Rapid Transition of the Hole Rashba Effect from Strong Field Dependence to Saturation in Semiconductor Nanowires

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The electric field manipulation of the Rashba spin-orbit coupling effects provides a route to electrically control spins, constituting the foundation of the field of semiconductor spintronics. In general, the strength of the Rashba effects depends linearly on the applied electric field and is significant only for heavy-atom materials with large intrinsic spin-orbit interaction under high electric fields. Here, we illustrate in 1D semiconductor nanowires an anomalous field dependence of the hole (but not electron) Rashba effect (HRE). (i) At low fields, the strength of the HRE exhibits a steep increase with the field so that even low fields can be used for device switching. (ii) At higher fields, the HRE undergoes a rapid transition to saturation with a giant strength even for light-atom materials such as Si (exceeding 100 meV Å). (iii) The nanowire-size dependence of the saturation HRE is rather weak for light-atom Si, so size fluctuations would have a limited effect; this is a key requirement for scalability of Rashba-field-based spintronic devices. These three features offer Si nanowires as a promising platform for the realization of scalable complementary metal-oxide-semiconductor compatible spintronic devices.

Coherent manipulations of electron spins in semiconductors by electrical means have been demonstrated [1–5]; however, it has proven difficult to find in tetrahedral semiconductors a strong Rashba effect, which is apparently needed for achieving efficient spin manipulation [5–7] in Rashba-effect-based spintronics devices [1,2,8]. This difficulty has stimulated searches of a strong Rashba effect in nonstandard nontetrahedral 3D materials [9–11] which, however, tend to be incompatible with current semiconductor technology. Thus far, studies of the electrical manipulation of spins using the Rashba effect have focused mostly on the electron Rashba effect (ERE), which is a third-order effect, leading to rather modest ERE as illustrated in Fig. 1 for InAs 1D nanowires as a function of either applied electric field [Fig. 1(a)] or nanostructure dimension [Fig. 1(b)]. For electrons, not only the Rashba effect is weak but its coupling to nuclear spins is strong, which leads to high spin decoherence rates, whose control remains the biggest challenge in quantum information hardware [2,6,12].

On the other hand, hole spins in semiconductors have weak coupling to nuclear spins and, therefore, have the potential for longer coherence times [2,12]. Nevertheless, there are but very few studies of hole Rashba effect (HRE) in semiconductors [2,7,12,14–16], likely because of the earlier focus on 2D systems, in which holes exhibit short spin lifetimes [6] and a negligible Rashba effect owing to

the lack of the k-linear spin splitting [14,15]. These two limiting factors have recently been overcome by replacing 2D semiconductor systems with 1D semiconductor nanowires [1–3,17]. In Ge-Si core-shell nanowires, experimentalists have observed an extremely long hole spin relaxation time $T_1 = 0.6$ ms [2] and a hole spin dephasing time $T_2 = 0.18$ μs [7]. A "giant" HRE in 1D nanowires has also recently been noted theoretically in band-structure calculations [18] (footnote 25 therein), and discussed by a qualitative model Hamiltonian theory [19], pointing to the possibility of a direct, first-order dipolar coupling of the 1D hole states to the applied electric field. Such a dipolar coupling yields a direct Rashba effect with a Hamiltonian $H_{DR} = eE_x U \tau_x \sigma_z$ [where E_x is an applied electric field perpendicular to nanowires, $U = \langle \psi_{h0_\pm} | (-x) | \psi_{h1_\pm} \rangle$ the dipolar coupling constant between the ground hole $\psi_{h0_\pm}$ and first excited hole $\psi_{h1_\pm}$ states, and τ_i and σ_i are the Pauli matrices acting on the orbital part $\{\psi_{h0}, \psi_{h1}\}$ and the spin part $\{+, -\}$ of eigenstates, respectively].

The possibility of manipulating carrier spins via the Rashba effect led to many ideas for electrically controlled spintronic devices, such as the Datta-Das spin field-effect transistor (SFET) [8]. However, as the drain current saturation of the field-effect transistor is essential to reach the maximum possible operating speeds, in practical applications of SFET-type devices, the saturation of the
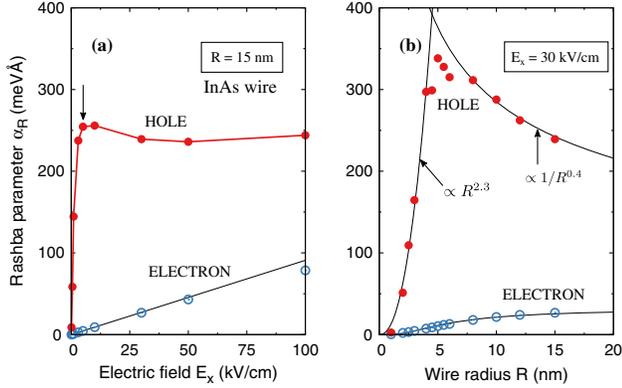
FIG. 1.   The strength of the electron and hole Rashba effects in 1D InAs nanowires. (a) Predicted Rashba parameter α_R as a function of electric field for both electrons (open circles) and holes (dots) in a $R = 15$ nm InAs nanowire, by performing atomistic pseudopotential method calculations. The vertical arrow separates the low-field region, where HRE depends strongly on field (an effect that can be used beneficially for applications in spintronic devices), and the intermediate field region where field saturation exists. The magnitude of the HRE at saturation is far larger than the ERE, and can reach giant values in nanowires even for light-atom materials such as Si. The black solid line represents a linear fit to electron α_R. (b) Same as in panel (a) but as a function of nanowire radius R, upon application of an electric field $E_x = 30$ kV/cm. In the case of holes, two solid curves represent the best fit of the rise and fall parts to $12.9 \times R^{2.3}$ and $715.9 \times R^{-0.4}$, respectively. In the case of electrons, the black solid line is the best fit to the well-known band-gap dependence of the ERE Rashba parameter [13].

drain spin current with applied electric field (and, thus, saturation of the Rashba effect) is essential, and is an elusive goal yet to be discovered. In this Letter, we find the following. (i) At low electric fields the strength of the Rashba effect for holes depends strongly on the electric field. The field-tunable HRE ranging from zero to large values, with an unexpected small electric field, is highly desirable for spintronic devices such as the Datta-Das SFET. (ii) At intermediate fields the HRE undergoes a rapid transition to saturation with a giant strength, even for light-atom materials such as Si. The emergence of saturation in the HRE ensures the Rashba effect in the saturation regime is immune from inevitable field fluctuations occurring in massive production or scalable applications [20]. These findings will probably boost efforts to further develop SFET [4,8,21], spin-orbit qubits [1,2,7], and quantum computing using Majorana states [22–26].

Method: Direct evaluation of the strength of the Rashba effect.—We use our previously developed atomistic material-dependent pseudopotential method to calculate the band structure of semiconductor nanowires under an applied electric field $\mathbf{E}$ (see Supplemental Material for details [27]). In the atomistic approach, one does not have to commit at the outset to a linear or nonlinear Rashba term, obtaining this information instead as output (not input)

from the quantum mechanical description of spin-orbit-coupling-induced interband coupling. We do not perform self-consistent Schrödinger-Poisson calculations because, as illustrated by Winkler [14] in 2D quantum wells, the strength of the Rashba effect is proportional to the averaged electric field rather than to the local field. Here, the former is an input variable. After solving the Schrödinger equation and obtaining the energy dispersion along k_z (a nanowire along z) for nanowires, as shown in Fig. 2(a), the spin splitting $\Delta E_{ss}(i, k_z)$ of the band i is fit to a power series in k_z, $\Delta E_{ss}(i, k_z) = 2\alpha_R^i k_z + \gamma^i k_z^3$. The coefficients extracted from the fit determine the Rashba parameters α_R of different subbands [28].

Electron Rashba effect in 1D nanowires.—(i) Field dependence: Fig. 1(a) shows the predicted Rashba parameters α_R of both ERE and HRE in a 15-nm-radius InAs nanowire as a function of applied electric field. We see that the ERE α_R increases approximately linearly with the electric field and then becomes sublinear when $E_x > 50$ kV/cm. The deduced ERE coefficient, defined as the slope of α_R in the linear region, is $r_{41}^e = \partial \alpha_R / \partial E_x = 90.9$ $e\text{Å}^2$, approaching the InAs bulk value of $r_{41}^{6c6c} = 117.1$ $e\text{Å}^2$ [14]. At very high fields, the ERE α_R exceeds 100 meV Å, comparable with the experimentally observed ERE $\alpha_R = 50$–100 meV Å in 2D InAs quantum wells or heterostructures [29]. (ii) Radius dependence: Fig. 1(b) shows the radius dependence of the ERE α_R for InAs nanowires under a fixed electric field of $E_x = 30$ kV/cm. We see that the ERE α_R increases initially with nanowire radius R and then begins to approach the bulk
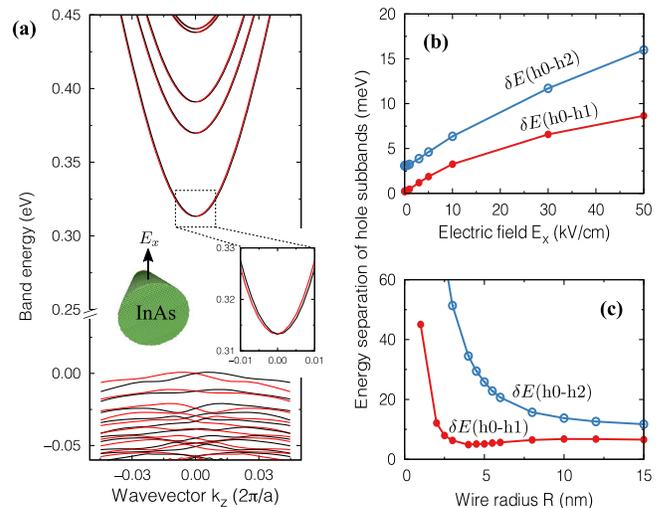

FIG. 2.   Energy separations of hole subbands in InAs nanowires. (a) Band structure of a $R = 15$ nm InAs nanowire under an electric field of 100 kV/cm. Inset: Schematic of an InAs nanowire under an electric field. (b) Energy separations of the first excited ($h1$) and second excited ($h2$) hole subbands relative to the ground hole subband ($h0$) at the zone center as a function of electric field E_x for the $R = 15$ nm InAs nanowire. (c) Energy separations as a function of nanowire radius R under an electric field $E_x = 30$ kV/cm.

asymptotic value at $R > 10$ nm. This monotonic, but non-linear, radius dependence of the ERE α_R is similar to the thickness dependence of the well-established ERE in 2D quantum wells, as demonstrated by the best fit [solid line in Fig. 1(b)] to the classical formulation of α_R developed for 2D electron gases [14]. The ERE α_R approaches an asymptotic limit of 34 meV Å as the radius increased, in excellent agreement with expected bulk InAs value of 35 meV Å under the same field [14]. These agreements with experimental data demonstrate the reliability and validity of the atomistic method used to predict the Rashba effect. See Fig. S1 (in Supplemental Material [27]) for detailed dependence of the ERE on wire sizes and applied fields as well as comparison with the closed form physical model.

Giant hole Rashba effect in 1D nanowires with a rapid saturation.—In sharp contrast to the ERE, the red lines in Fig. 1 exhibit an unusual size- and field-dependent HRE. (i) Field dependence: In a 15-nm-radius InAs nanowire, Fig. 1(a) shows that with increasing electric field, the HRE α_R develops a steep increase at the weak field, and then quickly saturates (with a saturation $\alpha_R^{\text{sat}} = 254$ meV Å) at a modest field of $E_x^{\text{sat}} = 5$ kV/cm, as opposed to a mild linear increase of the ERE α_R. The transition from the steep rise to the saturation occurs within an ultrasmall region of the electric field. This rapid saturation of the HRE satisfies the basic requirements for developing practical spintronic devices. The steep rise in the subsaturation region is linear with a huge slope of about $28\,000$ $e\text{Å}^2$ (termed as the Rashba coefficient r_{ss}), which is around 300 times larger than the ERE counterpart. The r_{ss} is so huge that the HRE α_R is highly tunable (from zero to 254 meV Å) even though it saturates at a modest field. The HRE α_R^{sat} is larger, by a factor of 5, than the ERE α_R at $E_{\text{sat}} = 5$ kV/cm for the 15-nm-radius InAs nanowire. The HRE α_R^{sat} is 2–5 times larger than reported values of the ERE α_R in InAs and InSb 2D electron gases [5,29], and is only 1 order of magnitude smaller than the giant Rashba parameters observed in the polar BiTeI [9] and on the surface of topological insulators [5]. (ii) Radius dependence: Compared with the ERE α_R, the radius dependence of the HRE α_R in 1D nanowires is also abnormal and nonmonotonic, as shown in Fig. 1(b). We see that HRE α_R increases rapidly as a $R^{2.3}$ power law, rising faster than the expected linear increase in Ref. [19], and then begins to decrease as a $R^{-0.4}$ power law once the maximum has been achieved (a large α_R of ~350 meV Å). The HRE α_R finally falls to its asymptotic zero value of the heavy-hole band in bulk. Such nonmonotonic size-dependent α_R, to the best of our knowledge, has not been reported in the literature. (iii) Material dependence: The strength of the conventional Rashba effect depends explicitly on two fundamental quantities: Γ-point direct band gap E_g and spin-orbit energy Δ_{so}; hence, we expect that it is strongest in InAs, modest in GaAs and Ge, but very weak in Si [14]. However, this is not necessary true for the HRE in nanowires since α_R implicitly depends on E_g and Δ_{so} in the direct Rashba Hamiltonian
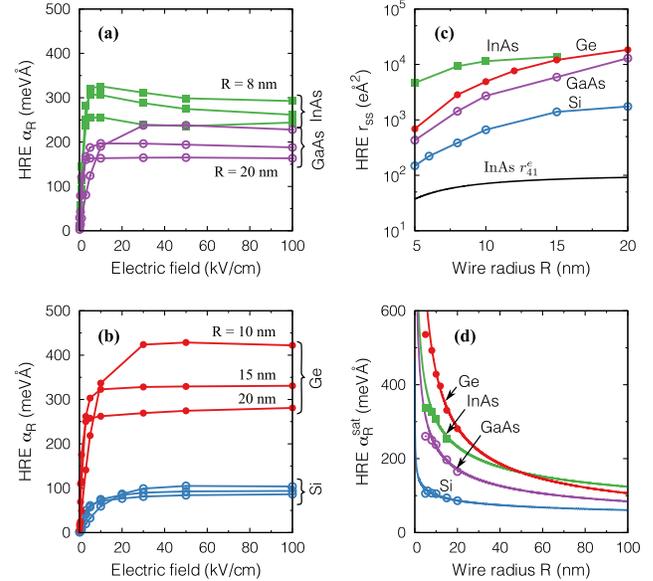

FIG. 3. Electrical response of the HRE in nanowires. The HRE α_R as a function of applied electric field for (a) GaAs and InAs nanowires and (b) Ge and Si nanowires with varying radius R. (c) Corresponding HRE coefficient r_{ss}^h in the subsaturation region as a function of nanowire radius R for InAs, GaAs, Ge, and Si nanowires. The black solid line represents the ERE coefficient r_{41}^e of InAs nanowires for comparison. (d) Saturation HRE α_R^{sat} decays as a $R^{-\lambda}$ power law toward its asymptotic zero value in bulk. The best fit indicates $\lambda = 0.39$, 0.44, 0.61, and 0.22 for InAs, GaAs, Ge, and Si nanowire materials, respectively.

H_{DR}. In Figs. 3(a) and 3(b), we compare predicted HRE α_R as a function of applied electric field in InAs, GaAs, Ge, and Si nanowires. All nanowires exhibit similar trends of the field-dependent HRE α_R as in InAs nanowires. Most of the significant features of the hole Rashba effect considered here are within weak electric fields (less than 50 kV/cm), where carrier density is low and, hence, a self-consistent Poisson-Schrödinger solution is not needed. Indeed, the electric field values required to archive saturation do not extend much beyond the transition point from strong to weak field-dependence (vertical arrow in Fig. 1). We summarize the deduced HRE r_{ss} and α_R^{sat} in Figs. 3(c) and 3(d), respectively. We find that both r_{ss} and α_R^{sat} highly, but nonmonotonically, depend on Δ_{so} and E_g. Figure 3(c) shows that the HRE r_{ss} even in Si nanowires is 1 order of magnitude larger than ERE r_{41}^e in InAs nanowires, giving the saturation HRE α_R^{sat} in Si nanowires around 110 meV Å, which is among the largest reported values in InAs and InSb electron systems [5,29]. The HRE α_R^{sat} in the saturation regime decays as a $R^{-\lambda}$ power law toward its asymptotic zero value in bulk. As shown in Fig. 3(d), the decay of the HRE α_R^{sat} is rather rapid for GaAs ($\lambda = 0.44$), InAs ($\lambda = 0.39$), and Ge ($\lambda = 0.61$) nanowires, but for light-atom Si nanowires the size dependence is weaker ($\lambda = 0.2$). Thus, for Si nanowires the saturation value of the HRE can be insensitive to size fluctuations over

a significant range of sizes, a key requirement for scalability of Rashba field-based spintronic devices.

The origin of the anomalous HRE in nanowires.—At first glance, we could not understand the anomalous field and radius dependences of the HRE α_R from the direct Rashba Hamiltonian $H_{DR} = eE_x U \tau_x \sigma_z$ alone since it is apparently linearly proportional to the external field E_x [19]. We note that H_{DR} couples with the last term of the effective Luttinger-Kohn Hamiltonian $H_{LK}^{eff} = A_+ + A_- \tau_z + C k_z \tau_y \sigma_x$ to lift the otherwise degenerate hole subbands with k-linear spin splitting [19] [where $A_\pm = \hbar^2 k_z^2 (m_{h0}^{-1} \pm m_{h1}^{-1})/4 \pm \Delta/2$, and $\Delta \propto R^{-2}$ is the energy separation between $h0$ and $h1$ subbands in the absence of external electric field, arising from the quantum confinement effect (QCE)], which is a key feature making 1D holes different from the electron counterpart as well as 3D bulk and 2D systems. The off-diagonal Hamiltonian matrix $\langle \psi_{h1_\pm} | H_{LK}^{eff} | \psi_{h0_\mp} \rangle = i k_z C$ and, hence, $C \propto 1/R$. We have to diagonalize the Hamiltonian of $H_{LK}^{eff} + H_{DR}$ (neglecting the weak H_R) following the procedure described in Ref. [19] to obtain the spin splitting $\Delta \epsilon_{ss}(k_z) = 2\alpha_R k_z$ with a Rashba parameter

$$\alpha_R = \frac{2eCUE_x}{\sqrt{\Delta^2 + 4e^2 U^2 E_x^2}}. \tag{1}$$

The denominator of Eq. (1) is the energy separation between $h0$ and $h1$ subbands (or $h0 - h1$ splitting): the first term (Δ) is due to the QCE, and the second term arises from the electric-field-induced quantum confined Stark effect (QCSE). The competition between these two energy contributions leads to the observed transition between two different electrical responses of the HRE α_R. If the QCE dominates the energy separation (i.e., $\Delta \gg 2eUE_x$), $\alpha_R \simeq 2eCUE_x/\Delta$, which is linearly proportional to the electric field E_x; if QCSE is predominant (i.e., $\Delta \ll 2eUE_x$), $\alpha_R \simeq C$, which is insensitive to the electric field E_x. Therefore, we attribute the observed emergence of the saturation of the HRE α_R to an electric-field-induced strong QCSE.

We now turn to examine the energy contributions to the $h0 - h1$ splitting. Figure 2(b) shows the predicted $h0 - h1$ splitting $\delta E(h0 - h1)$ as a function of the electric field for the $R = 15$ nm InAs nanowire using the atomistic pseudopotential method. For a particular nanowire, the contribution of the QCE to the $h0 - h1$ splitting is a electric field-independent constant of Δ, which is 0.5 meV for the $R = 15$ nm InAs nanowire. We attribute the change of $\delta E(h0 - h1)$ from Δ upon application of an electric field to the QCSE. In Fig. 2(b) we see that $\delta E(h0 - h1)$ raises quickly (from 0.5 meV at $E_x = 0$ to 1.9 meV at $E_x^{sat} = 5$ kV/cm) as increasing the electric field, illustrating a rapid transition in the dominant contribution from the QCE to the QCSE. In terms of Eq. (1), in the QCE-domainant scenario (i.e., when $E_x < E_x^{sat}$), $\alpha_R \simeq 2eCUE_x/\Delta$ which explains what we have observed a linearly field-dependent

HRE α_R for $E_x < 5$ kV/cm [Fig. 1(a)]. When $E_x > E_x^{sat}$ the QCSE is predominant in the $\delta E(h0 - h1)$ and $\alpha_R \simeq C$ in terms of Eq. (1); this explains the emergence of the saturation of the HRE α_R predicted by the atomistic pseudopotential method at $E_x > 5$ kV/cm [Fig. 1(a)].

Under a fixed electric field but varying the nanowire radius, the QCE will be the primary factor in the $h0 - h1$ splitting when nanowire is thin enough, whereas the QCSE is always the leading factor at extremely wide nanowires. Figure 2(c) shows that as the nanowire radius increases, $\delta E(h0 - h1)$ undergoes a change from a steep reduction to a radius independence for nanowires under a constant electric field $E_x = 30$ kV/cm. This change indicates a transition in the dominant energy contribution from the QCE at thin nanowires ($R < 5$ nm) to the QCSE at wide nanowires ($R > 5$ nm), considering that radius-independent splitting implies a negligible QCE. Regarding Eq. (1), $\alpha_R \simeq 2eCUE_x/\Delta \propto R^2$ for $R < 5$ nm and $\alpha_R \simeq C \propto 1/R$ for $R > 5$ nm, consistent with the atomistic pseudopotential method prediction that $\alpha_R \propto R^{2.3}$ for $R < 5$ nm, and $\alpha_R \propto 1/R^{0.4}$ for $R > 5$ nm, as shown in Fig. 1(b). Therefore, we ascribe the abnormal field and radius dependences of the HRE α_R in nanowires to the competition between the space-confinement-induced QCE and electric-field-induced QCSE on the $h0 - h1$ splitting. We also note in Figs. 2(b) and 2(c) that, in the QCSE-dominant scenario, the validity of the two-band approximation used in the model Hamiltonian approach is doubtful, as the first two subbands $h0$ and $h1$ are not well separated in energy from the next excited subband $h2$.

Possible device applications of the theoretical work.— As the drain-current saturation is an essential requirement in electronic field-effect transistors, the saturation of the electrically controlled Rashba effect is essential for practical applications of spintronic devices. The QCSE-induced saturation of the HRE under the applied electric field can remarkably improve the scalability of semiconductor spintronic devices that rely on the Rashba effect, considering that they can operate in the saturated region that is robust against the fluctuations in applied electric fields. In conjunction with a huge HRE r_{ss} (∼300 times larger than the ERE counterpart), which quantifies an ultrafast electrical response of the Rashba effect, the emergence of the rapid saturation of the HRE reflected as the raising of the Rashba effect over just a narrow range of the electric field is in fact an advantage of the current proposition, since it could lead to the realization of an ultrafast switch of the Rashba field from zero to a saturation value using only a small gate voltage [4,8,17]. In combination with the suppression of the Dyakonov-Perel spin relaxation in nanowires [30–32] and a remarkable reduction of hole spin-nuclear interaction [12], the unique HRE properties we have presented establish 1D hole nanowires as an attractive platform for semiconductor spintronics applications [1,2,8]. Specifically, in Si nanowires the HRE α_R^{sat} exceeds 100 meV Å over a wide range

of nanowire sizes, overcoming the major challenge of advanced Si spintronics owing to weak spin-orbit interaction in Si [6], and is not susceptible to fluctuations in nanowire sizes; this makes Si nanowires a promising avenue for the realization of scalable CMOS-compatible spintronics devices [2,7].

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splitting $\Delta_{so} = 0.38$ eV, InAs Kane's momentum matrix element $P^2/2m = 21.5$ eV, and $E_g(R)$ is the nanowire band gap. The predicted $E_g(R)$ of InAs nanowires under $E_x = 30$ kV/cm is described using $E_g(R) = E_g^b + \beta/R^\gamma$, where $E_g^b = 0.417$ eV is bulk InAs band gap, $\beta = 2.8$, and $\gamma = 1.6$.

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