

Correct implementation of polarization constants in wurtzite materials and impact on III-nitrides

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Supplemental Material

S1. POLARIZATION IN ZINCBLLENDE

There is an additional subtlety when calculating the formal polarization of the zincblende (ZB) structure that is related to the choice of unit cell. If the primitive unit cell is used for the calculation [with the origin chosen such that the Ga atom is at $(-1/8, -1/8, -1/8)$ and the N at $(1/8, 1/8, 1/8)$], then the result for III-nitrides will be what was determined in Ref. S1, Section III E. Specifically, the electronic part of the polarization vanishes, so the contribution simply comes from \mathbf{P}_{ion} of Eq. (2) of the main text:

$$\mathbf{P}_{\text{f}}^{\text{ZB}} = \frac{e\sqrt{2}a_{\text{WZ}}}{\Omega} \left(\frac{1}{4}, \frac{1}{4}, \frac{1}{4} \right), \quad (1)$$

where the a_{WZ} is the in plane lattice parameter of the wurzite (WZ) material (related to the ZB lattice constant by $\sqrt{2}$). The magnitude in the [111] direction is therefore $\sqrt{3}ea_{\text{WZ}}/2\sqrt{2}\Omega = e\sqrt{3}/2a_{\text{WZ}}^2$ [since the volume of the ZB primitive cell is $\Omega = (\sqrt{2}a_{\text{WZ}})^3/4$]. Though choosing a different origin of the cell may change the value by quanta of polarization, there are no lattice vectors \mathbf{R} of the primitive ZB cell [$\sqrt{2}a_{\text{WZ}}(1/2, 1/2, 0)$, $\sqrt{2}a_{\text{WZ}}(0, 1/2, 1/2)$ and $\sqrt{2}a_{\text{WZ}}(1/2, 0, 1/2)$] that will result in a quantum of polarization $e\mathbf{R}/\Omega$ that will take $\mathbf{P}_{\text{f}}^{\text{ZB}}$ to zero, and therefore ZB truly has a nonvanishing formal polarization. For the III-nitrides, we list the values of formal polarization for ZB along with WZ and the layered hexagonal (H) structure in Table I below.

We note that if a conventional eight-atom cubic unit cell is used, the results are misleading. The cubic cell volume is four times that of the primitive cell, $\Omega_c = 4\Omega$, and has four ‘‘dipoles’’ such as the one in Eq. (1); therefore, the magnitude of the polarization vector in the [111] direction is four times larger. Equation (1) now becomes:

$$\mathbf{P}_{\text{f}}^{\text{ZB}}(\text{cubic cell}) = \frac{e\sqrt{2}a_{\text{WZ}}}{\Omega_c} (1, 1, 1). \quad (2)$$

However, $\sqrt{2}a_{\text{WZ}}(1, 1, 1)$ is now given by the sum of lattice vectors of the *cubic cell* [$\sqrt{2}a_{\text{WZ}}(1, 0, 0)$, $\sqrt{2}a_{\text{WZ}}(0, 1, 0)$, and $\sqrt{2}a_{\text{WZ}}(0, 0, 1)$]; therefore it appears that $\mathbf{P}_{\text{f}}^{\text{ZB}}(\text{cubic cell})$ vanishes modulo a quantum of polarization. The calculation

TABLE I. Calculated formal polarizations, in units of C/m^2 , of wurtzite (WZ), zincblende (ZB) and layered hexagonal (H) GaN, AlN, and InN, all at the relaxed WZ in-plane lattice constant.

	$P_{\text{f}}^{(\text{WZ})}$	$P_{\text{f}}^{(\text{ZB})}$	$P_{\text{f}}^{(\text{H})}$
GaN	1.31	1.35	0
AlN	1.35	1.44	0
InN	1.03	1.07	0

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using the primitive cell is the rigorous result, as it is the smallest possible unit cell. For conventional unit cells of larger size, the quantum of polarization becomes smaller compared to the magnitude of the polarization vector, and the true values for the formal polarization cannot be ascertained.

S2. STRUCTURAL PARAMETERS AND BAND GAPS CALCULATED WITH THE HSE HYBRID FUNCTIONAL

TABLE II. Parameters for the III-nitrides calculated with HSE. Experimental data are listed for comparison.

	Property	HSE (this work)	Experiment ^a
GaN	a (Å)	3.205	3.189
	c (Å)	5.200	5.185
	u	0.377	0.377 ^b
	E_g (eV)	3.496	3.4-3.5
AlN	a (Å)	3.099	3.112
	c (Å)	4.959	4.982
	u	0.382	0.382 ^b
	E_g (eV)	6.044	6.1-6.3
InN	a (Å)	3.587	3.545
	c (Å)	5.762	5.703
	u	0.380	–
	E_g (eV)	0.646	0.6-0.8

^a From Ref. S2 unless otherwise specified.

^b From Ref. S3.

S3. EXPERIMENTAL DETERMINATION OF POLARIZATION FROM THE LITERATURE

The experimental data points in Fig. 2 of the main text were taken from various literature studies that were intended to determine the polarization constants in the InGaN/GaN or AlGaIn/GaN systems. We list these references in Table IV, V, VI, and III along with the reported values. Whether the actual measurement was bound charges at an interface or the field in a quantum well, we have converted the reported values to a polarization sheet charge for the purposes of Fig. 2 using the procedure outlined in Sec. V of the main text.

TABLE III. Experimental data for GaN/InGaIn/GaN quantum wells from optical (if not specified), holography, and CV measurements. In the cases where fields are reported in the reference, the bound charge is determined from the model described in the main text, Sec. V.

Reference	InGaIn content	Field (10^5 V/cm)	Bound charge ($10^{12}e^-/\text{cm}^2$)
S4	0.08	6.0	3.1
S5	0.10	13.6	7.2
S6	0.15	21.0	11.5
S7	0.12, 0.22	15.0, 29.0	8.1, 16.5
S8	0.10	3.5	1.9
S9	0.18, 0.15, 0.20	24.5, 27.0, 22.0	13.6, 14.8, 12.4
S10, S11, S12	0.07, 0.08, 0.08, 0.08, 0.08, 0.08, 0.09, 0.09, 0.09, 0.09, 0.09	10.5, 11.4, 11.1, 11.1, 12.6, 12.3, 12.9, 13.4, 13.7, 14.0, 14.0	5.5, 6.0, 5.8, 5.8, 6.6, 6.5, 6.8, 7.1, 7.2, 7.4, 7.4
S13	0.07	9.3	4.8
S14	0.15	13.4	7.33
S15	0.08	11.0	5.76
S16	0.09	19.0	10.0
S17	0.11		2.9
S18	0.20	31.0	17.5
S19	0.11	3.0	1.6
S20	0.10	9.0	4.8
S21	0.14, 0.14, 0.14	18.1, 21.2, 20.4	9.8, 11.5, 11.1
S22	0.16	12.0	6.6
S23	0.23	18.0	10.3
S23 (holography)	0.18	22	12.2
S24 (holography)	0.52	40.0	26.8
S25 (holography)	0.52	32.0	21.4
S26 (CV)	0.08		4.1
S27 (CV)	0.05, 0.09		1.8, 4.4

TABLE IV. Experimental data for GaN/AlGaN interfaces from Hall-effect measurements.

Reference	AlGaN content	Bound charge ($10^{12}e^-/\text{cm}^2$)
S28	0.09, 0.13, 0.17, 0.26, 0.31, 0.13, 0.18, 0.22, 0.22, 0.26, 0.29, 0.29, 0.31	3.9, 4.9, 8.7, 13.8, 15.0, 6.8, 7.2, 8.2, 11.0, 10.2, 10.1, 13.4, 13.5
S29	0.20, 0.20, 0.30, 0.35, 0.40, 0.40, 0.40, 0.40, 0.40, 0.37	9.8, 15.1, 19.1, 23.6, 28.5, 25.4, 24.1, 22.0, 19.7, 20.1
S30	0.33, 0.34, 0.38	13.2, 9.0, 10.5
S31	0.15	6.0
S32	0.15	7.9
S33	0.3 0	16.0
S34	0.05, 0.15	2.3, 6.7
S35	0.02, 0.06, 0.09, 0.14, 0.02, 0.05, 0.13, 0.15, 0.19, 0.24, 0.29	1.1, 2.1, 3.0, 3.3, 1.2, 1.6, 4.4, 4.6, 5.6, 6.5, 8.0
S36	0.12, 0.14, 0.14, 0.17, 0.17, 0.20, 0.23, 0.24, 0.26, 0.30, 0.31, 0.34, 0.36, 0.37	3.5, 4.6, 4.3, 5.6, 5.6, 6.5, 7.9, 8.8, 9.1, 10.7, 11.6, 12.3, 12.6, 14.0
S37	0.23	11.0
S38	0.16	7.3
S39	0.10, 0.13, 0.18	2.8, 4.1, 6.2
S40	0.10, 0.15, 0.20	4.1, 6.3, 8.7
S41	0.13, 0.23, 0.26, 0.36	7.3, 9.5, 11.0, 15.2
S42	0.22, 0.26, 0.32, 0.36	7.3, 9.0, 11.3, 12.0
S43	1.0	34
S44	0.20	13
S45	0.05, 0.15, 0.15, 0.15, 0.25, 0.35	3.0, 8.0, 7.5, 5.9, 9.9, 18.0
S46	0.23	9.8
S47	0.06, 0.10, 0.26, 0.33	1.0, 1.9, 1.4, 1.8
S48	0.72	35
S49	0.21, 0.21, 0.27, 0.33, 0.33, 0.40, 0.40, 0.49, 0.48	9.2, 10.1, 11.0, 11.5, 11.2, 12.9, 13.3, 16.9, 16.4
S50	0.15, 0.19, 0.18, 0.19, 0.20, 0.20, 0.23, 0.22, 0.26, 0.27, 0.26, 0.31, 0.31, 0.32, 0.32, 0.34, 0.35, 0.37, 0.37, 0.36, 0.43, 0.44, 0.46	0.7, 1.1, 1.4, 2.8, 3.0, 6.9, 6.4, 4.8, 11.2, 11.0, 8.7, 12.2, 13.0, 14.1, 9.8, 11.0, 9.6, 10.1, 11.4, 14.7, 13.6, 14.0, 14.3
S51	0.26	25

TABLE V. Experimental data for AlGa_N/Ga_N/AlGa_N quantum wells from optical and holography measurements. In the cases where fields are reported in the reference, the bound charge is determined from the model described in the main text, Sec. V.

Reference	AlGa _N content	Field (10^5 V/cm)	Bound charge ($10^{12}e^-/\text{cm}^2$)
S52	0.08, 0.08, 0.13, 0.17, 0.13, 0.17, 0.27, 0.27		3.8, 3.0, 5.6, 7.2, 7.4, 9.4, 14.2, 10.9
S53	0.15		2.0
S54	0.50	42.7	21.2
S55	0.20, 0.20	12.8, 8.3	6.4, 4.1
S55 (Holography)	0.20, 0.20, 0.20	12.8, 8.4, 6.9	6.4, 4.2, 3.4
S56	0.24	15.0	7.5
S57	0.17	8.3	4.1
S58	0.65	20	9.94
S59, S60	0.07	4.8	2.4
S61	0.14	5.1	2.5
S62	0.18, 0.11, 0.15	10.2, 9.3, 3.8	5.1, 4.6, 1.9
S63	0.18	12.3	6.1
S64	0.20, 0.50, 0.65, 0.80	11.9, 29.5, 33.9, 49.2	5.9, 14.6, 16.8, 24.5
S65	0.15	3.5	1.74
S57	0.11	4.5	2.24
S66	0.24, 0.18, 0.18, 0.15, 0.07, 0.18, 0.17, 0.16, 0.16	13.0, 13.0, 13.2, 9.0, 4.1, 13.3, 10.0, 10.0, 10.2	
S67	0.07, 0.15, 0.17, 0.18, 0.24, 0.18, 0.16, 0.16, 0.17	5.3, 11.7, 17.2, 16.9, 19.5, 13.8, 10.6, 10.2, 10.1	2.6, 5.8, 8.5, 8.4, 9.7, 6.9, 5.3, 5.1, 5.0
S68	0.15	14	7.0
S46	0.23		10.2
S47	0.06, 0.10, 0.26, 0.33	3.4, 3.1, 3.8, 3.4	1.7, 1.5, 1.9, 1.7
S69	0.31		11.0
S70			
S71	0.19	2.5	7.4

TABLE VI. Experimental data for Ga_N/AlGa_N interfaces from CV measurements.

Reference	AlGa _N content	Bound charge ($10^{12}e^-/\text{cm}^2$)
S72	0.22	1.3
S73	0.15	3.8
S50	0.33	10, 12
S74	0.09, 0.13, 0.17, 0.26, 0.31	3.8, 4.9, 8.7, 13.6, 15.0
S75	0.05, 0.12, 0.16	2.3, 6.8, 6.9
S26	0.13	7.1
S35	0.02, 0.06, 0.09, 0.14	0.9, 1.8, 2.0, 3.1
S51	0.26	7.0

S4. BOUND CHARGES AT NITRIDE INTERFACES

Here we present the specific equations used to generate Fig. 2 in the main text. As in the main text, we assume a coherent c plane interface of GaN and the alloy (InGa $_x$ N or AlGa $_x$ N), with the alloy layer under biaxial stress. The current practice in the field (black dashed curve in Fig. 2 of the main text) is to use the effective spontaneous (SP) polarization constants with respect to the zincblende (ZB) reference, without the correction term [$\Delta P_{\text{corr}}^{\text{ref}}$ introduced in Eq. (11) of the main text], and the proper piezoelectric (PZ) constants. (These values are usually taken from Ref. S76.) The resulting equation for Al $_x$ Ga $_{1-x}$ N/GaN is

$$\begin{aligned} \sigma_{\text{b}}^{(\text{ZB ref}),\text{prop}}(x) = & \Delta \tilde{P}_{\text{SP}}^{\text{int},(\text{ZB ref})} x - 2 \frac{(a_{\text{AlN}} - a_{\text{GaN}})x}{a_{\text{AlN}}x + a_{\text{GaN}}(1-x)} \left\{ e_{31}^{\text{AlN},\text{prop}} x + e_{31}^{\text{GaN},\text{prop}}(1-x) \right. \\ & \left. - [e_{33}^{\text{AlN},\text{prop}} x + e_{33}^{\text{GaN},\text{prop}}(1-x)] \frac{C_{13}^{\text{AlN}} x + C_{13}^{\text{GaN}}(1-x)}{C_{33}^{\text{AlN}} x + C_{33}^{\text{GaN}}(1-x)} \right\}, \end{aligned} \quad (3)$$

where $\Delta \tilde{P}_{\text{SP}}^{\text{int},(\text{ZB ref})}$ is

$$\Delta \tilde{P}_{\text{SP}}^{\text{int},(\text{ZB ref})} = P_{\text{eff}}^{\text{GaN},(\text{ZB ref})} - P_{\text{eff}}^{\text{AlN},(\text{ZB ref})}. \quad (4)$$

An identical set of equations are used for In $_x$ Ga $_{1-x}$ N/GaN, with InN instead of AlN.

The red solid curve in Fig. 2 corresponds to using the H ref (or ZB with the correction term) and the improper PZ constants:

$$\begin{aligned} \sigma_{\text{b}}^{(\text{H ref}),\text{imp}}(x) = & \Delta \tilde{P}_{\text{SP}}^{\text{int},(\text{H ref})} x - 2 \frac{(a_{\text{AlN}} - a_{\text{GaN}})x}{a_{\text{AlN}}x + a_{\text{GaN}}(1-x)} \left\{ \left(e_{31}^{\text{AlN},\text{prop}} - P_{\text{eff}}^{\text{AlN},(\text{H ref})} \right) x \right. \\ & \left. + \left(e_{31}^{\text{GaN},\text{prop}} - P_{\text{eff}}^{\text{GaN},(\text{H ref})} \right) (1-x) - [e_{33}^{\text{AlN},\text{prop}} x + e_{33}^{\text{GaN},\text{prop}}(1-x)] \frac{C_{13}^{\text{AlN}} x + C_{13}^{\text{GaN}}(1-x)}{C_{33}^{\text{AlN}} x + C_{33}^{\text{GaN}}(1-x)} \right\} \\ = & (\Delta \tilde{P}_{\text{SP}}^{\text{int},(\text{ZB ref})} + \Delta P_{\text{corr}}^{(\text{ZB ref})}) x - 2 \frac{(a_{\text{AlN}} - a_{\text{GaN}})x}{a_{\text{AlN}}x + a_{\text{GaN}}(1-x)} \left\{ \left(e_{31}^{\text{AlN},\text{prop}} - P_{\text{eff}}^{\text{AlN},(\text{H ref})} \right) x \right. \\ & \left. + \left(e_{31}^{\text{GaN},\text{prop}} - P_{\text{eff}}^{\text{GaN},(\text{H ref})} \right) (1-x) - [e_{33}^{\text{AlN},\text{prop}} x + e_{33}^{\text{GaN},\text{prop}}(1-x)] \frac{C_{13}^{\text{AlN}} x + C_{13}^{\text{GaN}}(1-x)}{C_{33}^{\text{AlN}} x + C_{33}^{\text{GaN}}(1-x)} \right\}, \end{aligned} \quad (5)$$

where

$$\Delta P_{\text{corr}}^{(\text{ZB ref})} = \frac{e\sqrt{3}}{2} \left(\frac{1}{(a_{\text{GaN}})^2} - \frac{1}{(a_{\text{AlN}})^2} \right), \quad (6)$$

and similarly for InGa $_x$ N/GaN.

S5. DIFFERENCE BETWEEN IMPLEMENTATIONS

The difference between the current practice in the field (ZB reference, no correction term, proper PZ) and our revised implementation (H reference, improper PZ constants) can be determined by taking the difference of Eq. (3) and Eq. (5). For the case of AlGa_N/Ga_N:

$$\begin{aligned}
\sigma_b^{(\text{H ref}), \text{imp}}(x) - \sigma_b^{(\text{ZB ref}), \text{prop}}(x) &= x \left[\Delta \tilde{P}_{\text{SP}}^{\text{int}, (\text{H ref})} - \Delta \tilde{P}_{\text{SP}}^{\text{int}, (\text{ZB ref})} \right] \\
&\quad - 2 \frac{(a_{\text{AlN}} - a_{\text{GaN}})x}{a_{\text{AlN}}x + a_{\text{GaN}}(1-x)} \left[-P_{\text{eff}}^{\text{AlN}, (\text{H ref})}(x) - P_{\text{eff}}^{\text{GaN}, (\text{H ref})}(1-x) \right] \\
&= x \left[\left(\Delta \tilde{P}_{\text{SP}}^{\text{int}, (\text{ZB ref})} + \Delta P_{\text{corr}}^{(\text{ZB ref})} \right) - \Delta \tilde{P}_{\text{SP}}^{\text{int}, (\text{ZB ref})} \right] \\
&\quad + 2 \frac{(a_{\text{AlN}} - a_{\text{GaN}})x}{a_{\text{AlN}}x + a_{\text{GaN}}(1-x)} \left[P_{\text{eff}}^{\text{AlN}, (\text{H ref})}(x) + P_{\text{eff}}^{\text{GaN}, (\text{H ref})}(1-x) \right] \\
&= x \Delta P_{\text{corr}}^{(\text{ZB ref})} + 2 \frac{(a_{\text{AlN}} - a_{\text{GaN}})x}{a_{\text{AlN}}x + a_{\text{GaN}}(1-x)} \left[P_{\text{eff}}^{\text{AlN}, (\text{H ref})}(x) + P_{\text{eff}}^{\text{GaN}, (\text{H ref})}(1-x) \right] \\
&= x \Delta P_{\text{corr}}^{(\text{ZB ref})} + 2\varepsilon_1(x) P_{\text{eff}}^{\text{AlGaN}, (\text{H ref})}(x).
\end{aligned} \tag{7}$$

We can gain some more insight by linearizing the first term in Eq. (7):

$$\begin{aligned}
x \Delta P_{\text{corr}}^{(\text{ZB ref})} &= x \frac{e\sqrt{3}}{2} \left(\frac{1}{(a_{\text{GaN}})^2} - \frac{1}{(a_{\text{AlN}})^2} \right) \\
&= x \frac{e\sqrt{3}}{2} \frac{1}{(a_{\text{GaN}})^2} \left(1 - \frac{(a_{\text{GaN}})^2}{(a_{\text{AlN}})^2} \right) \\
&= x P_{\text{f}}^{\text{GaN}, \text{ZB}} \left(1 - \frac{(a_{\text{GaN}})^2}{(a_{\text{AlN}})^2} \right) \\
&\simeq 2x P_{\text{f}}^{\text{GaN}, \text{ZB}} \left(1 - \frac{a_{\text{GaN}}}{a_{\text{AlN}}} \right) \\
&= -2P_{\text{f}}^{\text{GaN}, \text{ZB}} \left(x \frac{a_{\text{GaN}} - a_{\text{AlN}}}{a_{\text{AlN}}} \right) \\
&\simeq -2P_{\text{f}}^{\text{GaN}, \text{ZB}} \varepsilon_1(x)
\end{aligned} \tag{8}$$

So we see that the difference in implementations is

$$\begin{aligned}
\sigma_b^{(\text{H ref}), \text{imp}}(x) - \sigma_b^{(\text{ZB ref}), \text{prop}}(x) &\simeq 2\varepsilon_1(x) \left[P_{\text{eff}}^{\text{AlGaN}, (\text{H ref})}(x) - P_{\text{f}}^{\text{GaN}, \text{ZB}} \right] \\
&= 2\varepsilon_1(x) \left[x P_{\text{f}}^{\text{AlN}, \text{WZ}} + (1-x) P_{\text{f}}^{\text{GaN}, \text{WZ}} - P_{\text{f}}^{\text{GaN}, \text{ZB}} \right] \\
&= 2\varepsilon_1(x) \left[x \left(P_{\text{f}}^{\text{AlN}, \text{WZ}} - P_{\text{f}}^{\text{GaN}, \text{WZ}} \right) + \left(P_{\text{f}}^{\text{GaN}, \text{WZ}} - P_{\text{f}}^{\text{GaN}, \text{ZB}} \right) \right] \\
&= 2\varepsilon_1(x) \left[x \left(P_{\text{f}}^{\text{AlN}, \text{WZ}} - P_{\text{f}}^{\text{GaN}, \text{WZ}} \right) + P_{\text{eff}}^{\text{GaN}, (\text{ZB ref})} \right]
\end{aligned} \tag{9}$$

Therefore, the difference is small for small strains, and/or when there is a large cancellation of the terms in the square brackets. We see from Table I of the main text that $P_{\text{f}}^{\text{AlN}, \text{WZ}} - P_{\text{f}}^{\text{GaN}, \text{WZ}} = 0.039 \text{ C/m}^2 \sim -P_{\text{eff}}^{\text{GaN}, (\text{ZB ref})}$, hence the close agreement with between the black dashed and red solid curves in Fig. 2(b) of the main text (along with the relatively small magnitude of the strain). For the case of InGa_N, $P_{\text{f}}^{\text{InN}, \text{WZ}} - P_{\text{f}}^{\text{GaN}, \text{WZ}} = -0.286 \text{ C/m}^2$ which is the same sign as $P_{\text{eff}}^{\text{GaN}, (\text{ZB ref})}$, hence the larger discrepancy between the black dashed and red solid curves in Fig. 2(a) of the main text (also combined with a larger strain between InN and GaN).

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