite. Note that this cancellation would not happen if the spin-orbit coupling term were k-linear since the derivative of $\vec{B}_{int}$ would just be a constant. This is exactly what happens in the strained samples of GaAs where the spin splitting was explained by k-linear terms [17].

A related fact shows that, due to its symmetry, the bulk-Dresselhaus term produces no uniform magnetization in the bulk of the sample. This is an easily falsifiable prediction of our theory. The Hamiltonian (5) has two energy levels $E_\pm = \frac{\hbar^2}{2m} k^2 \pm B$ where $B = \sqrt{B_i B_i}$. The uniform magnetization $\langle \sigma_i \rangle$ induced by an electric current $J_j = \partial H / \partial k_j$ (due to the applied electric field E_j) can be easily computed in linear response, and one obtains:

$$\langle \sigma_i \rangle = \frac{2\pi e \tau}{\hbar} Q_{ij} E_j$$
$$Q_{ij} = \langle T \sigma_i J_j \rangle = \int \frac{d^3 k}{(2\pi)^3} \frac{n_{E_-} - n_{E_+}}{B^2} \left(B_i \frac{\partial B}{\partial k_j} - B \frac{\partial B_i}{\partial k_j} \right) \tag{8}$$

where $n_{E_\pm}$ are the Fermi functions of the two bands. By inspection, all the components of $B_i \frac{\partial B}{\partial k_j} - B \frac{\partial B_i}{\partial k_j}$ are odd in the components k_i and hence vanish under integration due to cubic symmetry. This leads to $\langle \sigma^i \rangle \equiv 0$. By contrast, a k-linear internal magnetic field, as in the strained samples, gives a finite uniform magnetization due to the fact that $\frac{\partial B_i}{\partial k_j}$ is a constant while B is isotropic in (and proportional to) k [17]. The bulk Dresselhauss term is most likely also the explanation of the contradiction between the observed spin splitting along the [110] and $[1\bar{1}0]$ directions, and the uniform magnetization on these directions. In [18] it is observed that although the spin splitting for $E||[110]$ is consistently larger than the spin splitting for the $E||[1\bar{1}0]$, the uniform magnetization for $E||[110]$ is usually lower than that for $E||[1\bar{1}0]$.

This can be very well explained by the missing bulk-Dresselhauss term in the case when this term subtracts from the splitting on the [110] direction but adds to the splitting in the $[1\bar{1}0]$ directions, which makes it qualitatively possible that the uniform magnetization observed be in agreement with the spin splitting. Quantitative modelling of this involves precise knowledge of the sample Hamiltonian (including the strain) which is currently not possible (mainly because of limited knowledge about out-of-plane spin-orbit coupling terms).

Even though it creates no uniform magnetization, the bulk Dresselhauss term does give rise to an intrinsic spin-Hall effect when under the action of an electric field. We define the spin current as usual ($\varepsilon = \hbar^2 k^2/2m$):

$$J_i^l = \frac{1}{2}\left\{\frac{\partial H}{\partial k_i}, \sigma^l\right\} = \frac{\partial \varepsilon}{\partial k_i}\sigma_l + \frac{\partial B_l}{\partial k_i}, \tag{9}$$

and the expanded expression for the Green's function $G(k, i\omega_n) = [i\omega_n - H]^{-1}$ as:

$$G(k, i\omega_n) = f(k, i\omega_n)(g(k, i\omega_n) + B_i(k)\sigma_i)$$
$$f(k, i\omega_n) = \tfrac{1}{(i\omega_n - \varepsilon(k))^2 - B^2}, \;\; g(k, i\omega_n) = i\omega_n - \varepsilon(k) \tag{10}$$

When subjected to the action of an electric field $\vec{E}$, the frequency dependent spin conductance (not including the vertex correction) can be found in linear response as:

$$J_i^l = \sigma_{ij}^l E_j; \quad \sigma_{ij}^l = \tfrac{Q_{ij}^l(\omega)}{-i\omega}; \quad Q_{ij}^l(i\nu_m) =$$
$$= \tfrac{1}{V\beta}\sum_{k,n} Tr[G(k, i(\omega_n + \nu_m))J_i^l(k)G(k, i\omega_n)J_j(k)] \tag{11}$$

Summing over the Matsubara frequencies $i\omega_n$, analytically continuing $i\nu_m \to \omega$, as well as omitting a dissipative term which vanishes upon momentum integration, we obtain the expression for the frequency dependent (reactive) spin conductivity:

$$\sigma_{ij}^l(\omega) = \frac{\hbar^2}{2m}\int \frac{d^3k}{(2\pi)^3}\frac{n_{E_-} - n_{E_+}}{B(B^2 - \omega^2)}k_i \epsilon_{lnr} B_n \frac{\partial B_r}{\partial k_j} \tag{12}$$

where $i, j, l, r, n = x, y, z$. Unlike the uniform magnetization case, the integrand is even in k and finite upon integration. Hence the spin current in the unstrained GaAs can be qualitatively explained by the presence of a intrinsic spin-Hall effect due to the bulk-Dresselhauss term. Working in spherical coordinates, substituting the explicit expression for the bulk Dresselhauss spin splitting $B_i(k)$, using the expression (valid for small γ) of the difference between the Fermi momenta of the two spin-split bands:

$$k_-^F - k_+^F \approx \frac{2m}{\hbar^2}\frac{B(k^F)}{k^F}; \quad k^F = \frac{k_+^F + k_-^F}{2}, \tag{13}$$

as well as integrating over the spherical angles, one obtains for the DC spin-Hall conductivity:

$$\sigma_{ij}^l = \frac{k^F}{12\pi^2}\epsilon_{lij}. \tag{14}$$

This is the intrinsic spin-Hall conductivity in the clean limit, $\hbar/\tau << B(k)$, which we call $\sigma_{intrinsic}^{clean}$. For the carrier concentration in [1] we have $k^F = 10^8 m^{-1}$ and we obtain $\sigma_{intrinsic}^{clean} = 200\Omega^{-1}m^{-1}$. This is much larger than the observed conductivity of $0.2 \sim 0.5\Omega^{-1}m^{-1}$. But this is expected since we have so far not taken the influence of disorder into account . In the experiment by Kato *et al.*, the lifetime broadening due to impurity scattering is much larger than the weak spin splitting due to the Dresselhauss coupling. The intrinsic spin-Hall effect is therefore in the dirty limit, and a significant reduction from the clean result is therefore expected. Note that the lifetime broadening due to impurity scattering leads to a *reduction* of the intrinsic spin-Hall conductivity. This is different from the extrinsic spin-Hall effect due to spin-orbit coupling to the impurity potential, which makes a small, but *positive* contribution to the spin-Hall conductivity.

To properly take into account disorder, one must perform a self-consistent calculation taking into account both the self-energy and the vertex correction. In the case of the electron Rashba model with a k-linear spin splitting, many groups have shown that the vertex correction cancels the intrinsic spin-Hall effect [19, 20]. However, this cancellation seems to be special to the k-linear spin splitting, and it has been shown that the vertex correction due to k^2 light/heavy hole splitting in the Luttinger model, or due to k^3 spin splitting in the heavy hole band, vanishes identically [8, 21]. We expect that for a similar reason, the vertex correction due to the k^3 Dresselhauss spin splitting would not cancel the intrinsic spin-Hall effect either. We will hence neglect the vertex correction and focus on the self-energy correction which is easy to extract analytically. The self-energy approximation to disorder can be simulated by letting $\omega = i\hbar/\tau$ in Eq. (12). The values in [1] are in the regime $\hbar/\tau >> B(k)$, we thus obtain:

$$\sigma_{ij}^l = \frac{\hbar^2}{2m}\frac{1}{(\hbar/\tau)^2}\int \frac{d^3k}{(2\pi)^3}\frac{n_{E_-} - n_{E_+}}{B}k_i \epsilon_{lnr} B_n \frac{\partial B_r}{\partial k_j} \tag{15}$$

which, upon momentum integration gives the lower bound for the spin conductivity:

$$\sigma_{ij}^k = \frac{4k_F}{105\pi^2}\left(\frac{\gamma k_F^3}{\hbar/\tau}\right)^2 \epsilon_{ijk}. \tag{16}$$

For the values $\gamma = 25eV\mathring{A}^3$, $k_F = 10^8 m^{-1}$ we obtain a bulk Dresselhauss spin splitting energy $\gamma k_F^2 \approx 0.025meV$ while $\hbar/\tau \approx 1.6meV$ for a sample of mobility $\mu = 1m^2/Vs$ as the one in the experiment. Using these values, we obtain for the intrinsic, disorder quenched spin conductivity $\sigma_{intrinsic}^{dirty} = 0.02\Omega^{-1}m^{-1}$. This lower bound is smaller than the measured conductivity (which is $0.2\Omega^{-1}m^{-1}$ for small electric field and $0.5\Omega^{-1}m^{-1}$ for large electric field. This is a lower bound for the spin conductivity since $\hbar/\tau$ is an upper bound for the frequency ω

in the dirty limit. Considering the uncertainty associated with the value of γ, the crudeness of the estimate, and the indirect determination of the experimental value, the agreement is reasonably good.

The application of strain induces two extra spin splittings in the Hamiltonian which are linear in the momentum k [17]. There is one structural inversion asymmetry (SIA) splitting of the form $\alpha(k_y\sigma_x - k_x\sigma_y)$, and a bulk-inversion asymmetry (BIA) of the form $\delta(k_x\sigma_x - k_y\sigma_y)$, where α and δ are strain dependent. For the values of the splitting in sample E used in [9] we have $\alpha/\hbar = 183 m/s$ and $\delta/\hbar = 112 m/s$. We observe that the splitting at the Fermi momentum is $0.011 meV$ for the SIA term and $0.007 meV$ for the BIA term. By contrast, the k^3 Dresselhauss coupling is $0.025 meV$, so it is likely that it will dominate (although not overwhelmingly) the spin current. Moreover, a vertex correction computation for the SIA or BIA term separately reveals that the spin current caused by these terms vanishes upon the introduction of impurities [19] (exact numerical diagonalization results [22, 23] are, however, at odds with [19]), whereas a vertex calculation for a k^3 term shows finite spin current [8, 21]. It is therefore plausible that the bulk Dresselhauss term dominates the spin-Hall transport even in the strained samples. This naturally explains the independence of spin current on the crystallographic directions of the applied electric field, since the bulk spin conductivity for the Dresselhauss term is direction independent. The experimental features observed can therefore be qualitatively explained by an intrinsic mechanism.

In conclusion, we have shown that without any spin splitting in the electron band, the extrinsic spin-Hall effect is far too small to explain the experimentally observed value of spin-Hall conductivity in [1]. In order to definitively determine the origin of the spin-Hall effect, we propose to carry out similar experiments in materials without any known intrinsic spin-orbit coupling, and a null result would give the definitive proof that the extrinsic spin-Hall effect is far below the current experimental sensitivity, and can not be the origin of the spin-Hall effect observed in Ref. [1]. We have shown that the experimental results are consistent with the interpretation of an intrinsic spin-Hall effect in terms of a bulk Dresselhauss term in the unstrained sample. Furthermore, this intrinsic spin-orbit coupling is consistent with the apparent absence of spin splitting observed (in the unstrained samples) in the spin drag experiment[9]. We also predict that the uniform magnetization in the unstrained bulk GaAs samples will be close to zero due to the symmetry of the k^3 Dresselhaus term. Since the experiment is carried out in a regime where the lifetime broadening due to impurity scattering is large compared to the spin splitting, the observed spin-Hall conductivity is significantly reduced from the value in the clean limit. It is argued that the k-linear terms in the strained GaAs samples [9, 17], although crucial for the appearance of a uniform magnetization, have a limited effect on the spin current due to the dominance of the Dresselhauss term, thereby qualitatively explaining the direction independence of the spin-Hall effect observed in the experiment.

We would like thank Y.K. Kato and and D. Awschalom for many useful discussions. B.A.B. acknowledges support from the Stanford Graduate Fellowship Program. This work is supported by the NSF under grant numbers DMR-0342832 and the US Department of Energy, Office of Basic Energy Sciences under contract DE-AC03-76SF00515.

[1] Y.K. Kato *et. al.*, Science, 11 Nov 2004 (10.1126/science.1105514); Science **306**, 1910 (2004).
[2] S. Murakami, N. Nagaosa, and S. Zhang, Science **301**, 1348 (2003).
[3] J. Sinova *et. al.*, Phys. Rev. Lett. **92**, 126603 (2004).
[4] M.I.D'yakonov and V. Perel, Phys. Lett. A **35**, 459 (1971).
[5] J. Hirsch, Phys. Rev. Lett. **83**, 1834 (1999).
[6] N. Mott, Proc. Roy. Soc. **124**, 425 (1929).
[7] J. Wunderlich *et.al.*, cond-mat/0410295.
[8] B. Bernevig and S. Zhang, cond-mat/0411457.
[9] Y. K. Kato *et. al.*, Nature **427**, 50 (2004).
[10] A. Crepieux and P. Bruno, Phys. Rev. B **64**, 014416 (2001).
[11] S. Murakami, N. Nagaosa, and S. Zhang, Science **301**, 1348 (2003) Supplementary Material.
[12] L. Berger, Phys. Rev. B **2**, 4559 (1970).
[13] P. Dresselhauss, C. Papavassiliou, and R. Wheeler, Phys. Rev. Lett. **68**, 106 (1992).
[14] T. Hassenkam *et. al.*, Phys. Rev. B **55**, 9298 (1997).
[15] B. Jusserand *et. al.*, Phys. Rev. B **51**, 4707 (1995).
[16] W. Knap *et. al.*, Phys. Rev. B **53**, 3912 (1996).
[17] B. Bernevig and S. Zhang, cond-mat/0408442, submitted to Phys. Rev. B.
[18] Y.K. Kato *et. al.*, Phys. Rev. Lett **93**, 176601 (2004).
[19] J. Inoue, G. Bauer, and L. Molenkamp, Phys. Rev. B **70**, 041303 (2004).
[20] E. Mishchenko, A. Shytov, and B. Halperin, cond-mat/0406730.
[21] S. Murakami, Phys. Rev. B **69**, 241202(R) (2004).
[22] K. Nomura *et. al.*, cond-mat/0407279.
[23] B. Nikolic, L. Zarbo, and S. Sauma, cond-mat/0408693.