

Accuracy of Circular Polarization as a Measure of Spin Polarization in Quantum Dot Qubits

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(Received 13 May 2003; published 15 December 2003)

A quantum dot spin light emitting diode provides a test of carrier spin injection into a qubit and a means for analyzing carrier spin injection and local spin polarization. Even with 100% spin-polarized carriers the emitted light may be only partially circularly polarized due to the geometry of the dot. We have calculated carrier polarization-dependent optical matrix elements for InAs/GaAs self-assembled quantum dots (SAQDs) for electron and hole spin injection into a range of quantum dot sizes and shapes, and for arbitrary emission directions. Calculations for typical SAQD geometries with emission along [110] show light that is only 5% circularly polarized for spin states that are 100% polarized along [110]. Measuring along the growth direction gives near unity conversion of spin to photon polarization and is the least sensitive to uncertainties in SAQD geometry.

DOI: 10.1103/PhysRevLett.91.257901

PACS numbers: 03.67.Lx, 73.63.Kv

There are several proposals for constructing a quantum bit using a spin confined to a quantum dot [1–4]. One method of initializing such a quantum bit is to electrically inject spin-polarized carriers into the quantum dot. Towards this end, recent experiments [5] have demonstrated a spin light emitting diode (spin-LED) in which spin-polarized carriers are injected into and recombine within InAs/GaAs self-assembled quantum dots (SAQDs). The emitted light is partially circularly polarized, with the degree of polarization providing a measure of the spin in the SAQDs. Besides its application to physical quantum bits, such a system provides information about spin transport and relaxation within the structure as a whole, which is important for the development of spin-based electronics (spintronics) [6,7]. Spin-LEDs have also been made using quantum wells for the recombination [8–11]. The conversion of electron spin to photon polarization is filtered through the selection rules associated with the quantum well or dot. The selection rules for quantum wells are already controversial, and essentially nothing is known about the selection rules for circular polarization in SAQDs. These can be complicated due to the presence of strain and uncertain geometry in SAQDs.

In Ref. [5], spin-polarized electrons or holes were injected along the [001] growth direction from a (Ga,Mn)As layer that was spin polarized along [110]. The light emitted along the [110] direction was found to be only $\approx 1\%$ circularly polarized, suggesting a small spin polarization within the SAQD. However, due to the selection rule uncertainty, a small photon polarization does not necessarily mean that the spin polarization within the SAQD is small.

In this Letter we present calculations of the circular polarization dependence of dipole recombination of spin-polarized states within a self-assembled InAs/GaAs quantum dot. This gives a measure of the efficiency with which spin-polarized SAQD states are converted into circularly polarized photons. The calculations are

done for a range of sizes and shapes. The polarization is independent of whether the injected spin-polarized carriers are electrons or holes. We find, however, that the SAQD geometry and emission direction strongly influence the observed circular polarization which varies from 0 to $\approx 20\%$ (for 100% polarized carriers). For a lens shaped SAQD there is a nonzero polarization for directions perpendicular to the growth direction only if the SAQD is elongated so as to break azimuthal symmetry. We also show that measuring along the growth direction gives near unity conversion of spin to photon polarization and is the least sensitive to uncertainties in SAQD geometry.

We consider the situation in which the electron spin is polarized along a direction d and the emitted light is observed along the same direction. The emitted light is characterized by its degree of polarization defined by

$$P_d = \frac{(I_d^+ - I_d^-)}{(I_d^+ + I_d^-)}, \quad (1)$$

where I_d^\pm is the intensity of light with \pm helicity. The InAs SAQD is taken to be an ellipsoidal cap, elongated along [110] and surrounded by GaAs (Fig. 1). More specifically, the geometry is determined by

$$(\hat{\mathbf{x}}_{[110]} \cdot \mathbf{x})^2/e + (\hat{\mathbf{x}}_{[1\bar{1}0]} \cdot \mathbf{x})^2/e + (\hat{\mathbf{x}}_{[001]} \cdot \mathbf{x})^2 = r^2, \quad (2)$$

where $\hat{\mathbf{x}}_d$ is a unit vector along the direction d , e is the elongation, and r is a scale determining the overall size of the SAQD. The ellipsoid is sliced along a (001) plane, giving the cap shown in Fig. 1. To account for variations and uncertainties in dot geometries, we consider a range of dot shapes, parametrized by the height h , the elongation e , and the width-to-height ratio w ,

$$h = 1.7 \text{ nm}, 2.3 \text{ nm}, 2.8 \text{ nm}, \quad (3)$$

$$e = d_{[110]}/d_{[1\bar{1}0]} = 1.0, 1.2, 1.4, \quad (4)$$

$$w = (d_{[110]} + d_{[1\bar{1}0]})/h = 12, 16, 20, \quad (5)$$

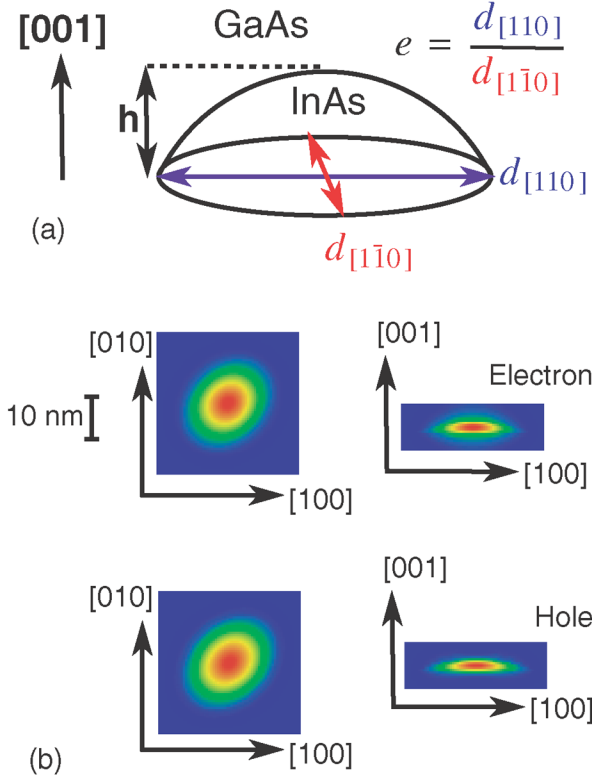


FIG. 1 (color online). (a) The quantum dot geometry. (b) Electron and hole wave functions for a dot with $e = 1.4$ and $h = 2.8$ nm.

where $d_{[110]}$ and $d_{[1\bar{1}0]}$ are the major axes along the indicated directions. We do not explicitly include composition gradients in the SAQD [12]. However, h may be regarded as an effective height after such effects are factored in.

Ground state electron and hole wave functions were calculated using 8-band strain-dependent $\mathbf{k} \cdot \mathbf{p}$ theory in the envelope approximation, by a method that has been described previously [13,14]. The parameters used, including the spin-orbit interaction (essential for nonzero polarization), are listed in Table I. All wave functions were computed numerically on a real space grid with spacing set to the unstrained lattice constant of GaAs. Since strain and confinement split the HH/LH degeneracy, all levels are doubly degenerate, with states that may be denoted $|\psi\rangle$ and $T|\psi\rangle$, which are time reverses of each other. Because the wave functions were computed with a spin-degenerate Hamiltonian, the state $|\psi\rangle$ has a random spin orientation. Spin-polarized states were constructed by taking a linear combination of the states comprising the doublet and adjusting the coefficient so as to maximize the expectation value of the pseudospin operator projected onto a direction d . That is, we find the complex number a that maximizes

$$\frac{[\langle\psi| + a^*\langle\psi|T]\hat{\mathbf{d}} \cdot \mathbf{S}[\psi\rangle + aT|\psi\rangle]}{(1 + |a|^2)}, \quad (6)$$

TABLE I. Material parameters used in the calculations [15]. The valence band offset (VBO) is the unstrained valence energy, determining the band alignment.

Parameter	InAs	GaAs
E_g	0.418 eV	1.519 eV
Δ_{so}	0.38 eV	0.341 eV
VBO	0.085 eV	0.0 eV
γ_1	19.67	6.98
γ_2	8.37	2.25
γ_3	9.29	2.88
E_P	22.2 eV	22.7 eV
a_c	-6.67 eV	-9.55 eV
a_v	1.67 eV	0.95 eV
b	-1.8 eV	-2.0 eV
d	-3.6 eV	-5.4 eV
a_{latt}	0.6058 nm	0.5653 nm
C_{xxxx}	832.9 GPa	1211 GPa
C_{xyyy}	452.6 GPa	548 GPa
C_{xyxy}	395.9 GPa	604 GPa

where the pseudospin operator in the 8-band model is given by

$$\mathbf{S} = \begin{pmatrix} \boldsymbol{\sigma}_{\Gamma_6} & 0 & 0 \\ 0 & \mathbf{J}_{\Gamma_8} & 0 \\ 0 & 0 & \boldsymbol{\sigma}_{\Gamma_7} \end{pmatrix} \quad (7)$$

and $\boldsymbol{\sigma}$ and \mathbf{J} are the spin-1/2 and spin-3/2 angular momentum operators respectively. The spin-polarized states found this way are the eigenstates in a small magnetic field oriented parallel to d , i.e., for $\mathbf{B} < (mc/e\hbar)\Delta E$, where ΔE is the energy splitting of the top two orbital conduction states (for electrons) or valence states (for holes). For our systems the minimum ΔE is 20 meV (for holes), thus $\mathbf{B} < 100$ T. Coulomb interaction between the electron and hole does not appreciably change the results (we find a maximum change in the polarization of 0.05P).

For spin-polarized electrons and unpolarized holes, the intensity for emission of circularly polarized light is given by

$$I_d^\pm = |\langle\psi_v|\hat{\boldsymbol{\epsilon}}_d^\pm \cdot \mathbf{p}|\psi_c\rangle|^2 + |\langle\psi_v|T\hat{\boldsymbol{\epsilon}}_d^\pm \cdot \mathbf{p}|\psi_c\rangle|^2, \quad (8)$$

where $|\psi_v\rangle$ and $|\psi_c\rangle$ are the conduction and valence states with spin oriented along $\hat{\mathbf{d}}$, \mathbf{p} is the momentum operator, and $\hat{\boldsymbol{\epsilon}}_d^\pm$ is the circular polarization vector for \pm helicity with propagation along the direction d . The corresponding expression for spin-polarized holes and unpolarized electrons is

$$I_d^\pm = |\langle\psi_v|\hat{\boldsymbol{\epsilon}}_d^\pm \cdot \mathbf{p}|\psi_c\rangle|^2 + |\langle\psi_v|\hat{\boldsymbol{\epsilon}}_d^\pm \cdot \mathbf{p}T|\psi_c\rangle|^2. \quad (9)$$

However, since T and \mathbf{p} anticommute, Eqs. (8) and (9) give identical results.

We first consider the case where the spins are polarized along [110]. Figure 2(a) shows the polarization for the [110] direction, $P_{[110]}$, as a function of dot geometry,

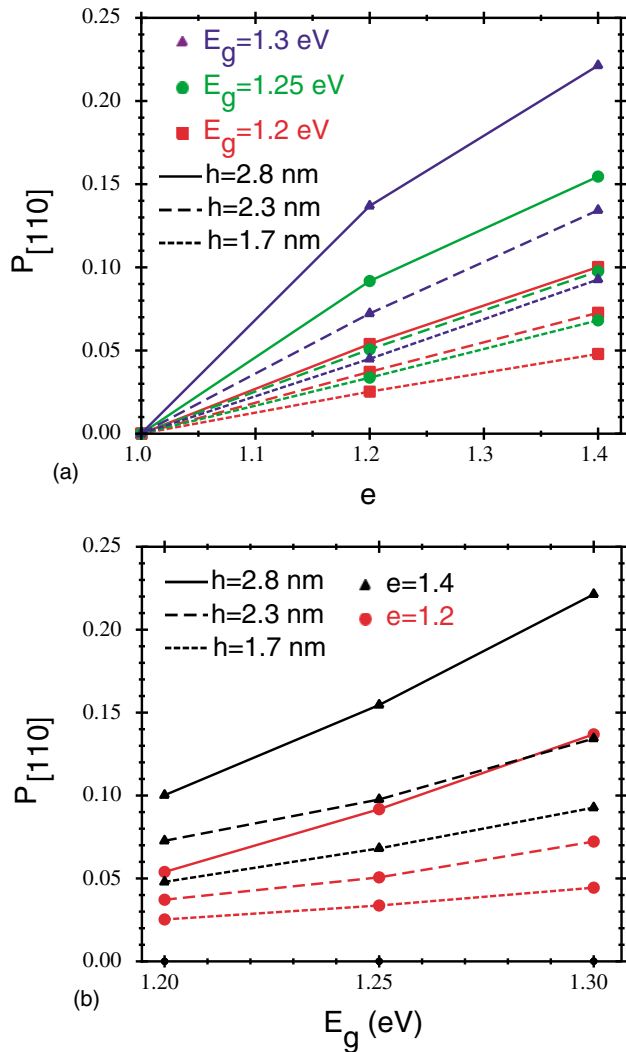


FIG. 2 (color online). (a) Polarization along [110], as a function of elongation. (b) Polarization along [110], as a function of band gap.

which is parametrized by the elongation e , the height h , and the band gap E_g . Rather than expressing results in terms of the width-to-height ratio w , we have linearly interpolated the final results between values of w so as to obtain P_d at convenient values of E_g .

For axially symmetric dots ($e = 1$) the polarization is zero, but increases as the dots become more elongated. The polarization also increases with increasing E_g with all other parameters held fixed. Finally, for a fixed elongation and fixed band gap, shorter dots have a larger polarization. Taken together, these indicate a general trend that the larger deviations from spherical symmetry result in larger polarization, whether comparing dimensions in the [110] vs [1 $\bar{1}$ 0] or [001] vs [110].

The magnitude of the polarization is of great interest, since the experimentally observed polarizations were only on the order of 1%. For the geometries considered, we find $P_{[110]} \lesssim 23\%$. Assuming nominal values $e = 1.2$,

$h = 2.3$, and $E_g = 1.25$ eV Fig. 2 shows that for 100% polarized carriers, the light should be 5% circular polarized. From this value of 0.05 for the conversion efficiency, we can infer that the observed 1% circular polarization [5] was generated by carriers that were $1/0.05 = 20\%$ polarized. As the polarization's dependence on elongation is roughly linear, an average elongation for a dot ensemble would produce an average polarization roughly given by Fig. 2(a) as well.

Figure 2(b) gives the polarization as a function of the band gap, showing the trend of increasing polarization with the band gap. The results of Fig. 2(b) disagree with the measurements [5] which show P independent of E_g for polarized electrons, and decreasing with increasing E_g for polarized holes. One possibility is that the polarized hole sample had growth conditions resulting in SAQDs with a size-dependent elongation. Another likely scenario is that the dynamics of hole relaxation into the SAQD are such that spin relaxation is stronger in smaller dots.

To further examine the polarization efficiency, we performed a second series of calculations in which P_d was computed as a function of the direction for a single dot geometry. Figure 3 shows the polarization as a function of the direction d for a SAQD. The maximum polarization is obtained along the growth direction, with $P_{[001]} \approx 0.98$. P_d is substantially smaller along [110] and [1 $\bar{1}$ 0], and zero for [100] and [010]. While clearly [001] is optimal, if one is restricted to the plane perpendicular to the growth direction, then [110] is the best choice, while [100] and [010] are the worst. It is important to note that the photon polarization is a result of SAQD geometry and strain and is not a crystallographic effect. [110] is singled out because the SAQD is elongated in that direction. Therefore, growth on a different substrate with different orientation will not remedy the poor spin conversion efficiency.

Besides the larger polarization, [001] has other advantages. For the SAQDs considered, $P_{[001]} \approx 1$ to within a few percent, in contrast to the large variation with geometry seen for $P_{[110]}$ and $P_{[1\bar{1}0]}$. Thus, measuring along [001] decreases the uncertainties due to the large uncertainties in SAQD geometry. Also, because the observed light must be collected within some solid angle, some of the emission will come from directions for which P_d is smaller than the nominal direction. From Fig. 3 we see that [001] has the advantage of having less curvature, thus decreasing effects from a nonzero collection angle.

We have shown that recombination of spin-polarized carriers in InAs/GaAs SAQDs results in only modest polarization of the light emitted perpendicular to the growth direction. The light obtains a circular polarization only for dots that are elongated so as to break azimuthal symmetry. These results explain the small polarization seen in recent experiments [5] and imply that the spin polarization of the carriers in the SAQDs in [5] was $\approx 20\%$. Measurement along [001] gives the most efficient conversion of spin to photon polarization. Finally, we

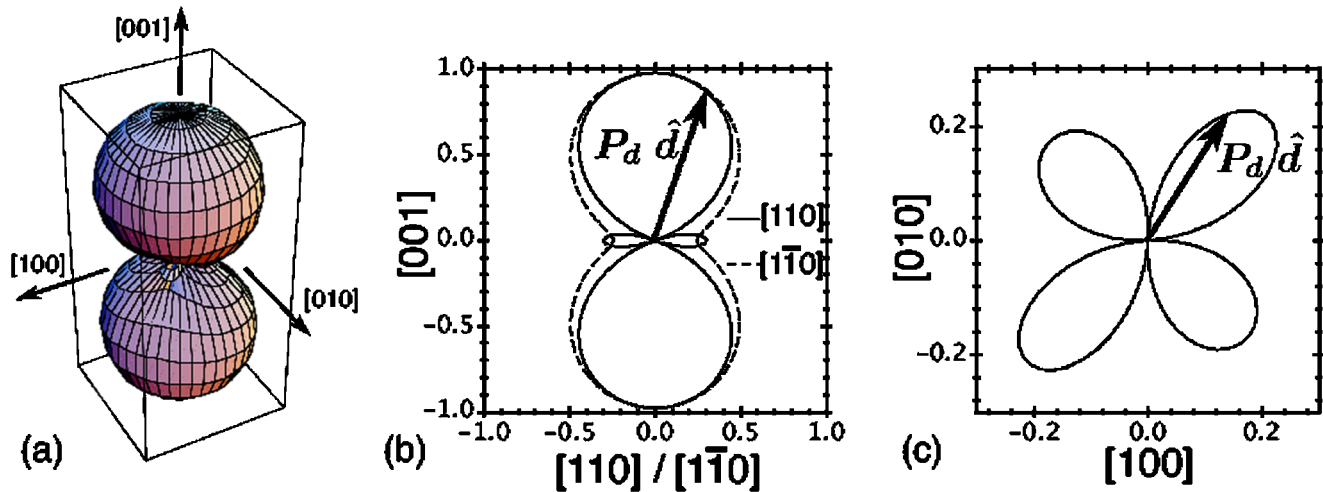


FIG. 3 (color online). Polarization as a function of spin polarization and light emission direction for a SAQD with $h = 2.8$ nm, $e = 1.4$, and $E_g = 1.36$ eV. The SAQD geometry was chosen to make the features more visible. (a) Surface showing $P_d \hat{d} = \hat{d}(I_d^+ - I_d^-)/(I_d^+ + I_d^-)$. (b) $P_d \hat{d}$ in the (110) and (1 $\bar{1}$ 0) planes. (c) $P_d \hat{d}$ in the (001) plane.

have determined that measurements done along the [001] direction will be less susceptible to uncertainties and variation in dot geometry, and to effects due to light being collected from a nonzero solid angle. The implications of these features for a particular SAQD qubit will depend on the details of the implementation. However, the anisotropy shown in Fig. 3 indicates that a SAQD differs significantly from an ideal isolated spin, and any qubit design must take this into account.

This work was supported by DARPA/ARO DAAD19-01-1-0490.

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- [1] D. Loss and D.P. DiVincenzo, Phys. Rev. B **57**, 120 (1998).
- [2] G. Burkard, D. Loss, and D.P. DiVincenzo, Phys. Rev. B **59**, 2070 (1999).
- [3] A. Imamoglu, D.D. Awschalom, G. Burkard, D.P. DiVincenzo, D. Loss, M. Sherwin, and A. Small, Phys. Rev. Lett. **83**, 4204 (1999).
- [4] J. Levy, Phys. Rev. Lett. **89**, 147902 (2002).
- [5] Y. Chye, M.E. White, E. Johnston-Halperin, B.D. Gerardot, D.D. Awschalom, and P.M. Petroff, Phys. Rev. B **66**, 201301(R) (2002).
- [6] G. A. Prinz, Phys. Today **48**, No. 4, 58 (1995).
- [7] S.A. Wolf, D.D. Awschalom, R.A. Buhrman, J.M. Daughton, S. von Molnár, and M.L. Roukes, Science **294**, 1488 (2001).
- [8] Y. Ohno, D.K. Young, B. Beschoten, F.M.H. Ohno, and D.D. Awschalom, Nature (London) **402**, 790 (1999).
- [9] D.K. Young, E. Johnston-Halperin, and D.D. Awschalom, Appl. Phys. Lett. **80**, 1598 (2002).
- [10] E. Johnston-Halperin, D. Lofgreen, R.K. Kawakami, D.K. Young, L. Coldren, A.C. Gossard, and D.D. Awschalom, Phys. Rev. B **65**, 041306(R) (2002).
- [11] M. Kohda, Y. Ohno, K. Takamura, F. Matsukura, and H. Ohno, Jpn. J. Appl. Phys. **40**, Pt. 2, L1274 (2001).
- [12] I. Kegel, T.H. Metzger, A. Lorke, J. Peisl, J. Stangl, G. Bauer, J.M. García, and P.M. Petroff, Phys. Rev. Lett. **85**, 1694 (2000).
- [13] C. Pryor, M.-E. Pistol, and L. Samuelson, Phys. Rev. B **56**, 10 404 (1997).
- [14] C. Pryor, Phys. Rev. B **57**, 7190 (1998).
- [15] I. Vurgaftman, J.R. Meyer, and L.R. Ram-Mohan, J. Appl. Phys. **89**, 5815 (2001).