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Band-gap narrowing in novel III-V semiconductors

S. C. Jain,[a] J. M. McGregor, and D. J. Roulston
Department of Electrical and Computer Engineering, University of Waterloo, Waterloo, N2L 3G1 Canada

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A predictive model for band-gap narrowing has been applied to several III-V semiconductors. Band-gap narrowing is expressed as $\Delta E_g = AN^{1/3} + BN^{1/4} + CN^{1/2}$; values for A, B, and C are predicted for these materials. The commonly used $N^{1/3}$ relation is shown to be valid for the p-type materials considered, but not for n-type materials.

It is well known that band-gap narrowing (BGN) has an important influence on optical properties and device performance in all semiconductors.[1-3] BGN has been extensively investigated in Si and GaAs, but very little is known about its influence on the performance of devices built using other materials.

The following simple expression may be used to predict BGN in any semiconductor:[4]

$$\frac{\Delta E_g}{R} = \frac{1.83}{r_s}\frac{\Lambda}{N_b^{1/3}} + \frac{0.95}{r_s^{3/4}} + \frac{\pi}{2}\frac{1}{r_s^{3/4}N_b}\left(1 + \frac{m^*_{\min}}{m^*_{\mathrm{maj}}}\right). \quad (1)$$

R is the effective Rydberg energy for a carrier bound to a dopant atom, and r_s is the average distance between majority carriers, normalized to the effective Bohr radius,

$$r_s = r_a/a, \quad (2)$$

where

$$r_a = (3/4\pi N)^{1/3}, \quad (3)$$

$$a = 4\pi\epsilon\hbar^2/m^*e^2. \quad (4)$$

Λ is a correction factor which accounts for anisotropy of the bands, in n-type semiconductors, and for interaction between the heavy- and light-hole bands in p-type semiconductors. N_b is the number of equivalent band extrema. m^*_{maj} and $m^*_{\min}$ are majority- and minority-carrier density-of-state effective masses, respectively. The first term in this expression is the exchange energy of the majority carriers. The band-gap shrinkage due to exchange interactions, neglecting screening, is given by

$$\Delta E_g(\mathrm{exch}) = 2e^2k_F/\epsilon_r\pi, \quad (5)$$

where k_F is the Fermi vector (see Eq. 3.6 in Ref. 5). Berggren and Sernelius have shown that the correct procedure is to subtract a term which accounts for screening from this expression. We have accounted for screening in an approximate way of replacing the "2" in Eq. (5) with "1.5."

The second term is the correlation energy, originally calculated by Mahan[6] for Si and Ge. Jain and Roulston[4] have shown that this expression may be used, in the normalized form given above, for other semiconductors, to a good approximation. The third term is the impurity interaction energy.[5] The expression for impurity interaction energy given by Lanyon and Tuft[7] is not generally acceptable; the BGN predicted by their expression decreases when the effective mass becomes small and/or the screening length becomes large. It is well known that the BGN is very large *because* the electron effective mass is small, and the screening length large,[8] a result contrary to the prediction of Lanyon and Tuft's expression.

To calculate the shift of the minority band, the result of Serre and Ghazali[9,10] was used, according to which the shifts of the two bands, divided by their effective masses, are equal, in the limit of high ($>10^{18}$ cm^{-3}) carrier concentration. However, the heavy- and light-hole bands move together into the gap due to heavy doping. To account for this, the average of heavy- and light-hole masses is used in the computation of the minority band-edge shift due to impurity interaction.[5] The use of $N_b = 2$ for all p-type semiconductors in Table I requires some explanation. Jain and Roulston[4] determined the Fermi level in p-type Si and p-type GaAs from extensive luminescence measurements reported in the literature. They found that the observed Fermi level was

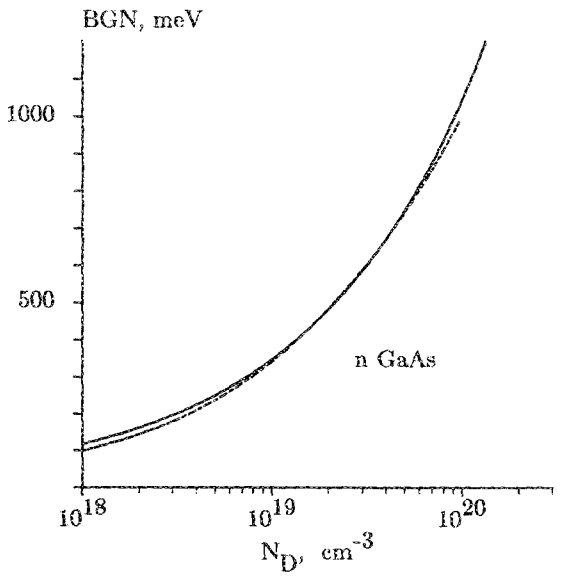

FIG. 1. n-type GaAs. Solid line is Eq. (1), dashed line in the theoretical result of Sernelius (see Ref. 8). Note very large BGN.

[a] Former address: Solid State Physics Laboratory, Delhi 110007, India, Present address: Clarendon Laboratory, Oxford OX1 3PU, U.K.

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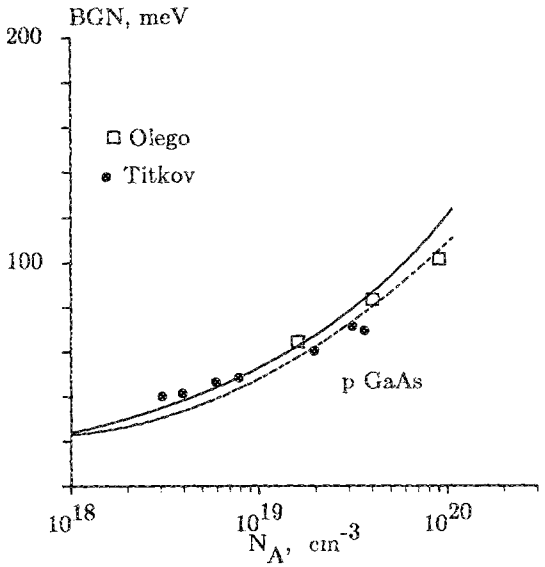

FIG. 2. p-type GaAs. Solid line is Eq. (1), dashed line is the theoretical prediction of Sernelius (see Reg. 12). Closed circles are the luminescence measurements of Titkov *et al.* (see Ref. 14); open squares those of Olego and Cardona (see Ref. 15).

higher by a factor of 1.5 than that calculated using the known densities of states, both at low temperature and at room temperature. To account for this, $N_b = 2$ was assumed for all p-type semiconductors.[4]

Equation (1) predicts BGN values for n- and p-type Si, n-type Ge, and p-type GaAs, which are in very good agreement with experimental results.[4] The results for these semiconductors and for n-type GaAs also agree extremely well with other many-body theories based on second-order perturbation theory and random-phase approximation (RPA) screening.[5,8,11–13] In Figs. 1 and 2, BGN values predicted by (1) in n- and p-type GaAs are plotted, along with the theoretical predictions of Sernelius[8,12] and experimental points from luminescence measurements.[14,15] Note that BGN in n-type GaAs is surprisingly large; however, Sernelius[8] has shown that this is consistent with luminescence measurements.

We now predict band-gap narrowing in heavily doped p- and n-type regions of several III-V semiconductors. Equation (1) may be rewritten in the form

$$\Delta E_g = A \times N^{1/3} + B \times N^{1/4} + C \times N^{1/2}. \quad (6)$$

Parameters used to calculate the A, B, and C coefficients, and hence band-gap narrowing, are listed in Table I. Calculated values of A, B, and C are given in Table II. In Fig. 3, calculated BGN for p-type InP, $In_{0.53}Ga_{0.47}As$, and GaSb is plotted versus N_A. In addition, experimental results of Titkov *et al.*[14] for p-type GaSb are plotted.

TABLE II. A, B, and C coefficients.

	$(A \times 10^{-9})$	$(B \times 10^{-7})$	$(C \times 10^{-12})$
p-GaAs	9.83	3.90	3.90
p-InSb	7.28	2.58	3.30
p-InAs	8.34	2.91	4.53
p-$In_{0.53}Ga_{0.47}As$	9.20	3.57	3.65
p-GaSb	8.07	2.80	4.12
p-InP	10.3	4.43	3.38
p-AlSb	11.5	5.30	3.53
p-AlAs	10.6	5.47	3.01
p-GaP	12.7	5.85	3.90
n-GaAs	16.5	2.39	91.4
n-InSb	12.2	1.09	604.
n-InAs	14.0	1.97	57.9
n-$In_{0.53}Ga_{0.47}As$	15.5	1.95	159.
n-GaSb	13.6	1.66	119.
n-InP	17.2	2.62	98.4
n-AlSb	10.1	3.09	8.27
n-AlAs	9.76	4.33	2.93
n-GaP	10.7	3.45	9.97

TABLE I. Assumed material constants.

	ϵ_r	m_e^*	m_{lh}^*	m_{hh}^*	N_b	A	Reference
p-GaAs	12.9	0.067	0.082	0.45	2	0.75	16
n-GaAs					1	1.00	
p-InSb	17.4	0.013	0.016	0.39	2	0.75	17, 16
n-InSb					1	1.00	
p-InAs	15.2	0.07	0.024	0.33	2	0.75	17, 16
n-InAs					1	1.00	
p-$In_{0.53}Ga_{0.47}As$	13.77	0.041	0.044	0.45	2	0.75	18, 19
n-$In_{0.53}Ga_{0.47}As$					1	1.00	
p-GaSb	15.7	0.041	0.06	0.32	2	0.75	14
n-GaSb					1	1.00	
p-InP	12.35	0.077	0.12	0.60	2	0.75	20
n-InP					1	1.00	
p-AlSb	11.6	0.11	0.11	0.40	2	0.75	17, 16
n-AlSb					6	1.00	
p-AlAs	12.0	0.50	0.49	1.06	2	0.75	17
n-AlAs					6	1.00	
p-GaP	11.0	0.13	0.17	0.67	2	0.75	17, 16
n-GaP					6	1.00	

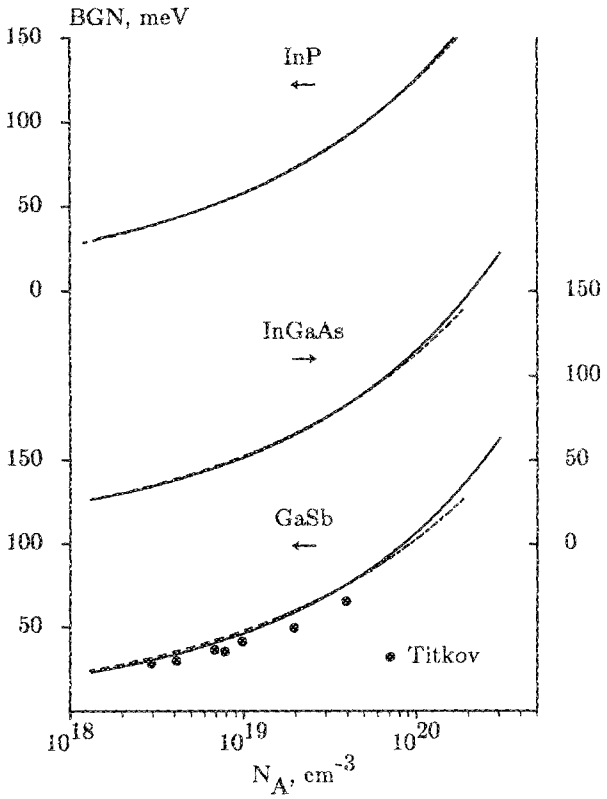

FIG. 3. From top to bottom, predicted BGN in p-type InP, $In_{0.53}Ga_{0.47}As$, and GaSb. Solid lines: Eq. (1). Dashed lines: fit to $a\times N^{1/3}$. For GaSb luminescence measurements of Titkov *et al.* are also plotted (closed circles).

In the past, ΔE_g (Ref. 21) has been found to have an $N_A^{1/3}$ dependence. Indeed, we find that in the p-type materials listed in Tables I and II, BGN may be fitted quite successfully to a $\Delta E_g = a\times N_A^{1/3}$ relation in the range $10^{18} < N_A < 10^{20}$. In Fig. 3 the dashed lines correspond to the $N_A^{1/3}$ fit, where $a = 2.69\times 10^{-8}$, 2.43×10^{-8}, and 2.22×10^{-8} eV cm^3 for InP, $In_{0.53}Ga_{0.47}As$, and GaSb, respectively. In p-type GaAs, $a = 2.6\times 10^{-8}$ gives a good fit. This would seem to be a happy coincidence; the correlation term, which is proportional to $N^{1/4}$, and the impurity term, which is proportional to N, are in roughly the right ratio so that their sum is proportional to $N^{1/3}$, as is the exchange term. This is not so when the impurity term is large, as it is in most of the n-type materials.

Note that in p-type GaAs, $a = 2.6\times 10^{-8}$, which is about 1.5 times as large as the extensively quoted value in Ref. 21. It is now known that optical absorption measurements yield a ΔE_g which is too small, because of the complication of free-carrier absorption.[22]

In bipolar device measurements, an *apparent* BGN is often obtained. To transform the true BGN ΔE_g to an apparent BGN ΔE_g^*, the Fermi–Dirac correction

$$\Delta E_g^* = \Delta E_g - E_f + kT\ln[F_{1/2}(E_f/kT)] \tag{7}$$

is applied, where

$$n = N_C F_{1/2}(E_f/kT), \tag{8}$$

$$p = N_V F_{1/2}(E_f/kT), \tag{9}$$

and $F_{1/2}(\eta)$ is the Fermi–Dirac integral of order one-half. For moderately, high-impurity concentrations, the apparent BGN is roughly linearly dependent on $\ln(N)$. At very-high-impurity concentrations, the apparent BGN *decreases* with increasing N. As the assumptions underlying (1) are not valid for $N < \approx 10^{18}$ cm^{-3}, the effective BGN for lower-impurity concentrations may be obtained by taking the slope of $\Delta E_g^*(N)$ around 10^{18}–10^{19} cm^{-3} and extrapolating back to $\Delta E_g^* = 0$.

A predictive model for band-gap narrowing has been applied to several novel III-V semiconductors. Experimental data are lacking for these materials, but reasonable agreement with luminescence data for GaSb was noted. BGN varies as $a\times N^{1/3}$ for most p-type, but not for n-type, semiconductors. The $N^{1/3}$ law should be regarded as empirical. For p-type GaAs, our value of a is around 1.5 times the value of Casey and Stern[21], but is in good agreement with recent results.

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