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Degree of polarization of luminescence from GaAs and InP as a function of strain: a theoretical investigation

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Abstract:

Experimentally it is known that the degree of polarization (DOP) of luminescence is a sensitive function of strain in III-V materials. It has been assumed that $DOP = -K_e (e_1 - e_2)$ and that the rotated degree of polarization (ROP) $= 2 K_e e_6$, where K_e is a positive calibration constant, e_1 and e_2 are the normal components of strain along perpendicular ‘1’ and ‘2’ directions, and $e_6 = e_{12}$ is the tensor shear strain. K_e has been measured experimentally for GaAs and InP.

In this paper, the results of a simple analytic determination of expressions for DOP as a function of strain are presented. Given the wide ranges reported for the strain deformation potentials b and d , it is not possible to give definitive and meaningful numerical values for expressions for DOP and K_e . However, the sensitivity of DOP to strain suggests that it might be possible to design simple experiments to provide accurate values for the deformation potentials.

The b and d deformation potentials might not be independent. For the results presented here and in the limit of isotropic material, an isotropic result for the DOP is found if $d = \sqrt{3} b$.

1. Introduction

1 The degree of polarization (DOP) of luminescence from III-V materials, such as GaAs and InP
2 and their alloys, is a sensitive function of strain [1–5]. DOP measurements [6–10] have been
3 applied to investigations of bonding strain [2, 4, 11–14], to understanding spectral properties
4 of lasers [15], to estimation of strain and photo-elastic effects owing to over-layers [16–18], to
5 identify dislocations [3, 5], to reliability investigations [19], to effects of strain on the operation
6 and yield of DFB lasers [20, 21], to growth related issues [22–25], and to characterize high power
7 lasers [10, 13, 19, 26].

8 Recently, Mokhtari *et al.* [27] used the DOP of photoluminescence technique to investigate the
9 occurrence of mechanical stress in vertical cavity surface emitting lasers (VCSELs), designed for
10 emission at 850 nm, in relation to the lateral oxidation process used to control current injection
11 and lateral optical confinement. Landesman *et al.* [28, 29] used the same technique to quantify
12 the anisotropic stress introduced in InP or GaAs substrates by the presence of thin and narrow
13 dielectric stripes on (100) surfaces. These stripes can play the role of hard masks for deep
14 reactive ion etching of InP or GaAs. Landesman *et al.* [29] demonstrated, using the DOP of
15 photoluminescence technique, that the reactive ion etching process itself can generate highly
16 anisotropic stress in the etched material, independent of the role of the hard mask layer.

17 Yan and Zhou [30] used DOP measurements to investigate bonding strain for p-up and p-
18 down superluminescent diode lasers. Fouchier *et al.* [31] extended the DOP technique to
19 cathodoluminescence (CL) measurements and demonstrated a strain sensitivity of 10^{-5} and spatial
20 resolution of the order of 100 nm on InP samples. Chen *et al.* [32] used DOP measurements in

21 their investigations of ZnO. Lin *et al.* [33] and Peloso *et al.* [34] applied polarization resolved
22 photoluminescence to the characterization of photovoltaic silicon wafers. Winterfeldt *et al.* [35]
23 used degree of polarization measurements to aid in the investigation of the factors limiting
24 the lateral beam parameter of 9xx nm high-power broad-area lasers. Hempel *et al.* [36] made
25 measurements on high-power lasers and provided a comparison of strain measurements by
26 photoluminescence, Raman, and DOP of electroluminescence. Matsui *et al.* [37] used results
27 from DOP measurements and finite elements simulations of strain in their investigations of
28 tuneable VCSELs. Pittroff *et al.* [38] used DOP measurements under the 200 μm wide stripe of
29 high-power III-V lasers to estimate the strain caused by different bonding approaches and found
30 no influence of mounting stresses on degradation for an optimized soldering process.

31 The DOP of photoluminescence (PL) is a local probe technique [39], much like photocurrent
32 spectroscopy [40] and cathodoluminescence [29, 31] are local probe techniques. However, DOP
33 measurements use the integrated luminescence [7]. This makes DOP measurements potentially
34 faster, simpler, and more sensitive than other local probe techniques that require spectral resolution
35 of the luminescence.

36 Strain estimation by analysis of the DOP of luminescence can be applied to both bulk and
37 nano-structures [41, 42]. Emission from nano-structures such as quantum wells (QWs) is
38 inherently polarized. Strain adds to the DOP of QWs [41]. The DOP for PL from the normal
39 to the plane of InGaAs QWs was found to be set by strained bonds across the interfaces of the
40 QWs [42]. Virtual force field (VFF) simulations revealed that the DOP of the PL was sensitive to
41 the assumed bond strengths for the binaries existing in the monolayers at the interfaces [43].

42 The spatial resolution for DOP measurements derived from PL is essentially diffraction limited.
43 Spatial resolution can be improved by using an electron beam to create luminescence, i.e.,
44 cathodoluminescence [29, 31]. The noise level for DOP measurements is typically 0.1%, which
45 translates roughly to a strain-equivalent noise level of $\approx 10^{-5}$ [4, 7]. The translation from DOP to
46 strain depends on an assumed functional dependence of DOP on strain and a calibration constant.
47 It was assumed that the DOP is proportional to the difference of two normal components of
48 stress or of strain, and the calibration constant K_e was experimentally determined [2, 3, 7]. It
49 was demonstrated that the difference of normal components of strain fit finite element method
50 (FEM) simulations of an experiment better than the difference of two normal components of
51 stress, and the calibration constant for InP was obtained from fits of these simulations to data [7].
52 The limiting noise source for DOP measurements using a rotating polarizer and a mechanical
53 chopper was investigated [44] and was found to a multiplicative noise from a beat frequency
54 between the polarizer and chopper frequencies.

55 In this paper the functional dependence of DOP on strain for III-V materials is investigated by
56 estimating the band-to-band transition rates for two orthogonal polarizations by using expressions
57 for the strain-dependant energy dispersion of the bands. The bands are assumed to be parabolic.
58 Boltzmann statistics and selection rules are used to find the DOP of luminescence. This leads to
59 an expression for the DOP as a function of strain and the calibration constant K_e is obtained from
60 this expression.

61 T. B. Bahder gave the matrix elements for an $8 \times 8 \mathbf{k} \cdot \mathbf{p}$ Hamiltonian for a uniformly strained
62 zinc-blende crystal [45, June 1990], with corrections to the results for the spin-orbit terms
63 published in October 1992 [46]. In January 1992 Bahder published approximate, analytic
64 dispersion relations for strained zinc-blende crystals [47]. These expressions are based on
65 perturbative expansions of the $8 \times 8 \mathbf{k} \cdot \mathbf{p}$ Hamiltonian, which reduced the dimensionality and
66 thus made it easier to find the eigenvalues. Generally the perturbative expansions are correct to
67 linear in strain and fourth-order in wave vector [47, RHS, pg 1630]. In addition, the eigenvalue
68 problem was linearized by using the average value of the diagonal elements for the energy in the
69 denominator of the Löwdin perturbation [47, LHS, pg 1640]. The $8 \times 8 \mathbf{k} \cdot \mathbf{p}$ Hamiltonian includes
70 strain-induced valence- and conduction-band mixing and is based on the usual second-order

71 Löwdin perturbation theory. The Luttinger four-band model with strain is recovered from
 72 Bahder's eight band model [45] if the asymmetry parameter B is set to zero and the band gap and
 73 spin-orbit splitting are taken to be large [45, Sec. III].

74 Bahder compared his approximate, analytic results to numerical computations of eigenvalues
 75 for the $8 \times 8 \mathbf{k} \cdot \mathbf{p}$ Hamiltonian and found them to be accurate for small $|\mathbf{k}|$, with small $|\mathbf{k}|$ being
 76 $< 0.33 \text{ nm}^{-1}$ [47]. Bahder notes in Ref. 17 of [47] that the original Hamiltonian neglects terms
 77 that are linear in \mathbf{k} , which might be important, and accuracy might be compromised for small \mathbf{k} .

78 Bahder used scaled parameters; see [47, Ref. 20]. The same scaling is employed here and
 79 thus k should be replaced with $k \times \sqrt{\hbar^2/(m_o q)}$, A_p^2 should be replaced with $A_p^2 \times m_o q/\hbar^2$,
 80 and P_o^2 should be replaced with $P_o^2 \times m_o q/\hbar^2$, where q is used to convert to eV. Physical and
 81 material constants and their symbols are defined in Appendix A.

82 Of interest to this work is that Bahder [45–47] did not specialize to biaxial strain, as would be
 83 found in strained layer epitaxy. The Hamiltonians that Bahder worked with have shear strain
 84 terms and thus analytic expressions contain shear strain terms.

85 2. Approach

86 We use Bahder's analytic expressions for the energy dispersion [47] and the $\mathbf{k} = 0$ eigenfunctions
 87 to calculate the strain-dependent spontaneous emission for two orthogonal polarizations. Using
 88 the $\mathbf{k} = 0$ eigenfunctions is an approximation to minimize the quantity of algebra that is required
 89 to find the calibration constant. It remains for corroboration to see if the approach is accurate.

90 The eigenfunctions are taken to be in a reference frame for \mathbf{k} along a z' direction. The original
 91 eigenfunctions must be rotated from the crystal coordinate system, which has x along [100], y
 92 along [010], z along [001], and \mathbf{k} along the z direction, to be in the \mathbf{k} -along- z' coordinate system.

93 Enders [48] notes that the Hamiltonian is at its simplest form when \mathbf{k} is along the z direction
 94 as some non-diagonal terms in the Hamiltonian are functions of k_x and k_y , and k_x and k_y
 95 are zero for \mathbf{k} along z . Any \mathbf{k} along an arbitrary direction z' is related to the components in the
 96 original z coordinate system by Euler rotations (see Appendix E). Enders also notes that a block
 97 diagonalisation of a Hamiltonian with \mathbf{k} can be perturbed by the rotation of the coordinate system.
 98 Enders proposed selective neglect of small terms that perturb the block diagonalisation. One can
 99 avoid the problem of block diagonalisation by using Bahder's analytic approximations [47].

100 To minimize subscripts we write tensors in a Voigt notation. The strain tensor $[e]$ is then, in
 101 this notation,

$$[e] = \begin{bmatrix} e_1 & e_6 & e_5 \\ e_6 & e_2 & e_4 \\ e_5 & e_4 & e_3 \end{bmatrix} = \begin{bmatrix} e_{xx} & e_{xy} & e_{xz} \\ e_{xy} & e_{yy} & e_{yz} \\ e_{xz} & e_{yz} & e_{zz} \end{bmatrix}, \quad (1)$$

102 with trace given by $\text{tr}([e]) = e_1 + e_2 + e_3$.

103 Ostromek [49] used Bahder's [45, 46] $8 \times 8 \mathbf{k} \cdot \mathbf{p}$ Kane Hamiltonian, which takes into account
 104 both the inversion asymmetry B and the \mathbf{k} -dependent spin-orbit interaction, to find through
 105 optimization a consistent set of band parameters for GaAs. Ostromek found the set of band
 106 parameters to be weakly dependent on the value of A_p , which couples the conduction band
 107 to higher lying bands. It was suggested $A_p = -14.7 \text{ eV \AA}^2$ with $E_p = 29.112 \text{ eV}$ or $A_p = 0$
 108 with $E_p = 22.827 \text{ eV}$. $B \neq 0$ as conduction band spin-splitting is observed, but Ostromek found
 109 inconsistent values for Kane non-parabolicity parameters with $B \neq 0$ [49, pg 14475]. We set
 110 $B = 0$ and ignore any spin-dependent splitting of the conduction band.

111 Photoluminescence occurs near the band edge where $|\mathbf{k}|$ is small. We thus restrict interest to
 112 small $|\mathbf{k}|$.

113 **2.1. Density of States**

114 Rather than calculating all possible transitions, we use an effective density of states that is a
 115 function of the effective masses. If a value for $|\mathbf{k}|$ is required, we use a value of $k = |\mathbf{k}|$ for which
 116 the spontaneous emission (i.e., luminescence) is a maximum.

117 We use Boltzmann statistics $\exp(-E/k_B T)$ and a parabolic band with a density of states
 118 $\rho(E) \propto \sqrt{E}$. The maximum value of $\sqrt{E} \exp(-E/k_B T)$ occurs at $E = k_B T/2$. The maximum
 119 value of $k \exp(-k^2/k_B T)$ occurs at $k = \pm \sqrt{k_B T/2}$. At 298 K, $k_B T = 25.7$ meV.

120 For a parabolic band, an effective density of states N_e can be defined such that the carrier
 121 density n is given by

$$n = N_e \exp((E_F - E_o)/k_B T) = 2 \left(\frac{m_e k_B T}{2 \pi \hbar^2} \right)^{3/2} \times \exp((E_F - E_o)/k_B T) \quad (2)$$

122 with E_F a quasi-Fermi energy and E_o the band edge energy. This effective density of states is
 123 proportional to $m_e^{3/2}$ with m_e an effective mass. The concept of an effective density of states can
 124 be extended to non-parabolic bands [50].

125 **3. Degree of Polarization (DOP)**

126 In the context of strain investigations, the degree of polarization (DOP) was defined to be [1, 7]

$$DOP_{\hat{\mathbf{h}} \times \hat{\mathbf{v}}} = \frac{L_{\hat{\mathbf{h}}} - L_{\hat{\mathbf{v}}}}{L_{\hat{\mathbf{h}}} + L_{\hat{\mathbf{v}}}} \quad (3)$$

127 where $\hat{\mathbf{h}}$ and $\hat{\mathbf{v}}$ are two orthogonal unit vectors in the plane of the surface that is being measured,
 128 $L_{\hat{\mathbf{q}}}$ is the measured irradiance for light polarized along a direction given by the unit vector $\hat{\mathbf{q}}$,
 129 $\hat{\mathbf{q}} = \hat{\mathbf{h}}$ or $\hat{\mathbf{v}}$, and the normal to the surface under study is given by the vector cross product $\hat{\mathbf{h}} \times \hat{\mathbf{v}}$.
 130 Usually the directions $\hat{\mathbf{h}}$ or $\hat{\mathbf{v}}$ are chosen to correspond to a feature of interest of the sample, such
 131 as $\hat{\mathbf{h}}$ parallel to the layers for a measurement from a cleaved facet of a laser, or $\hat{\mathbf{v}}$ parallel to a
 132 stripe for measurements from a (001) surface.

133 We also defined an ROP or rotated degree of polarization to be [3, 7]

$$ROP_{\hat{\mathbf{h}}' \times \hat{\mathbf{v}}'} = \frac{L_{\hat{\mathbf{h}}'} - L_{\hat{\mathbf{v}}'}}{L_{\hat{\mathbf{h}}'} + L_{\hat{\mathbf{v}}'}} \quad (4)$$

134 where the directions $\hat{\mathbf{h}}'$ and $\hat{\mathbf{v}}'$ are obtained by a -45 deg rotation about the normal to the surface,
 135 $\hat{\mathbf{h}} \times \hat{\mathbf{v}}$. Experimentally we determined that the DOP is proportional to the difference of the normal
 136 components of strain, $e_{hh} - e_{vv}$, and ROP is proportional to twice the tensor shear strain $2 e_{hv}$.

137 Given the definition of DOP as the ratio of the difference to sum, common factors cancel out
 138 and one need only retain relative terms. Thus to find an expression for $DOP_{\hat{\mathbf{h}} \times \hat{\mathbf{v}}}$ one should need
 139 only the strain-dependent shifts in energy of the light-hole (LH) and heavy-hole (HH) bands,
 140 the effective masses, and the wave functions for the bands. The wave functions are needed to
 141 calculate the polarization resolved photoluminescence.

142 **3.1. Calibration Constant K_e**

143 The calibration constant K_e is estimated by calculating values for the photoluminescences $L_{\hat{\mathbf{h}}}$ and
 144 $L_{\hat{\mathbf{v}}}$. To simplify calculation of K_e , the photoluminescence is assumed to originate from the band
 145 edges. Thus $k^4 \ll k^2$ and the bands can be assumed to be parabolic. The strain dependent shifts
 146 of the light-hole and heavy-hole bands are calculated using Bahder's analytic approximations [47].
 147 An effective density of states and Boltzmann statistics are used to obtain the relative contributions
 148 to the photoluminescences. The carriers, which have crystal momentum \mathbf{k} , are assumed to be

149 evenly divided amongst the two orthogonal directions $\hat{\mathbf{h}}$ and $\hat{\mathbf{v}}$. It is not necessary to attempt to
 150 calculate luminescences for carriers with \mathbf{k} along $\hat{\mathbf{h}} \times \hat{\mathbf{v}}$ as this is the direction of observation and
 151 electromagnetic radiation is a transverse wave – see Appendix C. Momentum matrix elements
 152 with \mathbf{p} along the direction of polarization are used to calculate the relative rates of emission of the
 153 polarized luminescences. It is assumed that the values calculated along two directions (\mathbf{k} along
 154 $\hat{\mathbf{h}}$ and $\hat{\mathbf{v}}$) are sufficient to describe accurately $L_{\hat{\mathbf{h}}}$ and $L_{\hat{\mathbf{v}}}$ (i.e., no integration over contributions
 155 from different directions, as in many cases the integrals are elliptic integrals). For calculations
 156 the z -direction is aligned with the crystal momentum of the carriers involved in the calculation
 157 and rotation of the coordinate system is used as necessary to obtain results in the observer's
 158 frame of reference.

159 Using a 2×2 L-K Hamiltonian with biaxial strain, the band edge (i.e., $\mathbf{k} = 0$) splitting of the
 160 light-hole and heavy-hole bands is given by $\Delta = 2 Q_e = \pm b (\text{tr}([e]) - 3 e_3)$:

$$H = \begin{bmatrix} -P + a \text{tr}([e]) - Q - Q_e & R + iS \\ R^* - iS^* & -P + a \text{tr}([e]) + Q + Q_e \end{bmatrix}, \quad (5)$$

161 since at the band edge and for biaxial strain (i.e., $e_1 = e_2$ and the shears strain $e_4, e_5, e_6 = 0$),
 162 $P = Q = R = S = 0$.

163 The standard L-K Hamiltonian with strain tends to be specialized to biaxial strain, as would be
 164 found in strained layer epitaxy [51, Eq. 4]. If the strain is not biaxial, then R and S are not zero
 165 at the band edge, and have real and imaginary components.

166 For arbitrary strain, the results obtained with a 2×2 L-K Hamiltonian and by Bahder [47] do
 167 not seem to be consistent.

168 Bahder states that his results reproduce, in the limit of no coupling to the conduction band or
 169 spin-orbit band, the results of Pikus and Bir [47, pg 1633]. Pikus and Bir used a Luttinger model
 170 that did not include mixing of the conduction and spin-orbit bands with the valence bands. We
 171 will work with the analytic approximations derived by Bahder [47].

172 3.2. Conduction Band Dispersion

173 Bahder's [47] expression for the conduction band dispersion E_c , neglecting strain and keeping
 174 only terms of order k^2 , is given below. The effects of the strain on the conduction band are not
 175 critical in calculation of the DOP, as the effects of these shifts are common to all transitions
 176 and thus cancel out in the determination of the DOP, Eq. (3). In the expression for E_c , A_p
 177 accounts for mixing with higher order bands [47]. Ostromeck [49] found for GaAs that $A_p = 0$
 178 and $E_p = 22.8$ or $A_p = -14.7$ and $E_p = 29.1$. Vurgaftman *et al.* [52] recommend $E_p = 28.8$ eV,
 179 which would suggest $A_p = -14.7 \text{ \AA}^2$.

$$\begin{aligned} E_c &= E_g + \left(k_x^2 + k_y^2 + k_z^2 \right) \left(\frac{1}{2} + A_p \frac{(10^{-10})^2 m_o q}{\hbar^2} + \frac{P_o^2 (E_g + 2/3 \Delta)}{E_g (E_g + \Delta)} \right) \\ &= 1.5177 + \left(k_x^2 + k_y^2 + k_z^2 \right) (0.5 - 1.916 + 8.9078). \end{aligned} \quad (6)$$

180 The recommended value for the GaAs conduction band effective mass at $T = 0$, in units of m_o , is
 181 $m_c = 0.067$ [52]. With $A_p = 0$ and $E_p = 22.8$, the expression above for E_c yields $m_c = 0.0662$,
 182 and with $A_p = -14.7$ and $E_p = 28.8$, the expression gives $m_c = 0.0669$. Given the results
 183 obtained, for GaAs we use $A_p = -14.6$ and $E_p = 28.8$ eV.

184 **3.3. Valence Band Dispersions**

185 Bahder's equation for the valence band energy as a function of $\mathbf{k} = (k_x, k_y, k_z)$ and strain
186 $[e]$ [47, Eq 9] is

$$E_v = E_v^{(0)} + E_v^{(1)} \pm \sqrt{E_k + E_{ks} + E_s} \quad (7)$$

187 with

$$E_v^{(0)} = -\left(k_x^2 + k_y^2 + k_z^2\right) \left(\frac{P_o^2}{3E_g} + \frac{\gamma_{1m}}{2}\right) + O(k^4) \quad (8)$$

188 and

$$\begin{aligned} E_v^{(1)} = & -a_v \text{tr}([e]) + \left(e_1 k_x^2 + e_2 k_y^2 + e_3 k_z^2\right) \left(\frac{P_o^2}{3E_g} \left(2 + \frac{a_p}{E_g}\right) - 2 \frac{b \gamma_{2m}}{\Delta_{so}}\right) \\ & + \left(k_x^2 (e_2 + e_3) + k_y^2 (e_1 + e_3) + k_z^2 (e_1 + e_2)\right) \left(\frac{a_p P_o^2}{3E_g^2} + \frac{b \gamma_{2m}}{\Delta_{so}}\right) \\ & + \left(e_4 k_y k_z + e_5 k_x k_z + e_6 k_x k_y\right) \left(\frac{4 P_o^2}{3E_g} - 2 \frac{\sqrt{3} d \gamma_{3m}}{\Delta_{so}}\right) \end{aligned} \quad (9)$$

189 and

$$\begin{aligned} E_k = & \left(k_x^2 + k_y^2 + k_z^2\right)^2 \left(\gamma_{2m} + \frac{P_o^2}{3E_g}\right)^2 \\ & + \left(k_x^2 k_y^2 + k_x^2 k_z^2 + k_y^2 k_z^2\right) (\gamma_{3m} - \gamma_{2m}) \left(3 \gamma_{3m} + 3 \gamma_{2m} + 2 \frac{P_o^2}{E_g}\right). \end{aligned} \quad (10)$$

190 Both $E_v^{(0)}$ and $E_v^{(1)}$ shift both the light-hole and the heavy-hole band, and do not contribute to
191 valence band splitting and to DOP. E_k is strain independent and contributes to the \mathbf{k} -dependant
192 splitting between the light and heavy holes, i.e, to the different effective masses of the valence
193 bands.

194 Bahder's E_{ks} has a form [47, Eq. 13] that selects strain along a given \mathbf{k} , which leads to DOP:

$$\begin{aligned} E_{ks} = & b \left(\gamma_{2m} + \frac{P_o^2}{3E_g}\right) \left(\left(k_x^2 + k_y^2 + k_z^2\right) \times \text{tr}([e]) - 3 k_x^2 e_1 - 3 k_y^2 e_2 - 3 k_z^2 e_3\right) \\ & - 2 \sqrt{3} d \left(\gamma_{3m} + \frac{P_o^2}{3E_g}\right) (e_4 k_y k_z + e_5 k_x k_z + e_6 k_x k_y), \end{aligned} \quad (11)$$

195 where b and d are valence band deformation potentials. Both b and d have wide ranges of
196 reported values and thus uncertainty [52].

197 From Bahder [47, Eq. 14], E_s is \mathbf{k} -independent and $\pm \sqrt{E_s}$ is the contribution to a valence
198 band-edge energy, i.e., $E_v(\mathbf{k} = 0) = -a_v \text{tr}([e]) \pm \sqrt{E_s}$, with

$$E_s = \frac{b^2}{2} \left((e_1 - e_2)^2 + (e_1 - e_3)^2 + (e_2 - e_3)^2\right) + d^2 \left(e_4^2 + e_5^2 + e_6^2\right), \quad (12)$$

199 E_s contributes to the splitting of the light and heavy hole bands, but is independent of \mathbf{k} and thus
200 does not contribute to DOP. In addition, E_s has a decreasing influence as \mathbf{k} increases from zero,
201 as can be deduced from Eq. (7) and Sec. 3.3.1.

202 3.3.1. Binomial Expansion

203 E_v , Eq. (7), has a square root dependence on $E_k + E_{k_s} + E_s$. Unless a binomial expansion can
 204 be made, the valence band energies are nonlinear in k^2 and thus difficult to work with.

205 In the absence of strain $E_{k_s} = E_s = 0$, and $\sqrt{E_k}$ gives the difference in masses for the light-hole
 206 band and the heavy-hole bands. Given the difference in masses of light and heavy holes and
 207 the relatively weak dependence of the light and heavy holes masses on strain, one might expect
 208 $E_k \gg (E_{k_s} + E_s)$ since E_{k_s} and E_s are strain dependent and E_k is strain independent.

209 Approximate E_v , Eq. (7), as a binomial series

$$E_v \approx E_v^{(0)} + E_v^{(1)} \pm \left(\sqrt{E_k} + \frac{E_{k_s} + E_s}{2\sqrt{E_k}} - O\left(\frac{(E_{k_s} + E_s)^2}{8E_k^{3/2}}\right) \right). \quad (13)$$

210 Specialize to $\mathbf{k} = (0, 0, k_z)$ to simplify the presentation and since determination of the
 211 calibration constant K_e requires calculation for light polarized parallel to \mathbf{k} ; E_s , Eq. (12), is
 212 independent of \mathbf{k} .

$$E_k(0, 0, k_z) = k_z^4 \left(\gamma_{2m} + \frac{P_o^2}{3E_g} \right)^2 \quad (14)$$

$$E_{k_s}(0, 0, k_z) = b \times k_z^2 \times \left(\gamma_{2m} + \frac{P_o^2}{3E_g} \right) (\text{tr}(e) - 3e_3) \quad (15)$$

213 Bahder's approximations kept only terms of order $k^2 e$ [47, pg 1633], thus one should be
 214 justified in ignoring the higher-order terms in the binomial expansion of the square root. The
 215 neglected term in Eq. (13) is, keeping only terms of lowest order in strain,

$$O\left(\frac{(E_{k_s} + E_s)^2}{8E_k^{3/2}}\right) \approx 0.22 \frac{(e_1 + e_2 - 2e_3)^2}{k_z^2}. \quad (16)$$

216 For sufficiently large k_z as compared to $e_1 + e_2 - 2e_3$, the binomial series approximation Eq.
 217 (13) converges to Eq. (7). For emission that is $k_B T/2$ above the band edge (for GaAs at room
 218 temperature, the band edge emission is at 871 nm, band edge + $k_B T/2 = 863$ nm, or 8 nm above
 219 the band edge), $k_z = 0.030 \sqrt{eV}$ for conduction band to light hole transitions and $k_z = 0.038 \sqrt{eV}$
 220 for conduction band to heavy hole transitions (for band edge + $k_B T$, $k_z > 0.043$).

221 The DOP is a sensitive function of strain. DOPs of $\pm 5\%$ are, for bulk material, extremely
 222 large and would be caused by strains of order 0.1%. Take $e_1 = 0.001$, $e_2 = 0.001$, $e_3 = -0.001$,
 223 and $k_z = 0.03$ to find in Eq. (16) that $O() < 6 \times 10^{-6}$. Thus one is justified in ignoring the higher
 224 order terms in the binomial expansion. Since E_s depends on the strain squared, this term can be
 225 neglected as compared to terms linear in strain, and the valence band energy for $\mathbf{k} = (0, 0, k_z)$
 226 can be written as

$$E_v(0, 0, k_z) \approx E_v^{(0)}(0, 0, k_z) + E_v^{(1)}(0, 0, k_z) \pm \left(k_z^2 \left(\gamma_{2m} + \frac{P_o^2}{3E_g} \right) - \frac{b}{2} (\text{tr}([e]) - 3e_{zz}) \right). \quad (17)$$

227 The splitting of light and heavy holes for $\mathbf{k} = (0, 0, k)$ relative to zero strain is then, to a good
 228 approximation,

$$\Delta = b (\text{tr}([e]) - 3e_3), \quad (18)$$

229 with one band shifted up by an amount $\Delta/2$ and the other band shifted down by $\Delta/2$. A
 230 direction-dependent strain shifting of the light hole energies as described by E_{k_s} , Eq. (11), leads
 231 to a DOP for strain.

232 A similar result to Eq. (17) can be obtained by completing the square in Eq. (13).

233 3.3.2. Free Surface

234 Since the surface that is under study in DOP measurements is typically a free surface, this
 235 imposes some constraints on the stresses and strains. Stress is force per unit area. $\sigma_{ij}dS$ is the
 236 component of force in the x_i direction that is transmitted across a surface element of area dS
 237 that is normal to x_j [53]. Thus if the ‘2’ direction is a normal to the free surface, then $\sigma_{22} = 0$,
 238 $\sigma_{12} = 0$ and $\sigma_{32} = 0$. Since stress and strain are symmetric second order tensors, $\sigma_{12} = \sigma_{21}$
 239 and $\sigma_{23} = \sigma_{32}$. For a cubic crystal, in Voigt notation, $\sigma_i = c_{44} e_i$, $i = 4, 5, 6$. Thus for a cubic
 240 crystal, if the shear stress is zero, the shear strain is zero. Since by assumption surface ‘2’ is a
 241 free surface, the normal component of stress $\sigma_2 = 0$ and two of the shear stresses equal zero:
 242 $\sigma_6 = \sigma_4 = 0$. The free surface constraints can be used to simplify the error term in the binomial
 243 expansion Eq. (13). In the crystal coordinate system and for a cubic crystal, $c_{11} = c_{22} = c_{33}$,
 244 $c_{44} = c_{55} = c_{66}$ and $c_{12} = c_{13} = c_{23}$.

245 3.4. Polarized Emissions: $L_{\hat{h}}$ and $L_{\hat{p}}$

246 3.4.1. $DOP_{[100] \times [001]}$

247 Consider \hat{h} along [100], \hat{p} along [001] and $\hat{h} \times \hat{p}$ along $[0\bar{1}0]$, and take x along [100], y along
 248 $[010]$, and z along [001]. In this section, note that \hat{h} and \hat{p} are definite directions.

249 Assume that the strain is biaxial, or sufficiently small that the expression Δ , Eq. (18), for the
 250 energy shifts with strain of the valence bands are accurate.

251 Take $\mathbf{k} = (0, 0, k)$. This gives energy shifts of $\pm b (\text{tr}([e]) - 3 e_3)/2$ for the light and heavy
 252 holes, relative to zero strain. For $\mathbf{k} = (k, 0, 0)$ the energy shifts are $\pm b (\text{tr}([e]) - 3 e_1)/2$. Note
 253 that selection of a direction for \mathbf{k} selects different energy shifts, with the direction of strain
 254 along the direction of \mathbf{k} : one shift depends on e_3 whereas the other energy shift depends on e_1 .
 255 Selection of the polarization for an electromagnetic wave selects the direction for \mathbf{p} and hence \mathbf{k} .

Given the energy shifts Δ , Eq. (18), the density of states (assuming a parabolic band
 approximation for small \mathbf{k} is appropriate) times the probability of occupation is, to within
 common factors which will cancel in calculation of the DOP, given by

$$P_{HH} = m_{HH}^{3/2} \exp\left(\frac{+b (\text{tr}([e]) - 3 e_3)}{2 k_B T}\right) \quad (19)$$

$$P_{LH} = m_{LH}^{3/2} \exp\left(\frac{-b (\text{tr}([e]) - 3 e_3)}{2 k_B T}\right). \quad (20)$$

The irradiance for light polarized in the z direction and produced by carriers with crystal
 momentum $\mathbf{k} = (0, 0, k)$ is

$$L_{\hat{p}}(0, 0, k) = |\langle CB | p_z | HH_1 \rangle|^2 P_{HH} + |\langle CB | p_z | LH_1 \rangle|^2 P_{LH} \\ + |\langle CB | p_z | HH_2 \rangle|^2 P_{HH} + |\langle CB | p_z | LH_2 \rangle|^2 P_{LH} \quad (21)$$

256 where $\langle CB |$ is the Bloch factor (basis function) for one of the conduction bands. See Appendices
 257 B and C. Equation (21) assumes incoherent interaction for luminescence from the conduction
 258 band to the the light-hole and heavy-hole bands. Given the broad emission from the band-to-band
 259 transitions, this is a reasonable depiction of the interaction for the luminescences from the bands.

260 After applying the selection rules (see Appendix B) and substituting for P_{HH} and P_{LH}

$$L_{\hat{p}}(0, 0, k) = \frac{2 |M|^2}{3} m_{LH}^{3/2} \exp\left(\frac{b (\text{tr}([e]) - 3 e_3)}{2 k_B T}\right). \quad (22)$$

261 A similar procedure gives an expression for the contributions to $L_{\hat{h}}$:

$$L_{\hat{h}}(k, 0, 0) = \frac{2 |M|^2}{3} m_{LH}^{3/2} \exp\left(\frac{b (\text{tr}([e]) - 3 e_1)}{2 k_B T}\right). \quad (23)$$

262 The total luminescence is the sum over values of \mathbf{k} , where \mathbf{k} gives the crystal momentum for
 263 the carriers involved in production of the luminescence . We use the luminescence calculated
 264 for \mathbf{k} along the two directions of the polarizer as a proxy for the total amount of light that is
 265 produced. Under this approximation, $L_{\hat{\mathbf{h}}} = L_{\hat{\mathbf{h}}}(k, 0, 0)$ and $L_{\hat{\mathbf{v}}} = L_{\hat{\mathbf{v}}}(0, 0, k)$.

Under the assumption that the strains are small (typically the magnitude of the strain is
 < 0.001), the exponential functions can be expanded in Taylor series, $\exp(x) = 1 + x + O(x^2/2)$,
 to obtain a simplified expression for the DOP:

$$DOP_{\hat{\mathbf{h}} \times \hat{\mathbf{v}}} = \frac{L_{\hat{\mathbf{h}}} - L_{\hat{\mathbf{v}}}}{L_{\hat{\mathbf{h}}} + L_{\hat{\mathbf{v}}}} \quad (24)$$

$$\approx \frac{3b}{4k_B T} (e_1 - e_3), \quad (25)$$

266 with the calibration constant K_e , $K_e > 0$, given by

$$K_e = \frac{-3b}{4k_B T} = \left| \frac{3b}{4k_B T} \right| \quad (26)$$

267 for $\hat{\mathbf{h}}$ along [100] and $\hat{\mathbf{v}}$ along [001].

268 Since $\exp(-b 3 e_3 / (2 k_B T)) = 1.122$ for $b = -2.0$ eV, $k_B T = 0.026$ eV, and $e_3 = 0.001$, and
 269 $1 + b 3 e_3 / (2 k_B T) = 1.115$, and since $\exp(b 3 e_3 / (2 k_B T)) = 0.8910$, and $1 - b 3 e_3 / (2 k_B T) =$
 270 0.8846 , differences $< 0.72\%$, clearly the expression for the calibration constant is accurate for
 271 strains $\lesssim 0.001$.

272 The magnitudes of process-induced strains in bulk devices and materials are typically < 0.001 ;
 273 thus the restriction to small strains to obtain the calibration constant K_e is not a significant
 274 problem. The approximate expressions for the energy dispersions given by Bahder [47] were
 275 obtained by keeping linear terms in the strain (or quadratic if the strain term was contained within
 276 a square root). Thus one would expect that expressions derived from Bahder's approximations
 277 should be accurate to no more than linear in strain.

278 Note that the deformation of the sample is, to a very good approximation, linear in the strain
 279 fields. One thus uses the principle of linear superposition to find the strain fields from multiple
 280 sources. The final strain field, which is the sum of all contributions from all sources, is used
 281 to find the DOP of the luminescence. If the final strain is sufficiently small, then the DOP is
 282 approximately linear in strain, and the principle of linear superposition holds for the DOP and a
 283 calibration constant can be defined. If the strain is not sufficiently small, then it appears that the
 284 DOP is not linear in the strain, and one cannot define a calibration constant. However, as a result
 285 of linearity in the deformation, small-in-amplitude features will lie on top of larger-in-amplitude
 286 features in the DOP and will not be masked by the larger features.

287 Figure 2 of [2] shows DOP linear over a range > 0.01 . From Table 2 of [7] and the related
 288 discussion, the points deviated from linear by no more than 0.6 in 26 when the calibrating force
 289 was doubled. For Fig. 3 of [7], a display gain of $10\times$ was used, which gives just off-scale signals
 290 of ± 2.90 percentage points relative to the green mid-point of the colour bar. The fit of DOP
 291 measurements to FEM simulations, as shown in Fig. 3(a) of [7], is remarkably good, which
 292 suggests that the DOP is linear over at least $\pm 3\%$. Assuming the calibration constant $K_e = 58$,
 293 then a DOP or ROP of 3% corresponds to a strain or strain difference of 5×10^{-4} ; a magnitude
 294 of strain which is within the region the small argument approximations, which were made in the
 295 derivation of Eq. (26), are accurate.

296 Typically we use a default display gain of $20\times$ to display false colour maps of the DOP and
 297 ROP. A display gain of $20\times$ gives just off-scale signals of ± 1.45 percentage points relative to the
 298 green mid-point of the colour bar. Experience has shown that DOPs for bulk material (i.e., not
 299 nanostructures) that are off-scale with the default display gains of $20\times$ indicate areas of concern.

300 For a calibration constant of 58, a DOP or ROP of 1.45% gives a difference of strain or a strain
 301 of $0.0145/58 = 2.5 \times 10^{-4}$.

302 The expression for the calibration constant K_e is based on the assumption that the energy
 303 splitting for the bands is given by Δ , Eq. (18). For small strains, the strain-squared terms can be
 304 ignored and Δ is accurate for small, but technologically interesting, arbitrary strain distributions.

305 Using the values listed in Appendix A, the calculated calibration constant $K_e = 58 \pm 30$ for
 306 GaAs and InP for \hat{h} along [100] and \hat{v} along [001]. Owing to the cubic symmetry of GaAs
 307 and InP, the calibration constant is the same for \hat{h} and \hat{v} equal to any of the equivalent crystal
 308 coordinate directions [100], [010], and [001].

309 Note that $DOP_{\hat{h} \times \hat{v}}$ can be written as $\Delta/(2 k_B T)$ where Δ is the light hole energy difference for
 310 \mathbf{k} along the two orthogonal directions \hat{h} and \hat{v} in the measurement plane.

311 3.4.2. \mathbf{k} not along z

312 The basis functions (Bloch factors) are defined for \mathbf{k} along z , with z along a $\langle 001 \rangle$ direction in the
 313 crystal coordinate system. The basis functions in other directions are obtained by rotation [48,54]
 314 of the $|S\rangle$, $|X\rangle$, $|Y\rangle$, $|Z\rangle$, $|\uparrow\rangle$, and $|\downarrow\rangle$ that are combined to form the conduction band, light hole,
 315 heavy hole, and spin orbit states. Momentum matrix elements such as $\boldsymbol{\varepsilon} \cdot \langle CB' | \mathbf{p} | \Psi' \rangle$ are
 316 required to calculate the relative amounts of light in a given polarization where $\langle CB' |$ represents
 317 the conduction band, $|\Psi' \rangle$ represents one of the valence band states for a given value of \mathbf{k} , and $\boldsymbol{\varepsilon}$
 318 is a unit vector that defines the polarization of the luminescence.

319 Let R_t and S_t be rotation operators for the spatial and spin components of a wave function.
 320 R_t and S_t commute since they operate on different Hilbert spaces, and S_t and \mathbf{p} commute since
 321 the momentum operator \mathbf{p} does not operate on spin. Both rotation operators are unitary. Thus
 322 $R_t R_t^\dagger = R_t^\dagger R_t = \mathbf{I}$ and $S_t S_t^\dagger = S_t^\dagger S_t = \mathbf{I}$ where \mathbf{I} is the identity operator.

323 The matrix elements are obtained by using rotated kets such as $|X'\rangle = R_t |X\rangle$ to form the
 324 the conduction band, light hole, and heavy hole states. Here R_t is a rotation matrix that aligns
 325 z with the direction of \mathbf{k} . These rotated states are used with the components of $\boldsymbol{\varepsilon} \cdot \mathbf{p}$ in the
 326 crystal coordinate system to calculate the matrix element M for the \hat{h} and \hat{v} polarized transitions.
 327 It appears that matrix elements using the rotated states and components of $\boldsymbol{\varepsilon} \cdot \mathbf{p}$ in the crystal
 328 coordinate system are equal to $\langle CB | p_z | \Psi \rangle$ with $\langle CB |$ and $|\Psi \rangle$ defined for \mathbf{k} along z and in
 329 the crystal coordinate system. This simplifies the calculations, particularly since Bahder [47]
 330 provided analytic expressions for the energy dispersions of the valence and conduction bands for
 331 arbitrary directions of \mathbf{k} .

332 Expressions for \hat{h} and \hat{v} not along a crystal coordinate axis are not as compact as for when \hat{h}
 333 and \hat{v} are along a direction of high symmetry. We take the limit as $E_g \rightarrow \infty$, which reduces
 334 Bahder's results from an 8×8 Hamiltonian to a 4×4 L-K Hamiltonian [45, Sec. 3] with
 335 an insignificant loss of accuracy for the estimation of the calibration constant, to reduce the
 336 complexity and space that the typeset equations would otherwise occupy. We found the limit has
 337 a $\approx 2\%$ effect on K_e . This loss of accuracy is insignificant as compared to the uncertainty in the
 338 material parameters, which are given in Appendix A.

339 3.4.3. $ROP_{\langle 001 \rangle}$

340 The DOP from a (001) surface (i.e., a $z = 0$ surface) for an alignment of the \hat{h} (horizontal)
 341 polarizer transmission axis at an angle of α with respect to the [100] or x -axis can be derived
 342 using the procedures described above. Consider two orthogonal directions (e.g., \hat{h} and \hat{v}) in the
 343 $z = 0$ plane. Let these two orthogonal directions be defined with respect to a counter-clockwise
 344 rotation about the z -axis, with the angle α measured with respect to the x -axis. The clockwise
 345 and counter-clockwise directions are defined for an observer looking at the origin from positive z .
 346 See Appendix D for more information.

347 Experimentally, the direction \hat{h}' for positive ROP (i.e., $L_{\hat{h}'} > L_{\hat{v}'}$) was chosen to be rotated by

348 -45 deg with respect to the direction $\hat{\mathbf{h}}$ for positive DOP, (i.e., $L_{\hat{\mathbf{h}}} > L_{\hat{\mathbf{v}}}$) [7, Fig. 1]. This choice
 349 leads to a calibration constant for ROP that has the opposite sign as for DOP.

350 General expressions for $DOP_{001}(\alpha)$ and $ROP_{001}(\alpha)$, in the limit of large E_g , are

$$DOP_{001}(\alpha) = \frac{2\sqrt{3}d \sin(2\alpha) \gamma_3 \epsilon_6 + 3b \cos(2\alpha) \gamma_2 (\epsilon_1 - \epsilon_2)}{2k_B T \sqrt{3 \sin^2(2\alpha) (-\gamma_2^2 + \gamma_3^2) + 4\gamma_2^2}} \quad (27)$$

351 and

$$ROP_{001}(\alpha) = \frac{-2\sqrt{3}d \gamma_3 \epsilon_6 \cos(2\alpha) + 3b \sin(2\alpha) \gamma_2 (\epsilon_1 - \epsilon_2)}{2k_B T \sqrt{3 \sin^2(2\alpha) (\gamma_2^2 - \gamma_3^2) + \gamma_2^2 + 3\gamma_3^2}} \quad (28)$$

with

$$\epsilon_1 = \cos^2(\alpha) e_1 + \sin^2(\alpha) e_2 - \sin(2\alpha) e_6 \quad (29)$$

$$\epsilon_2 = \cos^2(\alpha) e_2 + \sin^2(\alpha) e_1 + \sin(2\alpha) e_6 \quad (30)$$

$$\epsilon_3 = e_3 \quad (31)$$

$$\epsilon_6 = \cos(2\alpha) e_6 + \sin(2\alpha) \left(\frac{e_1 - e_2}{2} \right) \quad (32)$$

352 where the ϵ_i are the components of the strain tensor in the crystal coordinate system and the e_i are
 353 the components of the strain tensor in the DOP measurement coordinate system, which has been
 354 rotated by α about [001] (i.e., the z -axis). The horizontal direction $\hat{\mathbf{h}}$ is taken as the x' -axis in the
 355 rotated (or measurement) coordinate system. The vertical direction $\hat{\mathbf{v}}$ is along the axis of rotation,
 356 which is the [001] direction, i.e., the z -axis or z' -axis. The same angle α is used for both ROP
 357 and DOP; the -45 degree rotation from $\hat{\mathbf{h}}$ to $\hat{\mathbf{h}}'$ has been included in the equation for $ROP_{001}(\alpha)$.

358 A measurement for $\alpha = 0$ gives yields $DOP_{001}(0) = DOP_{[100] \times [010]}(0) = 3b(e_1 - e_2)/(4k_B T)$,
 359 which gives the calibration constant that was found previously, Eq. (26), for $\hat{\mathbf{h}}$ and $\hat{\mathbf{v}}$ along crystal
 360 coordinate axes.

361 For measurements from a (001) plane, with $\hat{\mathbf{h}}$ parallel to a cleaved $(1\bar{1}0)$ facet and $\hat{\mathbf{v}}$
 362 perpendicular to the cleaved facet, $\alpha = 45$ deg, giving

$$DOP_{001}(\alpha = \pi/4) = \frac{d \gamma_3 (e_1 - e_2) \sqrt{3}}{2k_B T \sqrt{\gamma_2^2 + 3\gamma_3^2}} = K_e (e_1 - e_2) \times \frac{d}{b} \times \frac{2\gamma_3}{\sqrt{3(\gamma_2^2 + 3\gamma_3^2)}} \quad (33)$$

363 and

$$ROP_{001}(\alpha = \pi/4) = -\frac{3b e_6}{2k_B T} = 2K_e e_6. \quad (34)$$

364 This $\alpha = 45$ deg example is the case for measurements of a $[1\bar{1}0]$ oriented oxide stripe on a (001)
 365 growth surface with $\hat{\mathbf{h}}$ across the stripe and $\hat{\mathbf{v}}$ along the length of the stripe [28, 29, 55].

366 A measurement of $ROP_{001}(\alpha = \pi/4)$ gives a measure of the tensor shear strain e_6 in the
 367 measurement system. For an isotropic medium we identified [3, 7]

$$ROP_{001} = 2K_e e_6. \quad (35)$$

368 The factor of 2 in the equation arises from recognition that $e_1 - e_2$ in the $\alpha = 0$ coordinate system
 369 equals $-2e_6$ in the $\alpha = -\pi/4$ coordinate system.

370 For GaAs, $ROP_{001}(\alpha = 0) = 1.85 e_6 d/(2k_B T)$ and the calibration constant equals

$$K_e = \left(\frac{1.85d}{3b} \right) \times \left(\frac{-3b}{4k_B T} \right) \quad (36)$$

371 where the expression for K_e has been arranged to show the difference between the DOP and
 372 the ROP calibration constants. Assuming that $d/b = 2.4$, then the calibration constant for
 373 $ROP_{001}(\alpha = 0)$ is found to be 1.475 times the calibration constant for DOP_{001} , rather than
 374 the isotropic value of unity times the calibration constant. If $d/b = 1.63$, then the calibration
 375 constants for $ROP_{001}(\alpha = 0)$ and $DOP_{001}(\alpha = 0)$ would be equal. For GaAs, Vurgaftman *et*
 376 *al.* [52, Table I] report $-1.66 < b < -3.9$ eV and $-2.7 < d < -6.0$ eV and recommend $b = -2.0$
 377 eV and $d = -4.8$ eV. The ratios for d/b of 1.63 and 2.4 lie within the reported ranges for the
 378 values of b and d .

379 Using Bahder's eight-band model, $ROP_{001}(\alpha = 0) = 1.84 e_6 d / (2 k_B T)$, which is not signifi-
 380 cantly different in magnitude than the value of $1.85 e_6 d / (2 k_B T)$ obtained by taking the limit of
 381 large E_g to obtain results from a four band model.

382 3.4.4. $DOP_{\langle 110 \rangle}$

383 We wish to calculate DOP and ROP for luminescence from a cleaved facet. A cleaved facet is
 384 a free surface and on a free surface the surface tractions must be zero for a body at rest. The
 385 '2' surface has been chosen as the cleavage plane. Thus the components e_4 and e_6 are zero, as
 386 discussed in Sec. 3.3.2.

387 Consider three coordinate systems: the crystal coordinate system, a primed system that is
 388 rotated about the z -axis of the crystal coordinate system by α radians, and a double-primed
 389 system that is obtained by rotation of β radians about the y' axis. See Appendix D and E for
 390 details.

391 Assume strains of e_1, e_2, e_3 , and e_5 in the facet coordinate system. For convenience we write
 392 e_2 and do not substitute the value owing to the free surface constraint. The components of
 393 the strain tensor $[\epsilon]$ in the crystal coordinate system are, as described in Appendix F, given by
 394 $[R_z(-\alpha)] \cdot [e] \cdot [R_z(-\alpha)]^T$ (or, depending on one's perspective, $[R_z(\alpha)]^T \cdot [e] \cdot [R_z(\alpha)]$) and are
 395 equal to

$$[\epsilon] = \begin{bmatrix} e_1 \cos^2(\alpha) + e_2 \sin^2(\alpha) & \sin(2\alpha)(e_1 - e_2)/2 & \cos(\alpha)e_5 \\ \sin(2\alpha)(e_1 - e_2)/2 & e_1 \sin^2(\alpha) + e_2 \cos^2(\alpha) & \sin(\alpha)e_5 \\ \cos(\alpha)e_5 & \sin(\alpha)e_5 & e_3 \end{bmatrix}. \quad (37)$$

396 The components of the strain tensor in the crystal coordinate system ϵ_i are used in the
 397 expressions for E_v to obtain the strain-induced splitting of the valence band.

398 We are interested in the calibration constant for a cleaved facet, thus we are interested in the
 399 case $\alpha = \pm\pi/4$. The rotation of β about the y' axis is used to align z'' along any direction in
 400 the plane of the facet. The rotation of β about the y' axis will be needed for a calculation of the
 401 DOP for an arbitrary direction in the plane of the facet and to calculate the ROP. We calculate the
 402 DOP for $\mathbf{k}_{x'} = (k, 0, 0)$ and $\mathbf{k}_{z'} = (0, 0, k)$ in the $x' y' z'$ facet coordinate system, which means
 403 that $\beta = 0$. Assuming that $\mathbf{k}_{x'}$ is parallel to a growth plane, then $\beta = 0$ would correspond to the
 404 usual alignment for a measurement of DOP (see Fig. 1 of [7]). The components of $\mathbf{k}_{x'}$ and $\mathbf{k}_{z'}$ in
 405 the crystal coordinate system are given by $[R_z(\alpha)]^T \cdot (k, 0, 0)^T$ and $[R_z(\alpha)]^T \cdot (0, 0, k)^T$ where
 406 $[R_z(\alpha)]$ is the rotation matrix for the coordinate transformation, which is a rotation about the
 407 z -axis by α radians. See Appendices D and E.

408 The calculation for the rate of luminescence for carriers with $\mathbf{k}_{z'} = \mathbf{k}_z$ proceeds as detailed
 409 previously, as the rotation does not affect the z -direction. The calculation for $\mathbf{k}_{x'}$ proceeds slightly
 410 differently as now the crystal momentum has components in both the x and y directions. In the
 411 crystal coordinate system, $\mathbf{k}_{x'} = (k \cos(\alpha), k \sin(\alpha), 0)$ and $\mathbf{k}_{z'} = \mathbf{k}_z = (0, 0, k)$ where k is the

412 magnitude of the crystal momentum. From Eq. (11),

$$\lim_{E_g \rightarrow \infty} E_{ks}(\cos(\alpha), \sin(\alpha), 0) = b \gamma_2 \left(\text{tr}([\epsilon]) - 3 \cos^2(\alpha) \epsilon_1 - 3 \sin^2(\alpha) \epsilon_2 \right) - \sqrt{3} d \gamma_3 \sin(2\alpha) \epsilon_6. \quad (38)$$

413 Two of the shear terms in Eq. (11) are zero because $k_z = 0$. The remaining shear term is
414 antisymmetric in α .

415 The energy difference for the DOP in the plane of the facet, $\Delta_f(\beta) = \Delta(\alpha = \pi/4, \beta)$, with
416 $\beta = 0$ is, from Eq. (11),

$$\Delta_f(\beta = 0) = + \frac{(d \gamma_3 \sqrt{3} + 3 b \gamma_2) e_1}{2 \mathcal{D}} + \frac{(-d \gamma_3 \sqrt{3} + 3 b \gamma_{2L}) e_2}{2 \mathcal{D}} - \frac{3 b e_3}{2} + \frac{(\mathcal{D} - 2 \gamma_2) \text{tr}([e]) b}{2 \mathcal{D}} \quad (39)$$

417 where the denominator $\mathcal{D} = \sqrt{\gamma_2^2 + 3 \gamma_3^2}$.

418 e_2 in the expression for $\Delta_f(\beta = 0)$ can be eliminated by substitution of the free surface
419 condition to obtain

$$\Delta_f(\beta = 0) = \frac{(-d \gamma_3 (c'_{12}/c'_{22} + 1) \sqrt{3} + (c'_{12}/c'_{22} - 1) (\mathcal{D} + \gamma_2) b) e_1}{2 \mathcal{D}} - \frac{(d \gamma_{3L} c'_{23}/c'_{22} \sqrt{3} + (c'_{23}/c'_{22} + 2) (\mathcal{D} + \gamma_2) b) e_3}{2 \mathcal{D}}. \quad (40)$$

420 For GaAs, with $d = 2.4 b$, $\Delta_f(\beta = 0) = 1.88 b e_1 - 1.22 b e_3$. For $d = 1.485 b$, $\Delta_f(\beta = 0) =$
421 $2.75 b (e_1 - e_3)/2$.

422 If $\Delta_f(\beta = 0) = 3 b (e_1 - e_3)/2$, then the calibration constant for DOP measurements with
423 $\beta = 0$ on cleaved facets (i.e., {110} surfaces) would be identical to the calibration constant for
424 DOP measurements on {001} surfaces with $\alpha = 0$. Given the calculations described here, this
425 would require $d = 1.485 b$ to obtain an $(e_1 - e_3)$ dependence but the magnitude of the calibration
426 constants for {001} and {110} surfaces would not be the same.

427 The axes for a calculation of ROP in the plane of the facet ($\alpha = \pi/4$) and in the usual alignment
428 (see Fig. 1 of [7]) are obtained for $\beta = \pm 45$ deg. Following the steps for a calculation of $ROP_{\bar{1}\bar{1}0}$,
429 one should find

$$\Delta_f(\beta = \pi/4) = - \frac{4 \sqrt{3} e_5 d \gamma_3}{\sqrt{\gamma_2^2 + 15 \gamma_3^2}} \quad (41)$$

430 which, for GaAs, equals $-1.76 e_5 d$. ROP is, as expected, proportional to the shear strain e_5
431 in the plane of the facet. For ROP_{001} , $\Delta(\alpha = 0) = -1.85 e_6 d$, which means that the calculated
432 ROP_{001} and $ROP_{\bar{1}\bar{1}0}$ calibration constants differ by about 1 part in 20. However, the recommended
433 value of $d = -4.8$ eV gives a calibration constant that appears to be about $1.6 \times$ larger than the
434 value that is expected, based on experimental measurements reported in [7].

435 The expression for $DOP_{\bar{1}\bar{1}0}$ is more complicated than the expressions for ROP or $DOP_{\langle 001 \rangle}$;
436 this owes to lack of symmetry as compared to other cases. For $ROP_{\bar{1}\bar{1}0}$, the two k 's are in the
437 plane of the facet and are mirror images along the [001] axis. These two directions are equivalent
438 crystal directions. For $DOP_{\bar{1}\bar{1}0}$, the two directions for k are along [110] and along [001]. These
439 directions are not equivalent directions in the crystal.

440 **4. Discussion**

441 Results presented in this paper suggest that for InP, $DOP_{\langle 1\bar{1}0 \rangle} = (1.32 e_1 - 0.80 e_3) b / (4 k_B T)$,
 442 where $d = 2.5 b$, which is the recommended ratio [52], has been used to eliminate d from the
 443 expression.

444 The calibration constant for InP was determined by fits of finite element method simulations to
 445 V grooves that were placed in a bending moment [7]. Least square fits of $-C_e (e_1 - e_3)$ were
 446 found to fit better to the data than fits of $-C_\sigma (\sigma_1 - \sigma_3)$, where $[\sigma] = [c][e]$ is the stress tensor
 447 and $[c]$ is the stiffness. This is surprising given that

$$\begin{aligned} \sigma_1 - \sigma_3 = & \\ & + \left(c_{11} - c_{13} - \frac{(c_{12} - c_{23}) c_{12}}{c_{22}} \right) e_1 - \left(\frac{(c_{12} - c_{23}) c_{23}}{c_{22}} + (c_{13} - c_{33}) \right) e_3 \quad (42) \\ & = (72.9 e_1 - 34.8 e_3) \times 10^9 \end{aligned}$$

448 where numerical values for a $\{110\}$ facet of InP have been substituted. Both the difference of
 449 stress and the theoretical expression for $DOP_{\langle 110 \rangle}$ have ‘excess’ e_1 . One would not necessarily
 450 expect a good fit of $e_1 - e_3$ to the data for a situation with excess e_1 , particularly given that fits
 451 of simulations using isotropic material properties did not fit as well as orthotropic simulations.
 452 These results suggest that the values of b and d are not accurate, or that the analysis is inaccurate.

453 Vurgaftman *et al.* [52, pg 5824] write

454 “The greatest uncertainty in the GaAs band structure parameters is associated with
 455 the deformation potentials, . . .”

456 “The various values for the deformation potential b varied between -1.66 and -3.9
 457 eV, although recent results tend toward the lower end of that range. We propose the
 458 following composite values [for GaAs]: $b = -2.0$ eV and $d = -4.8$ eV, which are
 459 consistent with the vast majority of measurements and several calculations.”

460 The calibration constant is a function of the deformation potential b ; a wide range of uncertainty
 461 in the value of b implies a wide range in the value of the calibration constant K_e . Vurgaftman *et al.*
 462 [52, pg 5829] in Table VI give the range of b for InP as $[-1.0, -2.0]$. In Table I of Ref. [52, pg
 463 5825], the range of b for GaAs is listed as $[-1.66, -3.9]$.

464 In addition, it was found that the best fit ROP calibration constant was found to be $1.3\times$
 465 larger than expected [7, pg 1817]. The factor of $1.3\times$ was explained at the time as owing
 466 to an uneven mounting surface providing an additional bending moment to the sample. The
 467 calculated expression for InP is $ROP_{\langle 110 \rangle} = -1.76 d e_5 / (2 k_B T)$. Using the recommended value
 468 of $d = -5.0$ for InP gives $ROP_{\langle 110 \rangle} = 2 \times 85 e_5$, which is $1.31\times$ larger than the expected $2 \times 65 e_5$.
 469 Given the results obtained, the assumption that the calibration constants for ROP and DOP are
 470 equal needs to be re-examined, as does the explanation for the difference in the constants found
 471 by fitting.

472 **4.1. Wishful Thinking on b and d ? Invariants of Second Order Tensors**

473 There are three principal invariants for a second rank tensor. These invariants are the same in any
 474 coordinate system obtained by rotations about the original coordinate system. The trace of a
 475 tensor is a principal invariant. For the strain tensor $[e]$ in Voigt notation, Eq. (1), the second
 476 principal invariant $I_2([e])$ is

$$I_2([e]) = e_1 e_2 + e_2 e_3 + e_1 e_3 + e_4^2 + e_5^2 + e_6^2. \quad (43)$$

477 The third principal invariant of a second rank tensor is the determinant of the tensor.

478 Consider the expression for $I_2([e - [\mathbf{I}] \text{tr}([e])/3])$ when the hydrostatic component of strain,
 479 which equals one third of the trace of the strain tensor, has been subtracted off of the diagonal
 480 elements of the strain tensor $[e]$. Here $[\mathbf{I}]$ is the identity matrix. For this case

$$I_2([e - [\mathbf{I}] \text{tr}([e])/3]) = \frac{(e_1 - e_2)^2}{6} + \frac{(e_2 - e_3)^2}{6} + \frac{(e_1 - e_3)^2}{6} + e_4^2 + e_5^2 + e_6^2. \quad (44)$$

481 $I_2([e - [\mathbf{I}] \text{tr}([e])/3])$ is a von Mises strain.

482 Compare the expression for $I_2([e - [\mathbf{I}] \text{tr}([e])/3])$ to Bahder's [47] expression for the strain-only
 483 contribution Eq. (12) to the valence band energy (7) and note that

$$E_s \Big|_{d=\sqrt{3}b} = -3 b^2 I_2([e - [\mathbf{I}] \text{tr}([e])/3]). \quad (45)$$

484 If $d = \sqrt{3} b$ then the strain-only contribution to the valence band energy, E_s , is invariant of the
 485 coordinate system.

486 4.1.1. Isotropic Material

487 For an isotropic material, $\gamma_2 = \gamma_3$, and there are only two independent elastic constants:
 488 $c_{11} = c_{22} = c_{33}$, $c_{12} = c_{23} = c_{13}$ with $c_{44} = c_{55} = c_{66} = (c_{11} - c_{12})/2$. Of the Luttinger
 489 parameters, γ_1 and γ_2 describe the coupling of the valence band basis states $|X\rangle$, $|Y\rangle$, and $|Z\rangle$
 490 to other states, and $\gamma_3 - \gamma_2$ is a measure of the anisotropy of the band structure.

491 Assuming $\gamma_3 = \gamma_2$, $d = \sqrt{3} b$, and using isotropic elastic constants,

$$DOP_{1\bar{1}0} = \frac{3b}{4k_B T} (e_1 - e_3) = -K_e (e_1 - e_3), \quad (46)$$

492 which is as expected, with K_e given by Eq. (26). For an isotropic material, the calculated
 493 DOP is proportional to the difference of the normal components of strain that are along the
 494 two orthogonal transmission axes of the polarizer, provided that $d = \sqrt{3} b$. For the isotropic
 495 case, the calculated $ROP = -3b/(2k_B T) e_5 = 2K_e e_5$, which also is as expected, provided that
 496 $d = \sqrt{3} b$; the isotropic ROP equals the bilinear product of $2K_e$ and the shear strain in the plane
 497 of the measured surface. These isotropic results are obtained if and only if the shear deformation
 498 potential $d = \sqrt{3} b$.

499 4.1.2. GaAs and InP: Cubic Materials

500 The calculated values of the DOP are closer to results obtained experimentally [7] if it is assumed
 501 that $d = \sqrt{3} b$. For this assumption and for GaAs,

$$DOP_{1\bar{1}0} = (1.0 e_1 - 0.89 e_3) \frac{b}{4k_B T} \quad (47)$$

502 by substitution of GaAs values into Eq. (40). For InP, the result is similar: $DOP_{1\bar{1}0} =$
 503 $(1.01 e_1 - 0.91 e_3) b/(4k_B T)$. For both InP and GaAs, the 'excess' e_1 is substantially reduced
 504 if $d = \sqrt{3} b$. For InP with $d = \sqrt{3} b$, the ratio of the e_1 coefficient to the e_3 coefficient is 1.12,
 505 whereas for the recommended ratio of $d = 2.5 b$, the ratio of the coefficients is 1.63. This first
 506 result with $d = \sqrt{3} b$ is consistent with experimental results [7] for the DOP calibration constant,
 507 where the trial function had no excess e_1 and appeared to fit the data well. For an isotropic
 508 material or for both \hat{h} and \hat{v} along crystal coordinate directions, $DOP = 3b \times (e_1 - e_3)/(4k_B T)$.

509 From Eq. (41) with $d = \sqrt{3} b$ and for GaAs,

$$ROP_{1\bar{1}0} = -1.02 \frac{3b}{4k_B T} \times 2e_5, \quad (48)$$

510 with the same numerical result for InP to two decimal places. The calculated calibration constant
511 with $d = \sqrt{3}b$ for $ROP_{1\bar{1}0}$ in GaAs is $1.02\times$ greater than for the isotropic case or for a $\{010\}$
512 plane. Experimentally the $ROP_{1\bar{1}0}$ calibration constant was found to be 1.3 ± 0.1 times greater
513 than the $DOP_{1\bar{1}0}$ calibration constant for InP [7].

514 With $d = \sqrt{3}b$, one finds that the calculated DOP appears to be closer to the experimentally
515 determined DOP, whereas the calculated ROP appears to be further from the experimental result.
516 The fit to the ROP data showed an asymmetry (see Fig. 3(b) of [7]) which was used to suggest
517 that an additional bending moment was added by the platform that supported the chip and that
518 this explained the finding of a ROP calibration constant that was $(1.3 \pm 0.1)\times$ the DOP calibration
519 constant.

520 Arbitrarily setting $d = \sqrt{3}b$ does not solve all discrepancies between data and calculation.
521 The results do suggest that it might be worthwhile to investigate further the relationship, if any,
522 between the deformation potentials.

523 The ratio of the experimentally determined calibration constants for GaAs and InP was found to
524 be $(50 \pm 10) : (65 \pm 10)$ [9]. Since the calibration constant is a linear function of the deformation
525 potential b and b is dominant in determining the calibration constant, this suggests that the ratio
526 of the strain deformation potentials for GaAs and InP should be roughly the same as the ratio of
527 the calibration constants. Thus one might expect $b_{\text{InP}} = (1.3 \pm 0.3) \times b_{\text{GaAs}}$.

528 5. Conclusion

529 Analysis of the degree of polarization (DOP) of luminescence is a useful and sensitive technique
530 to estimate strain in luminescent III-V materials and devices. Previously we assumed that
531 $DOP = -K_e(e_1 - e_2)$ and determined experimentally the calibration constant for GaAs and
532 InP, where e_1 and e_2 are normal strains near the surface being measured. The rotated degree of
533 polarization, or ROP, can be measured by rotating the transmission axes of the polarizer by -45
534 deg relative to the settings for a DOP measurement. The ROP is a measure of the shear strain
535 e_{12} , with assumed form $ROP = 2K_e e_{12}$. The calibration constant K_e was previously measured
536 experimentally and the assumed dependence of the DOP and ROP on strain were found to be
537 consistent with experimental data.

538 A simplified analytic determination of the dependence of DOP and ROP on strain is presented
539 here and discussed. This simplified analysis gives expressions for the calibration constant for InP
540 and GaAs, and for different surfaces. Analytic expressions for the band energies with arbitrary
541 crystal momentum, which were derived and published by T. B. Bahder [45–47], were used with
542 Boltzmann statistics, effective density of states, rotation of the band-edge Bloch factors (basis
543 functions), and selection rules for given polarizations of light, to obtain transitions rates and
544 hence the DOP and the ROP. To avoid elliptic integrals, the light along the two orthogonal
545 directions for the polarizer that define the ‘1’ and ‘2’ directions were used as proxies for the total
546 amount of light emitted in the selected polarization. The calibration constant K_e was found for
547 technologically interesting strains to be linearly dependent on the deformation potentials b , d , or
548 on both b and d , depending on the surface and the orientation of the polarizer transmission axes
549 relative to the crystal coordinate system.

550 The previously assumed forms for the DOP and ROP were found to be consistent with an
551 isotropic material, provided that the deformation potentials b and d were linearly related with
552 $d = \sqrt{3}b$. If $d \neq \sqrt{3}b$, then the DOP and ROP were not isotropic even though the material was
553 assumed to be isotropic. This fact raises some interesting questions.

554 Experimentally, the calibration constant K_e was measured on cleaved facets to be 65 ± 10
555 for InP [7, 9] and 50 ± 10 for GaAs [2, 3, 9]. These experimentally measured values for K_e
556 are consistent with the theoretically determined values for the calibration constant, given the
557 large range in the reported values for the deformation potentials b and d [52]. The calculated
558 relationship between DOP and strain for a (110) facet was found to be closer to experimental

559 results if it was assumed that $d = \sqrt{3} b$. Given the difference between the calibration constant for
560 GaAs and InP, it appears that $b_{\text{InP}} > b_{\text{GaAs}}$, and based on the ratios of the calibration constants,
561 $b_{\text{InP}} \approx 1.3 \times b_{\text{GaAs}}$.

562 Further work on determination of the calibration constant K_e and the relationship, if any,
563 between b and d is indicated. The degree of polarization of luminescence in InP and GaAs is a
564 sensitive function of strain. Careful measurements of the dependence of DOP and ROP on strain
565 might lead to better values for and understanding of the deformation potentials b and d .

566 Disclosures

567 The authors declare no conflict of interest.

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Table 1. Physical constants.

parameter	symbol	value	unit	remarks
electron mass	m_o	$9.10938356 \times 10^{-31}$	kg	
electron charge	q	$1.6021766208 \times 10^{-19}$	C	
Planck's constant	h	$6.62607004 \times 10^{-34}$	J·s	
	\hbar	$1.0545718 \times 10^{-34}$	J·s	
Boltzmann constant	k_B	$8.617333262 \times 10^{-5}$	eV·K ⁻¹	
	$k_B T$	25.68	meV	$T = 298$ K

Bahder used modified Luttinger parameters [47, Eq. A3]. In the limit of large E_g , the modified Luttinger parameters γ_{jm} equal the Luttinger parameters γ_j : $\lim_{E_g \rightarrow \infty} \gamma_{jm} = \gamma_j, j = 1, 2, 3$.

$$\gamma_{1m} = \gamma_1 - \frac{E_p}{3E_g + \Delta_{so}} \quad (\text{A.1})$$

$$\gamma_{2m} = \gamma_2 - \frac{E_p}{2(3E_g + \Delta_{so})} \quad (\text{A.2})$$

$$\gamma_{3m} = \gamma_3 - \frac{E_p}{2(3E_g + \Delta_{so})} \quad (\text{A.3})$$

Table 2. Material values [52]

parameter	symbol	GaAs	InP	unit	remarks
Luttinger parameter	γ_1	6.98	5.08		
Luttinger parameter	γ_2	2.06	1.60		
Luttinger parameter	γ_3	2.93	2.10		
modified Luttinger parameter	γ_{1m}	0.73	0.11		$T = 298$ K
modified Luttinger parameter	γ_{2m}	-1.06	-0.88		$T = 298$ K
modified Luttinger parameter	γ_{3m}	-0.19	-0.38		$T = 298$ K
band gap	E_g	1.519	1.4236	eV	$T = 0$ K
band gap	E_g	1.423	1.354	eV	$T = 298$ K
conduction band coupling	A_p	-14.7	-	eV \AA^2	
matrix element	E_p	28.8	20.7	eV	
matrix element	P_o^2	3.795	3.217	eV ²	$P_o^2 = E_p/2$
spin orbit splitting	Δ_{so}	0.341	0.108	eV	
conduction band	m_c	0.067	0.0795	m_o	$T = 0$ K
conduction band	m_c	0.0635	0.075 [†]	m_o	$T = 298$ K
heavy hole	m_{HH}	0.35	0.53	m_o	$T = 298$ K
light hole	m_{LH}	0.083	0.12	m_o	$T = 298$ K
E_g deformation potential	a	-8.33	-6.6	eV	$a = a_c + a_v$
valence band deformation potential	a_v	-1.16	-0.6	eV	
deformation potential	b	-2.0 ^{+0.34} _{-1.9}	-2.0 ^{+1.0} _{-0.0}	eV	note wide range
shear deformation potential	d	-4.8 ^{+2.1} _{-1.2}	-5.0 ^{+0.8} _{-0.0}	eV	note range
stiffness	c_{11}	118.0	102.2	GPa	crystal coordinate
stiffness	c_{12}	53.5	57.3	GPa	crystal coordinate
stiffness	c_{44}	59.0	44.2	GPa	crystal coordinate
stiffness	c'_{11}, c'_{22}	144.75	123.95	GPa	{110} facet
stiffness	c'_{33}	118.0	102.2	GPa	{110} facet
stiffness	c'_{12}	26.750	35.55	GPa	{110} facet
stiffness	c'_{13}, c'_{23}	53.5	57.3	GPa	{110} facet
stiffness	c'_{44}, c'_{55}	59.0	44.2	GPa	{110} facet
stiffness	c'_{66}	32.250	24.450	GPa	{110} facet

[†] The room temperature value for InP was determined by selecting $A_p = -9.98$ to match the recommended $T = 0$ value of 0.0795 [52, pg 5829], and using this value for A_p in Eq. (6). Using $A_p = 0$ gives values for m_c of 0.088 and 0.083 at $T = 0$ K and $T = 298$ K for InP.

692 B. Bloch Factors and Matrix Elements

The basis functions (Enders identifies these functions as Bloch factors [48, pg 544]) used by Bahder [45] are

$$CB_1 : |S\rangle |\downarrow\rangle \quad CB_2 : |S\rangle |\uparrow\rangle \quad (B.1)$$

$$LH_1 : \frac{-i}{\sqrt{6}} (|X\rangle + i|Y\rangle) |\downarrow\rangle + i\sqrt{\frac{2}{3}} |Z\rangle |\uparrow\rangle \quad LH_2 : \frac{i}{\sqrt{6}} (|X\rangle - i|Y\rangle) |\uparrow\rangle + i\sqrt{\frac{2}{3}} |Z\rangle |\downarrow\rangle \quad (B.2)$$

$$HH_1 : \frac{i}{\sqrt{2}} (|X\rangle + i|Y\rangle) |\uparrow\rangle \quad HH_2 : \frac{-i}{\sqrt{2}} (|X\rangle - i|Y\rangle) |\downarrow\rangle \quad (B.3)$$

$$SO_1 : \frac{-i}{\sqrt{3}} (|X\rangle - i|Y\rangle) |\uparrow\rangle + \frac{i}{\sqrt{3}} |Z\rangle |\downarrow\rangle \quad SO_2 : \frac{-i}{\sqrt{3}} (|X\rangle + i|Y\rangle) |\downarrow\rangle - \frac{i}{\sqrt{3}} |Z\rangle |\uparrow\rangle. \quad (B.4)$$

693 These Bloch factors are defined for \mathbf{k} along the z direction and the x , y , and z directions are
694 aligned along the [100], [010], and [001] directions of the crystal coordinate system.

695 The rate of transitions between two states $|\Psi_1\rangle$ and $|\Psi_2\rangle$ is proportional to $|M|^2$, the magnitude
696 squared of the momentum matrix element M , with

$$M = \langle \Psi_1 | \boldsymbol{\varepsilon} \cdot \mathbf{p} | \Psi_2 \rangle, \quad (B.5)$$

697 where $\boldsymbol{\varepsilon}$ is a unit vector that gives the polarization of the electromagnetic wave and \mathbf{p} is the
698 momentum operator. See Appendix C. For an electromagnetic wave that is polarized along the x
699 direction, $M = \langle \Psi_1 | p_x | \Psi_2 \rangle$.

700 The non-zero momentum matrix elements that connect the conduction band and the valence
701 band are $\langle S | p_x | X \rangle$, $\langle S | p_y | Y \rangle$, and $\langle S | p_z | Z \rangle$. The non-zero spin matrix elements are $\langle \downarrow | \downarrow \rangle$
702 and $\langle \uparrow | \uparrow \rangle$. These selection rules plus the Bloch factors for the conduction and valence bands are
703 required to calculate $L_{\hat{\mathbf{h}}}$ and $L_{\hat{\mathbf{v}}}$ and thus $DOP_{\hat{\mathbf{h}} \times \hat{\mathbf{v}}}$, Eq. (3).

704 C. Transition Rate

705 This Appendix follows Chapters 13 and 22 of Gasiorowicz's book, *Quantum Physics* [56].

706 The electric \mathbf{E} and magnetic \mathbf{B} fields are required to describe an electromagnetic field. The
707 coupled \mathbf{E} and \mathbf{B} components of an electromagnetic field can be combined into a vector potential
708 \mathbf{A} . Under certain conditions on the charge and current densities, a simple wave equation for the
709 vector potential \mathbf{A} can be obtained. The vector potential as a travelling wave is

$$\mathbf{A}(\mathbf{r}, t) = \sqrt{\frac{2\pi c^2 \mathcal{N} \hbar}{\omega \mathcal{V}}} \boldsymbol{\varepsilon} \exp i(\mathbf{k}_{\boldsymbol{\varepsilon}} \cdot \mathbf{r} - \omega t) \quad (C.1)$$

710 where $\boldsymbol{\varepsilon}$ is a unit vector that defines the polarization of the electromagnetic field, \mathcal{N} is the
711 refractive index, and \mathcal{V} is the volume of interest.

712 The classical force on an electron of reduced mass μ is given by the Lorentz force equation

$$\mu \frac{d^2 \mathbf{r}}{dt^2} = -e \left(\mathbf{E} + \frac{\mathbf{v}}{c} \times \mathbf{B} \right). \quad (C.2)$$

713 The Lorentz force equation is derivable if the Hamiltonian is taken as

$$H = \frac{1}{2\mu} \left(\mathbf{p} + \frac{e}{c} \mathbf{A} \right)^2 \quad (C.3)$$

714 i.e., replace \mathbf{p} with $\mathbf{p} + eA/c$. This Hamiltonian can be used with time-dependent perturbation
 715 theory to calculate the probability of a transition between two optically connected states.

716 The probability per unit time of a transition is

$$\Gamma = 2\pi\hbar \frac{2\pi e^2 \mathcal{N}}{\mu^2 \hbar \omega \mathcal{V}} |\langle \Psi_1 | e^{i\mathbf{k}_\varepsilon \cdot \mathbf{r}} \boldsymbol{\varepsilon} \cdot \mathbf{p} | \Psi_2 \rangle|^2. \quad (\text{C.4})$$

717 The total transition rate is determined by summing the probability over all states, modes, and
 718 polarizations. The total transition rate \mathcal{R} can be written as

$$\mathcal{R} = \frac{2\pi}{\hbar} |M|^2 \rho(E) \quad (\text{C.5})$$

719 where $\rho(E)$ is the density of final states and the equation is called Fermi's Golden Rule. The
 720 matrix element M describes the optical connection between the states and is given by

$$M = \langle \Psi_1 | e^{i\mathbf{k}_\varepsilon \cdot \mathbf{r}} \boldsymbol{\varepsilon} \cdot \mathbf{p} | \Psi_2 \rangle. \quad (\text{C.6})$$

721 For transitions in a crystal, the wave vector of the radiation \mathbf{k}_ε is significantly smaller than the
 722 crystal momenta \mathbf{k} of the carriers in the crystal that are involved in the transition, and can be
 723 ignored. Both Ψ_1 and Ψ_2 , which are Bloch functions, contain multiplicative factors of $\exp(i\mathbf{k}_1 \cdot \mathbf{r})$
 724 and $\exp(i\mathbf{k}_2 \cdot \mathbf{r})$, which leads to a Dirac delta function of $\delta(-\mathbf{k}_1 + \mathbf{k}_2 + \mathbf{k}_\varepsilon) \approx \delta(-\mathbf{k}_1 + \mathbf{k}_2)$ in
 725 the matrix element M to express conservation of \mathbf{k} [57]. The result is that

$$M = \langle \Psi_1 | \boldsymbol{\varepsilon} \cdot \mathbf{p} | \Psi_2 \rangle, \quad (\text{C.7})$$

726 a result that is needed [57, Eq. 4]. The relative rates of emission for two orthogonal polarizations
 727 can be determined from the preceding expressions.

728 For parabolic bands, \mathbf{k} and \mathbf{p} are parallel. The dot product with the polarization vector ensures
 729 that the light is a transverse wave. This means that to calculate the DOP, only \mathbf{k} that are in
 730 the plane of the measurement need to be considered (in the approximate analysis presented in
 731 this manuscript where the luminescences along principle directions are used as proxies for the
 732 integrated luminescence).

Baym [58, pg 282] shows for an isolated atom with Hamiltonian H_o that the matrix element
 can be written in terms of the dipole moment operator $\langle \Psi_1 | \boldsymbol{\varepsilon} \cdot \mathbf{r} | \Psi_2 \rangle$. By using $i\hbar \mathbf{p} = [\mathbf{r}, H_o]$,
 M can be expressed as:

$$M = \frac{1}{i\hbar} \boldsymbol{\varepsilon} \cdot \langle \Psi_1 | \mathbf{r} H_o - H_o \mathbf{r} | \Psi_2 \rangle \quad (\text{C.8})$$

$$= \frac{(E_2 - E_1)}{i\hbar} \langle \Psi_1 | \boldsymbol{\varepsilon} \cdot \mathbf{r} | \Psi_2 \rangle, \quad (\text{C.9})$$

733 which gives the matrix element in terms of the dipole moment. Only states with a non-zero
 734 dipole moment, such as $\langle S | x | X \rangle$, are considered optically coupled. The dipole moment and
 735 momentum matrix element are perhaps easier to visualize and understand than a density matrix
 736 approach [59]. Regardless, one must exercise caution to ensure that selection rules are followed.

737 D. Rotation Matrix

738 The defining features of tensors, vectors, and scalars are how they change under transformation
 739 of the coordinate system [53].

740 If scalars, vectors, and tensors represent physical objects, then magnitudes and directions
 741 should be independent of the choice of a coordinate system. Thus the components of a vector or
 742 a tensor must follow rules for transformations between coordinate systems.

743 Consider two Cartesian coordinate systems (i, j, k) and (i', j', k') with the same origin, but
 744 with the axes not necessarily aligned. The components of a vector A in the primed coordinate
 745 system are related to the components in the unprimed coordinate system by $(A_{x'}, A_{y'}, A_{z'})^T =$
 746 $[R] \times (A_x, A_y, A_z)^T$ where $[R]$ is the rotation matrix and is a 3×3 matrix. The rotation matrix
 747 $[R]$ is [60, pg 6]

$$[R] = \begin{bmatrix} i' \cdot i & i' \cdot j & i' \cdot k \\ j' \cdot i & j' \cdot j & j' \cdot k \\ k' \cdot i & k' \cdot j & k' \cdot k \end{bmatrix} = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix}. \quad (\text{D.1})$$

748 E. Euler's Angles

749 A rigid body in a 3D space requires three angles to specify its orientation relative to a frame
 750 of reference (i, j, k) . Euler's angles are one method to specify the orientation of a body with
 751 respect to a frame of reference. There are several conventions for specifying Euler's angles.
 752 The convention employed here is: Start with the (i', j', k') and the (i, j, k) coordinate systems
 753 aligned. Rotate counter-clockwise by an angle α about the k axis to obtain the (i'', j'', k'')
 754 basis. Rotate clockwise by an angle β about the j'' axis to obtain the (i''', j''', k''') basis. Finally,
 755 rotate counter-clockwise by an angle γ about the k''' axis. These three rotations will align the
 756 (i''', j''', k''') triad in an arbitrary direction in space. If $[R_z(\theta)]$ is a rotation matrix for rotation of
 757 θ about the k axis, then the rotation matrix for the three rotations is $[R_{z''}(\gamma)] \times [R_{y''}(\beta)] \times [R_z(\alpha)]$.
 758 The clockwise and counter-clockwise directions are defined from the perspective of an observer
 759 positioned on the positive side of the axis of rotation and facing the origin [60, pp 7 and 10–11].

$$[R_z(\alpha)] = \begin{bmatrix} \cos(\alpha) & \sin(\alpha) & 0 \\ -\sin(\alpha) & \cos(\alpha) & 0 \\ 0 & 0 & 1 \end{bmatrix} \quad [R_{y''}(\beta)] = \begin{bmatrix} \cos(\beta) & 0 & -\sin(\beta) \\ 0 & 1 & 0 \\ \sin(\beta) & 0 & \cos(\beta) \end{bmatrix} \quad (\text{E.1})$$

760 The intermediate steps in the rotations need not be written down. Given that the vector A has
 761 components (A_x, A_y, A_z) in the (i, j, k) coordinate system, then the components of the vector A
 762 in the (i''', j''', k''') coordinate system are

$$\begin{bmatrix} A_{x'''} \\ A_{y'''} \\ A_{z'''} \end{bmatrix} = [R_{z''}(\gamma)] \times [R_{y''}(\beta)] \times [R_z(\alpha)] \begin{bmatrix} A_x \\ A_y \\ A_z \end{bmatrix}. \quad (\text{E.2})$$

763 The inverse transformation is needed. Given some vector A with components $(A_{x'''}, A_{y'''}, A_{z'''})$
 764 in the (i''', j''', k''') coordinate system, the components of vector A in the (i, j, k) coordinate
 765 system are

$$\begin{bmatrix} A_x \\ A_y \\ A_z \end{bmatrix} = [R_z(-\alpha)] \times [R_{y''}(-\beta)] \times [R_{z''}(-\gamma)] \times \begin{bmatrix} A_{x'''} \\ A_{y'''} \\ A_{z'''} \end{bmatrix} \quad (\text{E.3})$$

766 Since $[R_z(-\alpha)] = [R_z(\alpha)]^T$ and $[R]^T[R] = [R][R]^T = [I]$ where $[I]$ is the identity matrix
 767 (i.e., rotation is a unitary transformation), negative rotations in the inverse order undo the
 768 transformation.

769 **F. Representation Quadric [53]**

770 The three components of a vector (A_1, A_2, A_3) transform under rotation of the basis (i.e. under
771 rotation of the coordinate system) as

$$A'_m = a_{mn}A_n = \sum_{n=1}^3 a_{mn}A_n \quad (\text{F.1})$$

772 where $a_{mn} = \hat{\mathbf{x}}'_m \cdot \hat{\mathbf{x}}_n$ [53, pg 10]. (A'_1, A'_2, A'_3) are the components of \mathbf{A} in the rotated basis
773 $(\hat{\mathbf{x}}'_1, \hat{\mathbf{x}}'_2, \hat{\mathbf{x}}'_3)$ and (A_1, A_2, A_3) are the components of \mathbf{A} in the original basis $(\hat{\mathbf{x}}_1, \hat{\mathbf{x}}_2, \hat{\mathbf{x}}_3)$. Note use of
774 the Einstein summation convention. Note also that Eq. (F.1) can be written in matrix form as
775 $(A'_1, A'_2, A'_3)^T = [R] \times (A_1, A_2, A_3)^T$, as presented in Appendices D and E.

776 The nine components T_{ij} of a second rank tensor $[T]$ transform under rotation of the basis as
777 $T'_{ij} = a_{ik} a_{jl} T_{kl}$ where T'_{ij} are the nine components in the rotated basis [53, pg 11]. The a_{nm} are
778 as defined for rotation of a vector.

779 Consider the equation for a second degree surface (i.e., a quadric, [53, pg 16]) where the
780 coefficients are 'symmetric' (i.e., $S_{mn} = S_{nm}$):

$$S_{mn} x_m x_n = 1. \quad (\text{F.2})$$

781 Rotate the basis and invert the rotation using the orthogonal property of rotation (i.e.,
782 $\hat{\mathbf{x}}'_i \cdot \hat{\mathbf{x}}'_j = \delta_{ij} = a_{ik} a_{jk}$, and $a_{ki} a_{kj} = \delta_{ij}$ since rotation is an unitary transformation) to obtain
783 $\hat{\mathbf{x}}'_m = a_{pm} \hat{\mathbf{x}}'_p$ and $\hat{\mathbf{x}}_n = a_{pn} \hat{\mathbf{x}}'_p$. Substitute the expressions for the components of $\hat{\mathbf{x}}$ into the
784 equation for a second degree surface (i.e., into the equation for the quadric):

$$S_{mn} x_m x_n = S_{mn} a_{pm} a_{qn} x'_p x'_q = a_{pm} a_{qn} S_{mn} x'_p x'_q = S'_{pq} x'_p x'_q. \quad (\text{F.3})$$

785 The coefficients of the quadric transform the same as a second rank tensor [53, pg 16]. Since
786 the coefficients of the quadric are symmetric, $S_{pq} = S_{qp}$, the components T_{mn} of a symmetric,
787 second rank tensor $[T]$ transform the same as the coefficients of a quadric. A quadric thus
788 provides a means to visualize a symmetric, second rank tensor and the surface $T_{mn} x_m x_n = 1$
789 is called the representation quadric of the tensor $[T]$ [53, pg 17].

790 The equation for the quadric surface, Eq. (F.2), can be written as a matrix equation

$$[x][S][x]^T = \begin{bmatrix} x_1 & x_2 & x_3 \end{bmatrix} \begin{bmatrix} S_1 & S_6 & S_5 \\ S_6 & S_2 & S_4 \\ S_5 & S_4 & S_3 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = 1, \quad (\text{F.4})$$

791 with the matrix $[S]$ written in a Voigt notation to reduce the number of subscripts.

792 Thus by analogy, a symmetric, second rank tensor can be written in matrix form. The properties
793 (e.g., principal axes, eigenvalues, eigenvectors, transformation, and principal invariants, which
794 are the trace, the determinate, and $S_{11}S_{22} + S_{22}S_{33} + S_{11}S_{33} - S_{12}^2 - S_{23}^2 - S_{13}^2$) of a quadric are
795 known. Thus, by analogy, the properties of a symmetric, second rank tensor are also known.

796 The transformation for a symmetric, second rank tensor, Eq. (F.3), can be calculated as
797 $[S] = [R]^T [S'] [R]$, where $[R] = [R(\alpha, \beta, \gamma)] = [R_z(\gamma)] \times [R_y(\beta)] \times [R_x(\alpha)]$ is the full rotation
798 matrix. Since rotation is a unitary transformation (i.e., $[R][R]^T = [R]^T[R] = [I]$), the inverse
799 transformation is $[S'] = [R][S][R]^T$ [53, pg 158].