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Strain-induced conduction-band spin splitting in GaAs from first-principles calculations

Athanasios N. Chantis,[1] Manuel Cardona,[2] Niels E. Christensen,[3] Darryl L. Smith,[1] Mark van Schilfgaarde,[4]
Takao Kotani,[4] Axel Svane,[3] and Robert C. Albers[1]
[1]*Theoretical Division, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA*
[2]*Max-Planck Institut für Festkörperforschung, Heisenbergstrasse 1, D-70569 Stuttgart, Germany*
[3]*Department of Physics and Astronomy, University of Aarhus, DK-8000 Aarhus C, Denmark*
[4]*School of Materials, Arizona State University, Tempe, Arizona 85287-6006, USA*

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We use a recently developed self-consistent *GW* approximation to perform first-principles calculations of the conduction-band spin splitting in GaAs under [110] strain. The spin-orbit interaction is taken into account as a perturbation to the scalar relativistic Hamiltonian. These are the calculations of conduction-band spin splitting under deformation based on a quasiparticle approach and, because the self-consistent *GW* scheme accurately reproduces the relevant band parameters, it is expected to be a reliable predictor of spin splittings. We also discuss the spin-relaxation time under [110] strain and show that it exhibits an in-plane anisotropy, which can be exploited to obtain the magnitude and sign of the conduction-band spin splitting experimentally.

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I. INTRODUCTION

The increasing prospect of utilizing spin electronics with conventional semiconductors calls for quantitative predictions of the spin relaxation of electrons in these materials.[1,2] In semiconductors without inversion symmetry, the spin-relaxation rate is related to the relativistic splitting in the conduction band; an effect that also induces spin precession, and is relevant for spin transport and injection.[3–6] In zinc-blende semiconductors, which are the most promising for spintronic applications, it is widely accepted that D'yakonov-Perel' (DP) (Ref. 7) is the dominant spin-relaxation mechanism. Generally speaking, this mechanism is present when the spin degeneracy of the conduction band is lifted. The spin splitting can be viewed as a **k**-dependent effective magnetic field $\mathbf{B}_{\text{eff}}(\mathbf{k})$, which, under certain scattering conditions, relaxes the average spin of the ensemble. The strength of the effective field depends on the material. In the general form we can add this field to the Hamiltonian as an effective Zeeman term $H(\mathbf{k})=(1/2)\sigma\cdot\mathbf{\Omega}$, where $\mathbf{\Omega}(\mathbf{k})$ (with the dimensions of energy) is proportional to $\mathbf{B}_{\text{eff}}(\mathbf{k})$. In the zinc-blende crystal structure, there is no inversion symmetry; this leads to an $\mathbf{\Omega}$ field with components[8,9]

$$\Omega_D^i = 2\gamma k_i(k_{i+1}^2 - k_{i+2}^2), \tag{1}$$

where $i=x,\ i+1=y,\ i+2=z$, the indices obey a cyclic relationship $(i+3=i)$, and γ is a constant that depends on the bulk properties of the material. This effective field was first introduced by Dresselhaus.[8] In uniaxially deformed crystals there is an additional effective field:[10–13]

$$\Omega_{\text{stress}}^i = C(\epsilon_{i,i+1}k_{i+1} - \epsilon_{i,i+2}k_{i+2}) + Bk_i(\epsilon_{i-2,i-2} - \epsilon_{i-1,i-1}), \tag{2}$$

where ϵ_{ij} is the strain tensor, and C and B are material-dependent constants. The first part of the effective field originates from off-diagonal components of the strain tensor while the second part originates from diagonal ones. The second part appears only due to the spin-orbit mixing of p and d states, and therefore should be much weaker than the first part.[14] However a numerical estimation of B has not yet been performed probably because of uncertainties concerning the Γ_{12} states.

The data for the values of γ, C, and B in various zinc-blende semiconductors are very sparse. The most studied case is GaAs. However, the experimental data for γ show a wide range of values between 11.0 and 34.5 eV Å^3.[15] Theoretical calculations of this parameter also show a wide range of predicted values. Calculations based on $\mathbf{k}\cdot\mathbf{p}$ method predict a value between 25 and 30 eV Å^3.[15] However, a first-principles calculation by Cardona *et al.*[16] predicted a value of 15 eV Å^3. Our recent first-principles calculation[17] predicted a value of 8.5 eV Å^3, a lot smaller than the commonly cited value of 27.5 eV Å^3. Recently, Krich and Halperin[18] used a semiclassical approach to estimate the effect of Ω_D on the mean and variance of the conductance in closed quantum dots, and compared the results of their model with the experiment in Ref. 19. They were able to reach a good agreement only when they used our value of γ, suggesting that the value of γ in GaAs must be around 9 eV Å^3.

Also our current knowledge of C and B in GaAs is far from being satisfactory. The magnitude of C was estimated experimentally in Refs. 20 and 21 to be 8.1 ± 2.5 and 3.9 eV Å, respectively. The values of C calculated with linear combination of atomic orbitals (LCAO) and pseudopotentials are 3.75 and 11.24 eV Å, respectively.[16] The calculations are able to define also the sign of C; in Ref. 16 it was found to be opposite to that of γ.[22] No other attempt has been made to calculate the sign of C since. To our knowledge the magnitude and sign of B has not been estimated experimentally or theoretically so far. D'yakonov *et al.*[10] showed that the spin-relaxation time has a very weak dependence on applied pressure upon application of [100] strain, possibly indicating that the magnitude of B is negligibly small.

In this work we use a recently developed *ab initio* method based on the *GW* approximation to predict these parameters for GaAs. We will try to answer the important questions about the strengths and signs of the spin splittings caused by the two mechanisms: Eqs. (1) and (2).

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II. METHOD

The GW approximation can be viewed as the first term in the expansion of the nonlocal energy dependent self-energy $\Sigma(\mathbf{r},\mathbf{r}',\omega)$ in the screened Coulomb interaction W. From a more physical point of view, it can be interpreted as a dynamically screened Hartree-Fock approximation plus a Coulomb hole contribution.[23] It is also a prescription for mapping the noninteracting Green function to the dressed one, $G^0 \to G$. In the quasiparticle self-consistent GW (QSGW) method, a prescription is given on how to map G to a new noninteracting Green function $G \to G^0$. This is used for the input to the next iteration; we repeat the procedure $G^0 \to G \to G^0 \to \ldots$ until convergence is reached. Thus QSGW is a self-consistent perturbation theory where the self-consistency condition is constructed to minimize the size of the perturbation. QSGW is parameter-free, independent of basis set, and of the local density approximation (LDA).[24] The method is described in great detail in Refs. 24 and 25. It has been shown that QSGW reliably describes the band structure in a wide range of materials.[17,26–28]

The QSGW method in the current implementation uses the full potential linear muffin tin orbital (FP-LMTO) method[29,30] so we make no approximations for the shape of the crystal potential. The smoothed LMTO basis includes orbitals with $l \leq l_{\max}=5$, and both $3d$ and $4d$ are included in the basis. $4d$ are added in the form of local orbitals[25]—an orbital strictly confined to the augmentation sphere, which has no envelope function at all. As QSGW gives the self-consistent solution at the scalar relativistic level, we add the spin-orbit operator, H_{SO}, as a perturbation (it is not included in the self-consistency cycle).

It has also been shown that the QSGW method systematically overestimates the fundamental band gap in semiconductors by an amount of a few tenths of an electron volt, independent of the magnitude of the gap.[26] This error is related to the fact that the vertex correction is not taken into account in the method and, when taken into account, a nearly perfect agreement with experiment is achieved.[31] Here, in order to obtain highly accurate results with less computational effort, we take a simple but somewhat heuristic approach to correct the error. We considered a "hybridized" QSGW+LDA Hamiltonian with

$$H_\alpha + H_{\mathrm{SO}} = H_{\mathrm{LDA}} + (1-\alpha)(\tilde{\Sigma} - V_{\mathrm{xc}}^{\mathrm{LDA}}) + H_{\mathrm{SO}}. \tag{3}$$

In Ref. 17 we found that, for all III-V and II-VI semiconductors studied, a value of $\alpha \approx 0.2$ gives excellent agreement of calculated band gap and other important band parameters with experiment.

All band parameters presented in Table I, except C and B, are calculated for the undistorted lattice structure. All signs are presented with the convention that the anion is at the origin and cation at (0.25,0.25,0.25). We see that overall the QSGW is in good agreement with experiment but the hybridized QSGW+LDA Hamiltonian is in even better agreement. For C and B we calculate self-consistently the self-energy and charge density under the corresponding deformation. We found that if instead we use the self-consistent self-energy of the undistorted structure, the value of C differs from that presented in Table I by $\approx 5\%$. In these calculations the atomic positions were allowed to relax within LDA in order to account for the displacement of the anion and cation sublattices relative to each other. For a pure shear deformation in the [111] direction, this displacement can be viewed as a length change Δl of the [111] bond described by the internal strain parameter ζ, $\Delta l = 3(1-\zeta)\epsilon/\sqrt{4}$. Our calculated value of ζ is 0.53, in good agreement with previous calculations[33,34]

TABLE I. Important band parameters for GaAs. $E_0=E(\Gamma_6^c)-E(\Gamma_8^v)$ and $E_0'=E(\Gamma_7^c)-E(\Gamma_8^v)$ are the energies of the first two conduction bands at the Γ point. Δ_{SO} and Δ_{SO}' are the spin-orbit splittings between Γ_8 and Γ_7 for valence and conduction bands, respectively. m_c^Γ/m is the conduction-band effective mass at Γ. Energies are in electron volts, γ is in eV Å^3, and C and B are in eV Å. An asterisk in front of the value indicates that this is a calculated value from another theoretical method.

	QSGW+LDA	QSGW	Expt
E_0	1.52	1.80	1.52[a]
$E_0'-E_0$	2.89	2.81	3.08[a]
Δ_{SO}	0.336		0.341[a]
Δ_{SO}'	0.174		
m_c^Γ/m	0.069	0.076	0.067[a]
γ	+8.5	+6.4	11.0–34.5[b]
C	+6.81	+5.39	3.9,[c] 4.0,[d] 5.3,[e] 8.1 ± 2.5,[f] *−3.74,[g] *−11.2,[h] *2.0,[i] *5.0,[j] *4.9[k]
B	+2.13	+1.7	

[a] From Ref. 32.
[b] From Ref. 15.
[c] From Table IX of Ref. 16, where only the absolute value is reported.
[d] From Ref. 14, where only the absolute value is reported.
[e] From Refs. 11 and 21, where only the absolute value is reported.
[f] From Ref. 20, where only the absolute value is reported.
[g] Calculated with pseudopotentials from Table IX of Ref. 16.
[h] Calculated with LCAO from Table IX of Ref. 16.
[i] Calculated with pseudopotentials from Ref. 14.
[j] Calculated with LCAO from Ref. 14.
[k] Calculated with the three-band $\mathbf{k}\cdot\mathbf{p}$ method from Ref. 11.

We apply two different deformations; the first of which is described by the following strain tensor:

$$\varepsilon = \begin{pmatrix} \epsilon_1 & \epsilon & 0 \\ \epsilon & \epsilon_1 & 0 \\ 0 & 0 & \epsilon_2 \end{pmatrix}, \tag{4}$$

where $\epsilon_1=0.0025186$, $\epsilon_2=-0.0049628$, and $\epsilon=0.0074814$. This tensor conserves the volume and induces the B related term in $\Omega_{\mathrm{stress}}^i$. To separate this term from the C related term, we also performed a calculation with a deformation described by the following strain tensor:

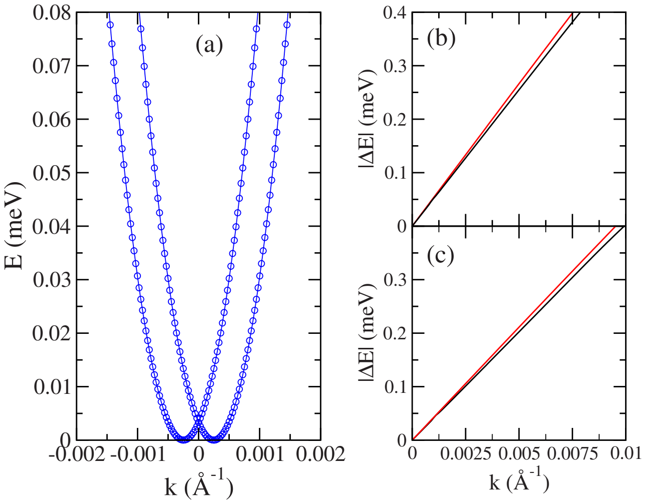

FIG. 1. (Color online) (a) The shift of the conduction-band minimum away from the Γ point in GaAs under deformation, given by Eq. (4) (hybridized method). (b) The magnitude of the conduction-band splitting along the [010] direction for the case of the hybridized Hamiltonian: red (gray) line with strain given by Eq. (4) and black line with strain given by Eq. (5). (c) is the same as (b) but for QS*GW* Hamiltonian.

$$\varepsilon = \begin{pmatrix} 0 & \epsilon & 0 \\ \epsilon & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}. \tag{5}$$

This strain tensor conserves the volume only to first order of deformation but only the first term (C related) is present in Ω^i_{stress}.

III. RESULTS

A. Spin splittings

In Fig. 1 we show the k dependence of the conduction-band splitting along [010] for the case of hybridized and QS*GW* calculations. Figure 1(a) shows the energy dispersion around the Γ point for the case of the hybridized Hamiltonian and the deformation given by Eq. (4). Along the [010] direction, Ω^i_D vanishes and the dispersion is given by

$$E_{\pm}(k) = \hbar^2 k^2/2m_{\text{eff}} \pm 1/2|A|k, \tag{6}$$

where

$$|A| = \sqrt{(C\epsilon)^2 + B^2(\epsilon_2 - \epsilon_1)^2}, \tag{7}$$

and the strain components were introduced in Sec. II. Correspondingly, the conduction-band minimum shifts to

$$k_{\pm} = \pm m_{\text{eff}}/2\hbar^2|A|. \tag{8}$$

In Figs. 1(b) and 1(c), we show the magnitude of the splitting along the [010] direction for the case of hybridized and QS*GW* Hamiltonians, respectively. The red (gray) lines are for strain given by Eq. (4) and black lines for strain given by Eq. (5). The slope of the red line is equal to

$$s_1 = \sqrt{(C\epsilon)^2 + B^2(\epsilon_2 - \epsilon_1)^2}, \tag{9}$$

while the slope of the black line is equal to

$$s_2 = |C||\epsilon|. \tag{10}$$

Hence

$$|C| = s_2/|\epsilon|, \tag{11}$$

and

$$|B| = \sqrt{s_1^2 - s_2^2}/|\epsilon_2 - \epsilon_1|. \tag{12}$$

The magnitudes of C and B, extracted with this procedure, are given in Table I. As it was pointed out in Ref. 35, this procedure is accurate only to the leading order of k and ε because it ignores the presence of quadratic terms that in principle are allowed by symmetry, and therefore can be present in the *ab initio* spin splitting but are absent in the Hamiltonian [Eq. (2)]. However, unlike the LDA calculations of Ref. 35, we did not detect any significant contribution to the spin splitting near the Γ point from those higher order terms. Considering the severe underestimation of GaAs band gap by LDA,[36] we suspect that such terms may be important for narrow gap semiconductors and/or higher strains, and will be investigated in future studies of such cases. As expected, in the case of the hybridized method, the magnitudes of C and B are slightly larger than in the QS*GW* because the hybridized band structure has a smaller band gap. However, the ratio of C/B remains nearly constant; it is equal to 3.197 in the hybridized method and 3.171 in QS*GW*. The magnitude of C is in good agreement with experiments in both the QS*GW* and the hybridized methods but the latter should be trusted more due to better agreement of the other band parameters with experimental values. We also note that in the experimental determination of C, the B terms were considered to be negligible. This corresponds to extracting the value of C directly from s_1; according to our calculations, this would yield an inaccurate value of C=7.14 eV Å with an error of 5%, much less than the experimental error in Ref. 20.

The Ω^i_D is highly anisotropic and completely vanishes in certain directions but is present for a general direction. It is therefore interesting to compare Ω^i_D with Ω^i_{stress}. We start by comparing C to γ. When we apply deformation [Eq. (5)], the dispersion along the [110] direction is

$$E(k) = \hbar^2 k^2/2m_{\text{eff}} \pm 1/4(\gamma k^3 + C\epsilon k). \tag{13}$$

Thus the Dresselhaus and the stress terms can either add or subtract, depending on the relative sign of $C\epsilon$ and γ. If they subtract the splitting will be zero at $k_{\text{rev}} = \sqrt{C/\gamma}\sqrt{\epsilon}$, i.e., the spin splitting reverses its sign at k_{rev}. In Table I it is seen that $\sqrt{C/\gamma}$=0.895 Å^{-1}, which means that, for the deformation [Eq. (5)], the spin splitting along [110] will change sign at k_{rev}=0.077 Å^{-1}. As shown in Fig. 2, ϵ can be either negative or positive; therefore such cancellation will always occur depending on the sign of the $C \cdot \epsilon \cdot k$ product. For example, if $k > 0$, whether it occurs for $\epsilon > 0$ or $\epsilon < 0$ depends on the sign of C. In Ref. 17 we determined the sign of γ according to conventions in Ref. 16. Here we will determine the sign of C relative to the sign of γ by simply plotting ΔE along [110]

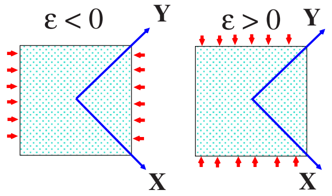

FIG. 2. (Color online) The left panel represents the applied deformation for $\epsilon < 0$ and the right panel for $\epsilon > 0$.

for positive and negative ϵ. In Fig. 3 we show such plot for the deformation [Eq. (5)] with positive and negative ϵ. The splitting is linear only in the vicinity of the Γ point; when away from the Γ point, the cubic term is clearly visible. For $\epsilon > 0$ the two contributions add [Fig. 3(a)] but for $\epsilon < 0$, they oppose each other [Fig. 3(b)]; for $k > 0.074$ Å^{-1}, the cubic term dominates and the splitting becomes positive. It is clear that C and γ have the *same sign* (according to the convention used here, they are both positive). The sign of B is defined in a similar way. We apply the deformation:

$$\epsilon = \begin{pmatrix} \epsilon_1 & 0 & 0 \\ 0 & \epsilon_1 & 0 \\ 0 & 0 & \epsilon_2 \end{pmatrix}, \qquad (14)$$

so that $\epsilon_2 = -2\epsilon_1$. Then the splitting along the [110] direction is $\Delta E \propto [\gamma k^3 + (\epsilon_1 - \epsilon_2) B k]$. If ΔE crosses zero for $(\epsilon_1 - \epsilon_2) > 0$ then B and γ have opposite signs, otherwise B and γ have the same sign. As can be seen in Fig. 4 we find that $B > 0$.

B. Spin relaxation

After having reliably determined the values of material parameters that dictate the spin-relaxation rate in GaAs, it will be interesting to estimate the spin-relaxation time for a deformation similar to the one given by Eq. (4). In the Appendix we have derived the average spin-relaxation time when both Ω_D and Ω_{stress} are present:

$$\frac{1}{\tau_{\perp,1}} = \gamma_l \left\{ \frac{1}{3}[(C\epsilon)^2 + (B\Delta\epsilon)^2]\frac{m^2}{\hbar^2}\langle v^2 \tau_p(E)\rangle + \frac{32}{105}\gamma^2 \frac{m^6}{\hbar^6}\langle v^6 \tau_p(E)\rangle \right\} + \frac{2}{3}\gamma_l B C \epsilon \Delta\epsilon \frac{m^2}{\hbar^2}\langle v^2 \tau_p(E)\rangle, \qquad (15)$$

$$\frac{1}{\tau_{\perp,2}} = \gamma_l \left\{ \frac{1}{3}[(C\epsilon)^2 + (B\Delta\epsilon)^2]\frac{m^2}{\hbar^2}\langle v^2 \tau_p(E)\rangle + \frac{32}{105}\gamma^2 \frac{m^6}{\hbar^6}\langle v^6 \tau_p(E)\rangle \right\} - \frac{2}{3}\gamma_l B C \epsilon \Delta\epsilon \frac{m^2}{\hbar^2}\langle v^2 \tau_p(E)\rangle, \qquad (16)$$

$$\frac{1}{\tau_{\parallel}} = \gamma_l \left\{ \frac{2}{3}[(C\epsilon)^2 + (B\Delta\epsilon)^2]\frac{m^2}{\hbar^2}\langle v^2 \tau_p(E)\rangle + \frac{32}{105}\gamma^2 \frac{m^6}{\hbar^6}\langle v^6 \tau_p(E)\rangle \right\}, \qquad (17)$$

where $\tau_p(E)$ is the momentum scattering time for an electron with energy E, v its velocity, ∥ denotes an axis parallel to the vector $\mathbf{N} = (0,0,1)$, and ⊥ perpendicular to it. Namely, $(\perp,1)$ and $(\perp,2)$ are the axes along the $[1\bar{1}0]$ and [110] crystal directions, respectively. We see that there is an in-plane anisotropy induced by the simultaneous presence of ϵ and $\Delta\epsilon = \epsilon_1 - \epsilon_2$ strain components (a similar anisotropy was observed for the circular piezobirefringence and confinement-induced circular birefringence in GaAs[37]). We can write the strain tensor [Eq. (14)] in these axes: $\epsilon = \epsilon_{i,j}\delta_{ij}$ with $\epsilon_{1,1} = \epsilon_{[110]} = \epsilon_1 + \epsilon$, $\epsilon_{2,2} = \epsilon_{[1\bar{1}0]} = \epsilon_1 - \epsilon$, and $\epsilon_{3,3} = \epsilon_{[001]} = \epsilon_2$. If we apply a uniaxial pressure (stress), p, along [110] in this system of coordinates, then using the compliance constants S_{11}, S_{12}, and S_{44}, we find $\epsilon_{[110]} = (S_{11} + S_{12} + S_{44}/2)p/2$, $\epsilon_{[1\bar{1}0]} = (S_{11} + S_{12} - S_{44}/2)p/2$, and $\epsilon_{[001]} = 2S_{12}p/2$, hence, $\Delta\epsilon = (S_{11} - S_{12})p/2$ and $\epsilon = (1/2)S_{44}p/2$. According to Eqs. (15) and (16), the difference between the inverse of the spin-relaxation time along $[1\bar{1}0]$ and [110] is equal to

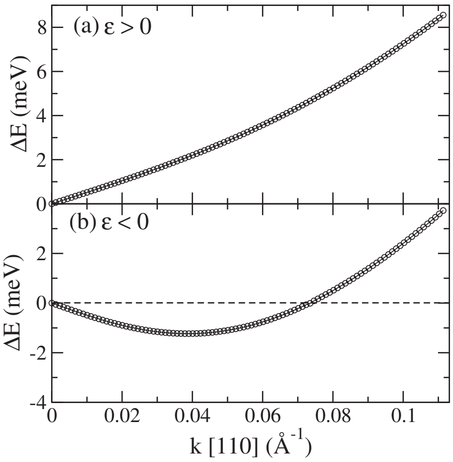

FIG. 3. (a) The conduction-band splitting along the [110] direction for the case of hybridized Hamiltonian, applied strain [Eq. (5)] for $\epsilon > 0$. (c) is the same as (a) but for $\epsilon < 0$.

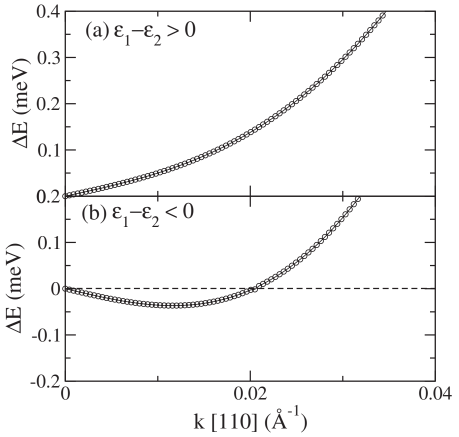

FIG. 4. (a) The conduction-band splitting along the [110] direction for the case of hybridized Hamiltonian, under deformation [Eq. (14)] with $(\epsilon_1 - \epsilon_2) > 0$. (b) is the same as (a) but for $(\epsilon_1 - \epsilon_2) < 0$.

$$\frac{1}{\tau_{\perp,1}} - \frac{1}{\tau_{\perp,2}} = \frac{BC}{6}\gamma_l \frac{m^2}{\hbar^2}\langle v^2 \tau_p(E)\rangle S_{44}(S_{11} - S_{12})p^2. \quad (18)$$

Hence, an experimental setup similar to the one described above should be able to measure a linear increase in the difference [Eq. (18)] with the square of applied pressure. The rate of increase should be proportional to BC. In the experiment of Ref. 10 the authors measured the increase in the spin-relaxation time with applied pressure along [100]. Such strain will only induce the B terms in Eqs. (15)–(17). If we assume that the applied strain is large enough to ignore the Dresselhaus term, then the spin-relaxation time should be isotropic and should increase linearly with the square of applied strain. However, unlike the experimental setup proposed here, the rate of increase is proportional to B^2. The experiment proposed here is independent of Dresselhaus terms no matter how small is the deformation, also the linear increase is proportional to CB instead of B^2 hence it may be easier to detect. Provided that the orientation of the As-Ga bond has been previously determined, this experiment can be used to find the sign of B relative to that of C from the sign of the difference [Eq. (18)].

IV. CONCLUSION

We have presented first-principles calculations of the magnitude and sign of bulk constants that govern the DP spin scattering in GaAs under strain. We find that both C and B have the same sign as γ. Our value of C is in good agreement with experiments. We have derived an expression for the spin-relaxation time of electrons under a strain given by Eq. (4) and showed that the in-plane spin relaxation is anisotropic in this case. We proposed an experiment that can exploit this anisotropy to deduce the magnitude and sign of B.

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APPENDIX: SPIN SCATTERING RATE

The momentum dependent spin-relaxation-time tensor is defined as

$$\frac{1}{\tau_{i,i}(k)} = \gamma_l \tau_p(E)(\overline{\Omega^2} - \overline{\Omega_i^2}), \quad (A1)$$

and

$$\frac{1}{\tau_{i,j}(k)} = \gamma_l \tau_p(E)(\overline{\Omega_i \Omega_j}) \quad (i \neq j). \quad (A2)$$

Here $i=x,y,z$ and the overbar denotes averaging over all directions of $\mathbf{k}$. $\tau_p(E)$ is the momentum scattering time for an electron with energy E and

$$\gamma_l = \frac{\displaystyle\int_{-1}^{+1} \sigma(\cos\theta)[1 - P_l(\cos\theta)]\, d\cos\theta}{\displaystyle\int_{-1}^{+1} \sigma(\cos\theta)(1 - \cos\theta)\, d\cos\theta}, \quad (A3)$$

where $\sigma(\cos\theta)$ is the electron-scattering cross section and P_l the Legendre polynomials. Here it is assumed that the electron scattering is elastic, the electron energy spectrum is isotropic, and the scattering cross section $\sigma(\mathbf{k},\mathbf{k}')$ depends only on the scattering angle θ. $\mathbf{\Omega}$ is the total effective field and in our case we can write

$$\mathbf{\Omega} = \mathbf{\Omega}_D + \mathbf{\Omega}_{\text{stress}} \quad (A4)$$

with the components, as given in Eqs. (1) and (2). We apply a strain similar to that of tensor Eq. (4) with the constraint $\epsilon_2 = -2\epsilon_1$ so as to conserve the volume. Then

$$\begin{cases} \Omega^x_{\text{stress}} = C\epsilon k_y + B\Delta\epsilon k_x, \\ \Omega^y_{\text{stress}} = -[C\epsilon k_x + B\Delta\epsilon k_y], \\ \Omega^z_{\text{stress}} = 0, \end{cases} \quad (A5)$$

where $\Delta\epsilon = (\epsilon_1 - \epsilon_2)$. To facilitate the discussion, let us write also explicitly the components of the Dresselhaus field:

$$\begin{cases} \Omega^x_D = 2\gamma k_x(k_y^2 - k_z^2), \\ \Omega^y_D = 2\gamma k_y(k_z^2 - k_x^2), \\ \Omega^z_D = 2\gamma k_z(k_x^2 - k_y^2). \end{cases} \quad (A6)$$

Then we can write

$$\overline{\Omega_x^2} = \overline{(\Omega^x_{\text{stress}})^2} + \overline{(\Omega^x_D)^2} + 2\overline{\Omega^x_{\text{stress}}\Omega^x_D}. \quad (A7)$$

The first integral on the right-hand side (RHS) is

$$\begin{aligned} \overline{(\Omega^x_{\text{stress}})^2} &= (C\epsilon)^2\overline{k_y^2} + (B\Delta\epsilon)^2\overline{k_x^2} + (2CB\epsilon\Delta\epsilon)\overline{k_x k_y} \\ &= \frac{1}{3}[(C\epsilon) + (B\Delta\epsilon)^2]k^2. \end{aligned} \quad (A8)$$

The second integral on the RHS is

$$\overline{(\Omega^x_D)^2} = 4\gamma^2\overline{k_x^2(k_y^2 - k_z^2)^2} = \gamma^2 k^6 \frac{16}{105}. \quad (A9)$$

The third integral on the RHS is

$$\overline{\Omega^x_{\text{stress}}\Omega^x_D} = (C\epsilon\gamma)\overline{k_x k_y(k_y^2 - k_z^2)} + (B\Delta\epsilon\gamma)\overline{k_x^2(k_y^2 - k_z^2)} = 0.$$

So we get

$$\overline{\Omega_x^2} = \frac{1}{3}[(C\epsilon)^2 + (B\Delta\epsilon)^2]k^2 + \gamma^2 k^6 \frac{16}{105}. \quad (A10)$$

In a similar way we obtain $\overline{\Omega_y^2} = \overline{\Omega_x^2}$ and

$$\overline{\Omega_z^2} = \gamma^2 k^6 \frac{16}{105}. \quad (A11)$$

For the off-diagonal components, we get

$$\overline{\Omega_x\Omega_y} = \overline{\Omega_y\Omega_x} = \overline{\Omega_D^x\Omega_D^y} + \overline{\Omega_D^x\Omega_{\text{stress}}^y} + \overline{\Omega_{\text{stress}}^x\Omega_D^y} + \overline{\Omega_{\text{stress}}^x\Omega_{\text{stress}}^y}. \tag{A12}$$

The first three integrals on the RHS are equal to zero. With the form of strain field given by Eq. (A5), the last term can be written as

$$\begin{aligned}\overline{\Omega_{\text{stress}}^x\Omega_{\text{stress}}^y} &= -(C\epsilon)^2\overline{k_yk_x} + (B\Delta\epsilon)^2\overline{k_xk_y} - CB\epsilon\Delta\epsilon\overline{(k_x^2+k_y^2)}\\ &= -\frac{2}{3}CB\epsilon\Delta\epsilon k^2.\end{aligned} \tag{A13}$$

All other $\overline{\Omega_i\Omega_j}$ are equal to zero. Therefore according to Eqs. (1) and (2) for the spin-relaxation time of an electron with energy E, we find

$$\begin{aligned}\frac{1}{\tau_{x,x}(k)} &= \frac{1}{\tau_{y,y}(k)}\\ &= \gamma_l\tau_p(E)\left\{\frac{1}{3}[(C\epsilon)^2+(B\Delta\epsilon)^2]k^2+\gamma^2k^6\frac{32}{105}\right\},\end{aligned} \tag{A14}$$

$$\frac{1}{\tau_{z,z}(k)} = \gamma_l\tau_p(E)\left\{\frac{2}{3}[(C\epsilon)^2+(B\Delta\epsilon)^2]k^2+\gamma^2k^6\frac{32}{105}\right\}, \tag{A15}$$

$$\frac{1}{\tau_{x,y}(k)} = \frac{1}{\tau_{y,x}(k)} = -\gamma_l\tau_p(E)\frac{2}{3}(BC\epsilon\Delta\epsilon)k^2. \tag{A16}$$

Then the average spin-relaxation time is

$$\begin{aligned}\frac{1}{\tau_{x,x}} = \frac{1}{\tau_{y,y}} = \gamma_l\Bigg\{&\frac{1}{3}[(C\epsilon)^2+(B\Delta\epsilon)^2]\frac{m^2}{\hbar^2}\langle v^2\tau_p(E)\rangle\\ &+\frac{32}{105}\gamma^2\frac{m^6}{\hbar^6}\langle v^6\tau_p(E)\rangle\Bigg\},\end{aligned} \tag{A17}$$

$$\begin{aligned}\frac{1}{\tau_{z,z}} = \gamma_l\Bigg\{&\frac{2}{3}[(C\epsilon)^2+(B\Delta\epsilon)^2]\frac{m^2}{\hbar^2}\langle v^2\tau_p(E)\rangle\\ &+\frac{32}{105}\gamma^2\frac{m^6}{\hbar^6}\langle v^6\tau_p(E)\rangle\Bigg\},\end{aligned} \tag{A18}$$

$$\frac{1}{\tau_{x,y}} = \frac{1}{\tau_{y,x}} = -\frac{2}{3}\gamma_lBC\epsilon\Delta\epsilon\frac{m^2}{\hbar^2}\langle v^2\tau_p(E)\rangle, \tag{A19}$$

where $v=\hbar k/m$ and the brackets $\langle\ \rangle$ denote averaging over energies. For example, for the Maxwell distribution, $\langle v^{2r}\tau_p(E)\rangle = (\frac{k_BT}{m})^r(2r+1)!!\tau_p$.

By transforming the above tensor to the principal system of coordinates, we obtain

$$\begin{aligned}\frac{1}{\tau_{\perp,1}} = \gamma_l\Bigg\{&\frac{1}{3}[(C\epsilon)^2+(B\Delta\epsilon)^2]\frac{m^2}{\hbar^2}\langle v^2\tau_p(E)\rangle\\ &+\frac{32}{105}\gamma^2\frac{m^6}{\hbar^6}\langle v^6\tau_p(E)\rangle\Bigg\}+\frac{2}{3}\gamma_lBC\epsilon\Delta\epsilon\frac{m^2}{\hbar^2}\langle v^2\tau_p(E)\rangle,\end{aligned} \tag{A20}$$

$$\begin{aligned}\frac{1}{\tau_{\perp,2}} = \gamma_l\Bigg\{&\frac{1}{3}[(C\epsilon)^2+(B\Delta\epsilon)^2]\frac{m^2}{\hbar^2}\langle v^2\tau_p(E)\rangle\\ &+\frac{32}{105}\gamma^2\frac{m^6}{\hbar^6}\langle v^6\tau_p(E)\rangle\Bigg\}-\frac{2}{3}\gamma_lBC\epsilon\Delta\epsilon\frac{m^2}{\hbar^2}\langle v^2\tau_p(E)\rangle,\end{aligned} \tag{A21}$$

$$\begin{aligned}\frac{1}{\tau_{\parallel}} = \gamma_l\Bigg\{&\frac{2}{3}[(C\epsilon)^2+(B\Delta\epsilon)^2]\frac{m^2}{\hbar^2}\langle v^2\tau_p(E)\rangle\\ &+\frac{32}{105}\gamma^2\frac{m^6}{\hbar^6}\langle v^6\tau_p(E)\rangle\Bigg\},\end{aligned} \tag{A22}$$

where $\parallel$ denotes axis parallel to the vector $\mathbf{N}=(0,0,1)$ and $\perp$ denotes axis perpendicular to it. Namely, $(\perp,1)$ and $(\perp,2)$ are the axes along the $[1\bar{1}0]$ and $[110]$ crystal directions, respectively. Equations (A20) and (A21) signal an in-plane anisotropy induced by the simultaneous presence of ϵ and $\Delta\epsilon$.

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