

# A SIMPLE EXPRESSION FOR BAND GAP NARROWING (BGN) IN HEAVILY DOPED Si, Ge, GaAs AND $\text{Ge}_x\text{Si}_{1-x}$ STRAINED LAYERS

S. C. JAIN† and D. J. ROULSTON‡

Department of Electrical and Computer Engineering, University of Waterloo, Ontario, Canada N2L 3G1

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**Abstract**—This paper presents simple but accurate closed form equations for Band Gap Narrowing (BGN) for  $n$  and  $p$  type, Si, Ge, GaAs and  $\text{Ge}_x\text{Si}_{1-x}$  alloys and strained layers. The equations are derived by identifying the four components of BGN: exchange energy shift of the majority band edge, correlation energy shift of the minority band edge and impurity interaction shifts of the two band edges. In the simple parabolic band approximation, the BGN is determined by the effective masses of the carriers and the relative permittivity of the semiconductor. For real semiconductors, known corrections due to anisotropy of the bands, due to multi-valleys in a band and due to interactions between sub-bands are used. The values of BGN for  $n$  Si,  $n$  Ge and  $n$  and  $p$  GaAs calculated using this simple formulation agree closely with the theoretical values calculated by other authors using advanced but complex many body methods and the Random Phase Approximation for screening effects. For  $p$  Si and  $p$  Ge ours appear to be the first calculations taking all interactions into account. Experimental values of BGN for all semiconductors except for  $p$  Ge for which no data could be found, are also in very good agreement with our theory.

The Fermi level for  $n$  and  $p$  Si and  $p$  GaAs is determined using the published luminescence data. In heavily doped  $p$  type semiconductors, the values are found to be considerably smaller than those calculated using the known values of the effective density of states. The values of apparent BGN for  $n$  and  $p$  Si and  $p$  GaAs calculated using experimentally determined Fermi levels are in remarkably good agreement with the experimental values derived from device measurements. All results are presented in a form which lends itself to numerical computer simulation studies.

## NOTATION

$a$	effective Bohr radius
$\Delta E_g$	band gap narrowing
$\Delta E_g^a$	apparent band gap narrowing
$\Delta E_F^{\text{FD}}$	Fermi Dirac correction
$E_F$	Fermi level measured from Majority band edge
$\epsilon$	dielectric constant
$\Lambda$	correction factor
$m_d$	effective density of state mass of a carrier divided by free electron mass
$m_e$	effective density of state mass of electron divided by free electron mass
$m_h$	effective density of state mass of hole divided by free electron mass
$n, p$	carrier (electron or hole) density
$N$	dopant concentration, $N_A$ or $N_D$ ; complete ionization is assumed, $N = n$
$N_A$	acceptor concentration
$N_D$	donor concentration
$N_b$	number of valleys in the conduction or valence band
$N_v$	effective density of states in the valence band
$n_{i0}$	intrinsic carrier density
$n_{ie}$	effective intrinsic carrier density
$R$	effective Rydberg energy
$r_a$	average distance between impurity ions
$r_s$	many body parameter

## 1. INTRODUCTION

In view of its importance in determining the performance of bipolar devices, extensive work has been done on band gap narrowing (BGN) in  $n$  Si (and  $n$  Ge) during the last 35 yr. Early work on BGN (see for example Refs[1–6]) has been reviewed in Refs[7–10]. Subsequent work has shown that the classical theories[2–4] used in the early years do not predict the BGN correctly; a quantum mechanical description is required[7,11–19].

Mahan[11] wrote a theoretical paper in which he considered all possible interactions which affect the band shifts due to heavy doping and calculated the BGN in  $n$  Si and  $n$  Ge. Mahan's approach was elegant in that he used the many-body technique and still obtained very simple expressions for the BGN. Subsequent work of Berggren and Sernelius[13] based on second order perturbation theory and RPA[13] calculations showed however that since Mahan had assumed the impurity atoms to be distributed in a periodic lattice in Si and in Ge, his results for band gap shift due to carrier impurity interaction were in error. The results of the theory of Berggren and Sernelius[13] are in reasonable agreement with the experimental results of Wagner and del Alamo[20] in the high density regime where the theory is applicable. Wagner and del Alamo also determined the BGN at room temperature using luminescence measurements. Though the scatter was rather large,

†Present address: Delft Institute of Microelectronics, TU Delft, Postbus 5053, 2600 GB Delft, The Netherlands. Formerly at the Clarendon Laboratory, Oxford, U.K. and the Solid-State Physics Laboratory, Delhi, India.

‡Part of this work was done by this author at Department of Materials, University of Oxford, U.K.

the results generally agreed with theory[22,23] which suggests that BGN at room temperature is 10–20 meV larger than BGN at low temperature. If the doping density is not high, the theories of Mahan and Berggren *et al.* do not apply. Serre and Ghazali[12], Bennett and Lowney[14] and Lowney[24] have calculated BGN using Klauder's theory of multiple scattering[25] which is valid for all doping concentrations.

Sernelius[15,16] and other authors[7,17,26–32] have done considerable theoretical and experimental work on GaAs. Extensive work has been done recently on measurements of apparent BGN in GaAs devices by Lundstrom and co-workers[26–29], by Tiwari and Wright[30] and by de Lyon *et al.*[31].

More work on BGN is required. So far apparent BGN (different from physical BGN but more convenient for predicting the effective intrinsic carrier concentration  $n_i$ , the quantity of most importance in analysis of bipolar devices) determined by device measurements does not seem to agree[26] with that derived from theoretically determined BGN[14] (see Section 4). The results obtained by second order perturbation theory or by Klauder's theory of multiple scattering are not in convenient form to interpret experiments and design devices. The calculations are time consuming and have to be performed for each case separately. The effect of changing any one parameter, say effective mass[33], cannot be determined conveniently since closed form expressions for BGN have not been obtained. These results are not convenient for developing CAD tools. There is a large discrepancy between the apparent BGN of *p* GaAs determined experimentally and by theory[14,26–29]. No theoretical work using modern many body theories and including all effects on BGN has been done on *p* Si or *p* Ge, presumably because modelling of the valence band is more difficult[16,32–34]. In view of the recent interest in heterostructures based on *p* type heavily doped Ge–Si alloys, *p* type Si and *p* type Ge have acquired great importance.

In this paper we discuss BGN in the high density regime (dopant concentration more than  $1 \times 10^{18} \text{ cm}^{-3}$ ) in *n* and *p* type Si, Ge, GaAs and Ge–Si alloys. Our approach is essentially the same as that of Mahan, the aim being to obtain simple closed form analytical expressions for BGN and apparent BGN which are suitable for interpreting experiments, for use in computer aided design, and for predicting behaviour of devices based on new materials such as Ge–Si, InGaAs, GaAsP and other semiconductor alloys. Theoretically, our approach is less rigorous. It is rather an approach with the purpose of constructing a simple expression for BGN useful for practical CAD analysis of devices.

The organization of the paper is as follows. In the next section (Section 2) we discuss the various contributions (exchange, correlation and impurity interaction shifts of the band edges) to BGN and

examine the validity of existing expressions which have been used for these contributions. We discard those which are of doubtful validity and select an appropriate expression for each contribution. We modify the selected expressions suitably and express them in reduced form so that a simple expression applicable to all semiconductors can be constructed. We make a key approximation which enables us to make these expressions applicable to *p* type semiconductors. In Section 3, we calculate numerical values of BGN for *n* and *p* Si, *n* and *p* Ge and *n* and *p* GaAs using this expression and compare them with other available theoretical and experimental[35–43] results for these semiconductors. We find that the Fermi level in *p* type semiconductors cannot be calculated using the existing values of density of states. We determine the Fermi level accurately by analysing large number of luminescence spectra available in the literature. Using these Fermi levels, and the simple expression developed in Section 2, values of apparent BGN are calculated and compared with device measurements[23,26–31,43–48] in Section 4. A method to predict the apparent BGN of new semiconductors is suggested in this section. The method can be used for predicting BGN in new materials like Ge–Si, InGaAs and GaAsP alloys which are acquiring great technological importance. In view of the recent interest in bipolar transistors based on Si–Ge strained layers (see Section 5 for references), we also calculate the BGN in these alloys and strained layers for low Ge fractions in Section 5. The empirical equations for apparent BGN, suitable for numerical computer simulation studies, are given in Section 6. Section 7 gives a brief summary of the main results of this paper.

## 2. THEORY

### 2.1. Normalizing parameters

We will normalize the various energies by the effective Rydberg energy  $R$  and express the doping concentration in terms of the dimensionless parameters  $r_s$ .  $R$  and  $r_s$  are given by [7]:

$$R = \frac{13.6m_d}{\epsilon^2} \text{ eV} \quad (1)$$

$$r_s = \frac{r_a}{a} \quad (2)$$

where  $r_a$  is half the average distance between the impurity atoms and  $a$  is the effective Bohr radius given by:

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

and

$$a = \frac{0.53\epsilon}{m_d} \times 10^{-8} \text{ cm.} \quad (4)$$

Here  $N$  is the doping concentration,  $\epsilon$  is the dielectric constant and  $m_d$  is the effective density of state mass of the carriers in the majority band divided by the free electron mass. The semiconductor is assumed to be uncompensated and all impurities ionized so that  $N$  is also the concentration of free carriers.

There are four major contributions[11] to the BGN: (1) shift  $\Delta E_{x(maj)}$  of the majority band edge due to exchange interaction; (2) shift  $\Delta E_{cor(mino)}$  of the minority band edge due to carrier-carrier or electron-hole interaction, also designated as the correlation energy[11]; (3) shift  $\Delta E_{i(maj)}$  of the majority band edge due to carrier-impurity interactions; and (4) shift  $\Delta E_{i(mino)}$  of the minority band edge due to carrier-impurity interactions. The shifts  $\Delta E_{x(maj)}$  and  $\Delta E_{cor(mino)}$  are also known as shifts due to many-body interactions, or simply many-body shifts. All shifts are into the band gap and the total band gap narrowing  $\Delta E_g$  or BGN is obtained by numerically adding all the shifts[11–13],

$$\Delta E_g = \Delta E_{x(maj)} + \Delta E_{cor(mino)} + \Delta E_{i(maj)} + \Delta E_{i(mino)}. \quad (5)$$

Work of Berggren and Sernelius[13] shows that use of Thomas Fermi screening does not give accurate results for many body-shifts of the two band edges. It is necessary to calculate these shifts using Random Phase Approximation (RPA) for screening. In addition to Thomas Fermi and RP approximations, there is a third approach known as Plasmon Pole Approximation (PPA) which can be used to calculate these shifts. Abram *et al.*[18] and Sterne and Inkson[19] have shown that proper use of PPA simplifies the procedure considerably (as compared to RPA procedure) and gives results in close agreement with full RPA calculations.

We discuss below how we obtain simple expressions for these four shifts which give results in close agreement with full RPA calculations.

## 2.2. Exchange energy

The expression for shift in the majority and band edge due to exchange interactions is[1,7,11,13]:

$$\Delta E_{x(maj)} = \frac{fe^2(3\pi n)^{1/3}}{\epsilon\pi} \quad (6)$$

where  $e$  is the electronic charge. For a simple parabolic band and if the effect of screening is neglected,  $f = 1$ , a value used by Mahan. The correct procedure is however to take  $f = 2$  and calculate (using many body methods) and subtract a density dependent quantity to take into account the effect of screening[7,13,18]. In order to obtain a simple expression including the effect of screening, we calculated the numerical values of  $\Delta E_{x(maj)}$  including the effect of screening for Si, Ge and GaAs. We found that  $f = 1.5$  gives approximately the correct effect of screening for all semiconductors in the doping range  $1 \times 10^{18} - 1 \times 10^{20} \text{ cm}^{-3}$ . Expression (6) has to be further modified to take into account the effect of  $N_b$  equivalent valleys in the band (e.g. 6 in the conduc-

tion band of Si), for the anisotropy of the conduction bands in  $n$  semiconductors and for interactions between the light and the heavy hole bands in the case of  $p$  semiconductors. These corrections are different for different semiconductors. Including the effect of  $N_b$  multiple sub-bands[11], representing by  $\Lambda$  the correction factor due to anisotropy in the conduction bands of Si and Ge and due to interactions between the light and the heavy hole valence bands in  $p$  semiconductors and converting eqn (6) to dimensionless parameters, we obtain:

$$\frac{\Delta E_{x(maj)}}{R} = 1.83 \frac{\Lambda}{N_b^{1/3}} \frac{1}{r_s}. \quad (7)$$

Application of this formula to  $n$  type semiconductors is straightforward. Modelling  $p$  type semiconductors requires further considerations. Extensive work on the calculation of the exchange energy of holes in the valence band in  $p$  Si and  $p$  Ge was done in the 1970s to interpret experiments on the formation of electron-hole liquid drops in highly excited intrinsic Si and Ge at low temperatures. A survey of this literature shows that the values of the exchange energy in the valence band were sensitive to the method used to calculate the energy and to the assumptions made for modelling the heavy hole and the light hole bands[49]. We use a value 0.75 for  $\Lambda$ [7,49] for reduction in the exchange energy due to interaction between the light and the heavy hole bands. Additional difficulties arise in modelling the valence band when the  $p$  type semiconductor is heavily doped. For Si these difficulties were noted by Barber[33] and more recently by Dumke[34,35]. From the measurements of luminescence generated by circularly polarized light in  $p$  GaAs, Miller *et al.*[32] have concluded that the conventional effective hole mass of 0.47 cannot be used to model the valence band of heavily doped  $p$  type GaAs. It is known that both the light hole and the heavy hole bands shift by the same amounts due to heavy doping even though the hole density in the heavy hole band is considerably larger[13,17]. The luminescence caused by the light holes is comparable to that caused by the heavy holes[16] in spite of their small numbers. In short, the effect of a light hole band cannot be taken into account simply by taking an effective hole mass derived from the heavy hole and the light hole masses. Different authors have used different mechanisms to account for these complications. Mahan has used one single value of 0.33 for the hole effective mass in  $n$  Si even when the number of holes is small. Berggren and Sernelius[13] have treated the two hole bands as equivalent with an average hole mass of  $(m_h + m_l)/2$  in the approximate calculation of impurity shift of the valence band in  $n$  Si (see eqn 3.17 of their paper). Conventionally, the valence band is represented by one band (i.e.  $N_b = 1$  in eqn 7) with an effective mass derived from the masses of the light and heavy hole bands. We have used, somewhat empirically, the assumption that  $N_b = 2$  in eqn (7) for

all  $p$  semiconductors we have considered in this paper. Some justification for this assumption can, however, be given.

The luminescence experiments support strongly our approximation of  $N_b = 2$  in  $p$  Si and  $p$  GaAs. It was noted by Schmid *et al.*[38] and by Dumke[34,35] that in  $p$  Si, the Fermi level  $E_F$  determined by using the conventional density of state formula:

$$N = N_v F_{1/2} \left( \frac{E_F}{kT} \right) \quad (8)$$

is considerably larger than the value determined directly from the observed luminescence spectra. We have determined the Fermi levels for  $p$  Si and  $p$  GaAs using the published data of luminescence spectra[32,41–43] for different doping concentrations. Detailed results at room temperature will be discussed in Section 4; we give below in Table 1 the result for one doping each for both  $p$  Si and  $p$  GaAs at 4.2 K. It can be seen that the experimental values are considerably smaller than the conventional values determined using the usual density of states values,  $1.04 \times 10^{19} \text{ cm}^{-3}$  for the valence band in Si and  $7.0 \times 10^{18} \text{ cm}^{-3}$  in GaAs at room temperature[50].

Our approximation  $N_b = 2$  increases the density of states by a factor  $2^{2/3}$  for  $p$  type semiconductors and reduces the Fermi level by approximately the required amount so that it agrees with the observed values. We could have increased the density of states by increasing the effective mass of the hole. However in this case the significance of the light hole band as a separate band is lost. This choice has no effect on the calculation of Fermi level but influences the Fermi wave vector, the exchange energy and the BGN significantly. To illustrate this point further, for calculating the density of states in the conduction band of  $n$  Si, it does not matter whether we take the effective electron mass as 0.33 with  $N_b = 6$  or as  $0.33 \times 6^{2/3} = 1.09$  and ignore the fact that  $N_b = 6$ . In the latter case however, there is a large error in the calculation of the Fermi vector and the exchange energy if  $N_b$  is not taken as 6. Note that in our simple formulation, the exchange energy does not involve the effective mass but depends significantly on  $N_b$ . Taking  $N_b = 2$  and not increasing the effective mass emphasizes the importance of the light hole band consistent with the discussion given in the previous paragraph and gives correct values of Fermi level and of BGN. We cannot provide a full theoretical justification for assuming  $N_b = 2$  for the valence band in heavily doped  $p$  semiconductors and this should be

regarded as an empirical assumption to explain a large body of the experimental data.

With these approximations, eqn (7) for the shift of band edge due to exchange interactions can be used for all semiconductors.

The effect of screening on exchange energy calculated using the more accurate Random Phase Approximation (RPA) is considerably different from that using Thomas Fermi screening[13]. Numerical calculations show that the values given by eqn (7) agree with RPA calculations within 3–5 meV for  $n$  Si[13] and for  $n$  and  $p$  GaAs[15,16]. They also agree with the results of Abram *et al.*[18] obtained by using Plasmon Pole Approximation (PPA).

### 2.3. Correlation energy shift $\Delta E_{\text{cor(mino)}}$ of the minority band

This is the shift of the minority band due to electron hole interaction, also known as the correlation energy shift. Berggren *et al.* have calculated this energy for  $n$  Si and  $n$  Ge using the RPA method since Thomas–Fermi screening gives wrong results for this shift also. Mahan used the PPA method and was able to derive an analytical expression for this energy. The final expression given by Mahan involves an integral and the ratio of the effective masses of holes and electrons as multiplying factors. Sterne and Inkson[19] have pointed out that this result is in error and if the expressions leading to the final results are correctly evaluated, the ratio of the effective masses disappears. Our calculations agree with Stern and Inkson and with this correction, this shift of the minority band depends entirely on the properties of the majority band. Mahan found that the integral is weakly dependent on the dopant concentration and the value of the integral could be taken as constant at 0.8 for  $n$  Si and  $n$  Ge in the high doping regime. The integral is also weakly dependent on  $N_b$  and we can use the same value (i.e. 0.8 of the integral) for all semiconductors, to a good approximation. The final result can be written as:

$$\frac{\Delta E_{\text{cor(mino)}}}{R} = \frac{0.95}{r_s^{3/4}} \quad (9)$$

We have already mentioned that RPA or PPA calculations are required to obtain accurate values of the correlation energy. For  $n$  Si, values obtained using eqn (9) are in close agreement with those calculated using RPA by Berggren and Sernelius[13]. At  $N_D = 10^{18} \text{ cm}^{-3}$ , the value given by eqn (9) is 13 meV, by RPA it is 14 meV. Similar agreement is

Table 1. Comparison of Fermi level values measured from valence band edge;  $E_F(\text{Lum.})$ , determined from luminescence measurements and  $E_F(N_v)$ , calculated by using eqn (8) and converting them to 4.2K assuming that  $N_v$  varies as  $T^{1.5}$ . The luminescence values are for the data from the papers of Schmid *et al.*[38] for  $p$  Si and of Olego and Cardona[43] for  $p$  GaAs

	$T(\text{K})$	$N$	$E_F(N_v, \text{meV})$	$E_F(\text{Lum.}, \text{meV})$
$p$ Si	4.2	$1.04 \times 10^{20}$	140	96
$p$ GaAs	4.2	$9.0 \times 10^{19}$	166	115

obtained at higher doping concentrations and for  $n$  and  $p$  type GaAs[15,16].

#### 2.4. Impurity interaction energy shift $\Delta E_{i(maj)}$ of the majority band

There are several expressions available in the literature to describe the shift of the majority band due to carrier impurity interaction. Mahan has discussed the results based on the Born approximation, derived by Lanyon and Tuft[46], and his own result based on periodic distribution of the impurity ions. For  $n$  type Si almost all expressions give numerically similar results for the majority band and any one of them can be used to get the right numerical answers. However we found that all these expressions are unacceptable for general applications to all semiconductors for one reason or the other. The expression that Mahan derived, based on the periodic distribution of the impurity atoms in the semiconductor, gives the shift of the minority band in the wrong direction leading to a large error in the final results. Mahan has pointed out that inconsistency arises in using the expression based on Born's approximation. The value of  $\Delta E_{i(maj)}$  calculated using the expression originally given by Lanyon and Tuft for correlation energy[46] and generalized by Mahan to include the case of impurity scattering, decreases with a decrease of the inverse screening length. This implies that for lighter particles (e.g. electrons in the conduction band of  $n$  GaAs) which have a large screening length, the shift should be very small. This is contrary to the well known result for  $n$  GaAs[15]. Lanyon and Tuft's result also implies that the BGN in compensated semiconductors or in the space charge layer of a junction device should be small. This is contrary to the results obtained by Lowney[51] and by Jain *et al.*[52] for the space charge layer and by Serre and Ghazali[12] and others for compensated materials. We do not discuss here the reasons for these discrepancies, but simply note that the Lanyon and Tuft expression for impurity interaction shift can not be used generally for all semiconductors.

The expression derived by Berggren and Sernelius[13] using Thomas–Fermi screening is free from these difficulties. Thomas–Fermi screening is known to be accurate in the heavy doping regime for the majority band[7]. This expression can also be written in the reduced form as:

$$\frac{\Delta E_{i(maj)}}{R} = \frac{1.57}{N_b r_s^{3/2}} \quad (10)$$

applicable to all semiconductors.

#### 2.5. Impurity interaction energy shift, minority band

We make use of the result proved by Serre and Ghazali and by Berggren and Sernelius that the shift of the majority and minority band edges into the gap due to impurity interaction divided by their effective masses are equal[12,13]. The corresponding

expression for the minority band can therefore be written as:

$$\frac{\Delta E_{i(mino)}}{R} = \frac{R_{(mino)}}{R} \frac{1.57}{N_b r_s^{3/2}} \quad (11)$$

where  $R$  is the Rydberg energy for the minority carrier band. Following Berggren and Sernelius, we use the average of the heavy hole and the light hole masses in calculating the  $R_{(mino)}$  in  $n$  type semiconductors [only for the purpose of calculating  $\Delta E_{i(mino)}$ ]. We emphasize again that the shifts of the minority band are in the opposite direction though we have not included explicitly the negative sign in these shifts; numerically they are to be added to the shifts of the majority band to obtain the BGN values.

The discrepancy in the values of  $\Delta E_{i(maj)} + \Delta E_{i(mino)}$  calculated using eqns (10) and (11) and by RPA[13] is 8 meV at  $10^{20} \text{ cm}^{-3}$ . Though this is larger than the discrepancy in the values of exchange and correlation energies discussed earlier, it is still small; it causes an overall error in the value of BGN less than 3%.

By substituting the values of various shifts from eqns (7) and (9)–(11) in eqn (5), we obtain the following simple expression for the BGN applicable to all semiconductors

$$\frac{\Delta E_g}{R} = 1.83 \frac{\Lambda}{N_b^{1/3} r_s} + \frac{0.95}{r_s^{3/4}} + \left[ 1 + \frac{R_{(mino)}}{R} \right] \frac{1.57}{N_b r_s^{3/2}} \quad (12)$$

This is the final expression we use in the next section for calculating the band gap narrowing of  $n$  and  $p$  type Si, Ge and GaAs. Note that from now on we use no adjustable parameter in going from one semiconductor to another and calculating their BGN values. We use only the known values of the parameters with  $N_b = 2$  for all  $p$  semiconductors.

### 3. BGN OF $n$ AND $p$ TYPE Si, Ge AND GaAs

#### 3.1. Values of parameters

Using eqn (12), the BGN can be calculated for any semiconductor provided the values of the required parameters for the semiconductor are known. We give below in Table 2 the parameters used in our calculations.

The values of electron and hole masses and dielectric constant for Si and Ge are given in Refs[11] and[13], and for GaAs in Refs[15] and[16]. The anisotropy corrections are discussed in Refs[11] and[13] and we have calculated this correction, quoted in the table, approximately. We have found the correction small and negligible in Si, a result in agreement with Berggren and Sernelius. The correction due to exchange interactions for  $p$  type semiconductors is discussed in Ref[7]. The values of  $R$  and  $a$  are calculated using eqns (1) and (4). Note that  $R$  without any subscript is for the majority band. Using these values, we calculate the numerical values of the prefactors in eqn (12) for different semiconductors

Table 2. Values of the parameters used in the calculations for the BGN for different semiconductors. The symbol (\*) on the values of  $R_{(\text{min})}$  for  $n$  type semiconductors indicates that average of heavy and light hole masses have been used in this calculation[13]

	$n$ Si	$p$ Si	$n$ Ge	$p$ Ge	$n$ GaAs	$p$ GaAs
$\epsilon$	11.4	11.4	15.4	15.4	13.0	13.0
$m_e$	0.33	0.33	0.22	0.22	0.0665	0.0665
$m_h$	0.59	0.59	0.36	0.36	0.47	0.47
$N_b$	6	2	4	2	1	2
$\Lambda$	1	0.75	0.84	0.75	1	0.75
$R$ (meV)	34.5	61.7	12.6	20.6	5.4	38.1
$R_{(\text{min})}$ (meV)	35.4*	34.5	11.2*	12.6	21.4*	5.4
$a$ (Å)	18.3	10.2	37.1	22.7	103.6	14.6

and obtain the equations for  $\text{BGN} = \Delta E_g$  given below.

For  $n$  Si:

$$\Delta E_g = 10.23 \left( \frac{N}{10^{18}} \right)^{1/3} + 13.12 \left( \frac{N}{10^{18}} \right)^{1/4} + 2.93 \left( \frac{N}{10^{18}} \right)^{1/2} \quad (13)$$

For  $p$  Si:

$$\Delta E_g = 11.07 \left( \frac{N}{10^{18}} \right)^{1/3} + 15.17 \left( \frac{N}{10^{18}} \right)^{1/4} + 5.07 \left( \frac{N}{10^{18}} \right)^{1/2} \quad (14)$$

For  $n$  Ge:

$$\Delta E_g = 8.67 \left( \frac{N}{10^{18}} \right)^{1/3} + 8.14 \left( \frac{N}{10^{18}} \right)^{1/4} + 4.31 \left( \frac{N}{10^{18}} \right)^{1/2} \quad (15)$$

For  $p$  Ge:

$$\Delta E_g = 8.21 \left( \frac{N}{10^{18}} \right)^{1/3} + 9.18 \left( \frac{N}{10^{18}} \right)^{1/4} + 5.77 \left( \frac{N}{10^{18}} \right)^{1/2} \quad (16)$$

For  $n$  GaAs:

$$\Delta E_g = 16.30 \left( \frac{N}{10^{18}} \right)^{1/3} + 7.47 \left( \frac{N}{10^{18}} \right)^{1/4} + 90.65 \left( \frac{N}{10^{18}} \right)^{1/2} \quad (17)$$

and for  $p$  GaAs:

$$\Delta E_g = 9.71 \left( \frac{N}{10^{18}} \right)^{1/3} + 12.19 \left( \frac{N}{10^{18}} \right)^{1/4} + 3.88 \left( \frac{N}{10^{18}} \right)^{1/2} \quad (18)$$

### 3.2. BGN in $n$ and $p$ Si

The values of BGN in  $n$  Si and  $p$  Si calculated using eqns (13) and (14) are shown in Figs 1 and 2 respectively. It is seen that the values of BGN in  $p$  Si are larger than those in  $n$  Si throughout the whole range of impurity concentration. The calculated values for  $N_D = 1 \times 10^{20} \text{ cm}^{-3}$  are 118 meV for  $n$  Si and 150 meV for  $p$  Si. We will see later that this yields a difference between  $p$  and  $n$  Si for apparent BGN which is consistent with available published data[47]. The BGN data for both  $n$  and  $p$  type silicon derived from luminescence measurements are also shown. Since luminescence measurements are made at 4.2 K, and in principle the high density theories are valid close to 0 K, comparison of luminescence data with the calculated values is very appropriate. The agreement between theory and experiment is good except

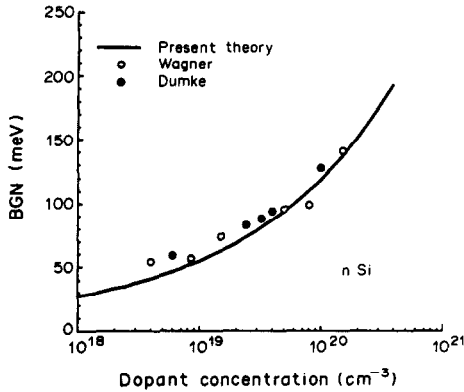


Fig. 1. Values of BGN in  $n$  Si calculated using eqn (13) are compared with the experimental luminescence values taken from the papers of Wagner and del Alamo[20] and of Dumke[35].

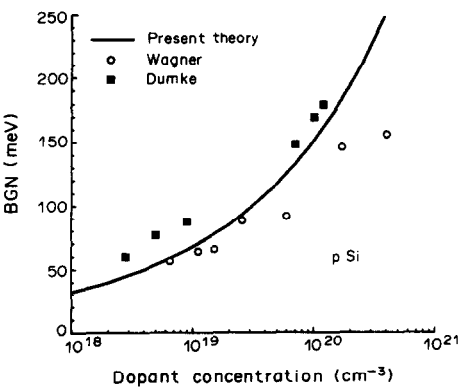


Fig. 2. The values of BGN in  $p$  Si calculated using eqn (14) are compared with the experimental luminescence values taken from the papers of Wagner and del Alamo[20] and of Dumke[34].

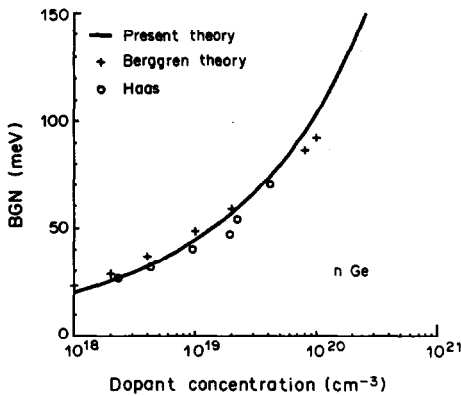


Fig. 3. The values of BGN for *n* Ge calculated using eqn (15) are compared with the results obtained by Berggren and Sernelius[13] and with the experimental values obtained by Haas[1] from optical absorption measurements.

for the *p* Si data of Wagner at very high dopings. In his earlier paper (Wagner 1984, quoted in Ref.[20]), Wagner had determined values of BGN from the low energy cut off of the luminescence peak. The BGN values determined in this manner were higher; and at high dopings, the values determined by this method are in better agreement with theory for *p* Si.

Our values for *n* Si are about 10 meV smaller than the theoretical values of Berggren and Sernelius[13]. Their theory is very sophisticated and it is very gratifying that the agreement between their results and our results is quite satisfactory. We are not aware of any theoretical values of BGN for *p* Si in the recent literature.

### 3.3. BGN in *n* and *p* type Ge

The BGN values calculated using eqn (15) for *n* Ge and eqn (16) for *p* Ge are displayed in Figs 3 and 4 respectively. The band gap narrowing values derived from optical absorption measurements by Haas[1] are also shown and are in good agreement. The theoretical values of Berggren and Sernelius[13] and our values are also in good agreement. We could not find

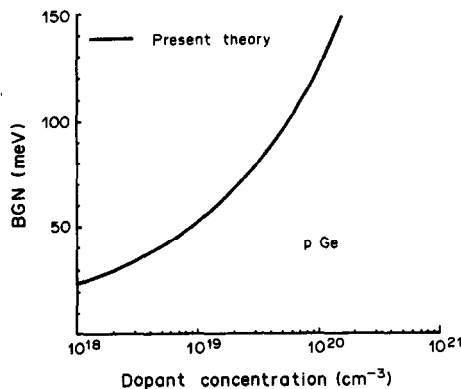


Fig. 4. The values of BGN in *p* Ge calculated using eqn (16) are displayed in the figure. We are not aware of any other BGN values for this material with which we could compare our results.

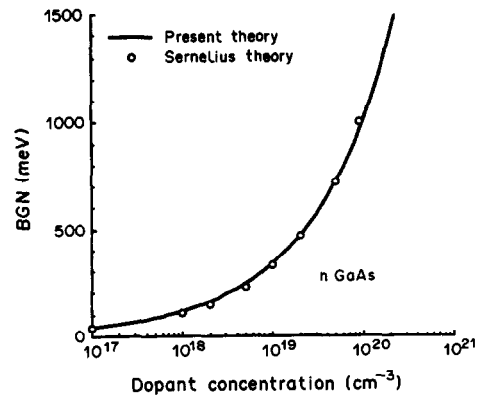


Fig. 5. The BGN values of *n* GaAs calculated using eqn (17) are shown and compared with the values of Sernelius[15]. Though the values are surprisingly very high, Sernelius has shown that the values are in reasonable agreement with the limited luminescence data available for this semiconductor.

any theoretical or experimental values of BGN for *p* Ge for comparison with our values. The calculated values of BGN for  $N = 1 \times 10^{20} \text{ cm}^{-3}$  are 125 meV for *p* Ge and 102 meV *n* Ge. As in the case of Si, the values for *p* Ge are higher than the values for *n* Ge. The values for Ge are lower than the value for Si mostly because of the larger dielectric constant of Ge. We found that BGN values are not sensitive to small changes in the values of effective masses; they are more sensitive to the values of dielectric constant. The exchange term in the BGN is independent of the effective mass, the correlation term increases as the  $1/4$  power of the mass and the impurity term for the majority band decreases as  $-1/2$  power of the mass; the two effects are small and partly cancel each other.

### 3.4. BGN in *n* and *p* type GaAs

Finally we display the calculated values of *n* and *p* type GaAs in Figs 5 and 6. The values of BGN in

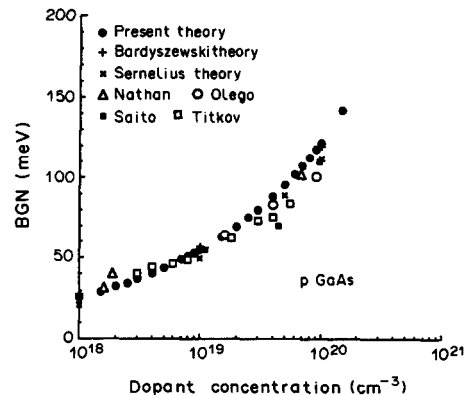


Fig. 6. The BGN values for *p* GaAs calculated using eqn (18) are shown and compared with other theoretical and experimental values. The theoretical values are from the papers of Sernelius[16] and Bardyszewski and Yevik[17]. The experimental values are from the luminescence measurements of Nathan *et al.*[41], Olego and Cardona[43], Saito *et al.*[40] and Titkov *et al.*[42].

$n$  GaAs are startlingly high, a result of very low electron mass and single conduction band valley as shown in Table 2. The values at  $N = 1 \times 10^{20} \text{ cm}^{-3}$  is 1006 meV! The values calculated by Sernelius[16] are also shown. The agreement between his results and our theory is excellent; it is within the error involved in reading his values from the figure. Sernelius has shown that the results of his theory are in reasonable agreement with the available luminescence data. At  $N_D > 10^{19} \text{ cm}^{-3}$ ,  $E_F$  comes close to the  $L$  and  $X$  sub-bands and this causes further complications in the calculations of BGN. It is possible that in this high doping range the results in Fig. 5 are not reliable. Recent experiments of Yao and Compaan[53] suggest that observed BGN in  $n$  GaAs is considerably lower than that given in Fig. 5 at  $N_D = 10^{19} \text{ cm}^{-3}$ .

The calculated values of BGN for  $p$  GaAs using eqn (18) are in good agreement with the theoretical results of Sernelius[6] and of Bardyszewski and Yevick[17], also shown in Fig. 6. We have shown the values of these authors only at a few values of doping to avoid crowding of data points and curves in the figure. The BGN values derived from the luminescence data of Nathan *et al.*[41], Olego and Cardona[43], Saito *et al.*[40] and Titkov *et al.*[42] are also shown. Except for one or two data points, the agreement is very satisfactory. The BGN for  $N = 1 \times 10^{20} \text{ cm}^{-3}$  in  $p$  GaAs is 122 meV.

#### 4. APPARENT BAND GAP NARROWING

As we mentioned earlier, comparison of BGN with luminescence measurements made at low temperatures is straightforward. The determination of apparent BGN at 300 K however requires knowledge of the Fermi level and effect of temperature on BGN. We first discuss the method by which we determine the Fermi level, calculate the so called "Fermi Dirac correction" and convert BGN to apparent BGN. We then discuss briefly the possible magnitude of the temperature correction which should be applied to BGN. Finally we give the calculated values of apparent BGN for  $p$  and  $n$  Si and  $p$  GaAs and compare them with the corresponding experimental values of apparent BGN.

##### 4.1. Fermi Dirac correction and determination of apparent BGN

In the low doping regime, the product of the concentration of electrons and holes, the so called  $pn$  product, remains constant and is given by:

$$pn = n_{i0}^2 \quad (19)$$

where  $n_{i0}$  is the intrinsic carrier concentration in the semiconductor. This relation implies that the minority carrier concentration is suppressed by the same factor by which the majority carrier concentration increases on doping the crystal. When the doping is high, the band gap is reduced and the value

of  $n_{i0}$  increases to a larger value  $n_{ie}$  and becomes dependent on the doping concentration  $N$ . At higher doping concentrations, Fermi Dirac statistics shows that the Fermi level rises rapidly in the majority band and the minority concentration is suppressed by a larger amount reducing somewhat the enhancement of  $n_{i0}$  due to BGN. Taking into account the effect of reduction of band gap and of the Fermi Dirac statistics, the final result for the  $pn$  product can be written as[45]:

$$pn = n_{i0}^2 \exp\left(\frac{\Delta E_g}{kT}\right) \exp\left(\frac{-E_F}{kT}\right) F_{1/2}\left(\frac{E_F}{kT}\right). \quad (20)$$

Equation (20) can be written as:

$$pn = n_{i0}^2 \exp\left(\frac{\Delta E_g^a}{kT}\right) = n_{ie}^2 \quad (21)$$

with

$$\Delta E_g^a = \Delta E_g + \Delta E^{FD} \quad (22)$$

and

$$\Delta E^{FD} = kT \ln \left[ \exp\left(\frac{-E_F}{kT}\right) F_{1/2}\left(\frac{E_F}{kT}\right) \right] \quad (23)$$

and where  $n_{ie}^2(N)$  is the effective value of  $n_{i0}^2$  (it is the actual  $pn$  product at any doping level  $N$ ),  $\Delta E_g^a$  is the apparent or effective band gap narrowing (apparent BGN) and  $\Delta E^{FD}$  is the Fermi Dirac correction. The Fermi Dirac correction is always negative and apparent BGN is always smaller than BGN. Apparent BGN =  $\Delta E_g^a$  is very convenient in describing minority carrier transport in devices and developing computer codes. The values of Fermi Dirac correction  $\Delta E^{FD}$  calculated using eqn (23) at room temperature are shown in Fig. 7 for different values of Fermi level. The correction is very large for large values of Fermi level, i.e. at large doping concentrations. To calculate and apply this correction to BGN, we still need the values of Fermi level at room temperature as a function of doping concentration.

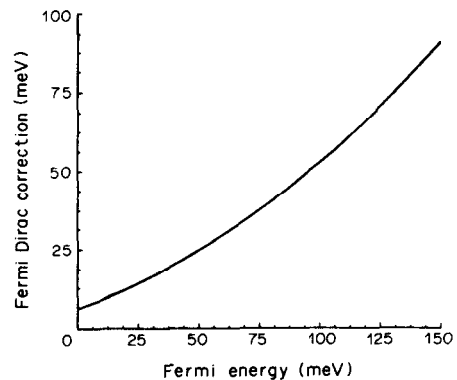


Fig. 7. The Fermi Dirac correction as a function of values of Fermi energy calculated at room temperature using eqn (23).



We have seen in Section 2 that for  $p$  semiconductors the Fermi level cannot be calculated by using eqn (8) and the conventional value of the density of states. If we use the calculated Fermi level, the error caused in apparent BGN can be up to 30–50 meV at high doping concentrations and the predicted values of apparent BGN become too low compared to the experimental values.

#### 4.2. Determination of Fermi level in $p$ semiconductors

Dumke[34,35] and Olego and Cardona[43] have shown that accurate values of Fermi level can be obtained from the low temperature measurements of luminescence in heavily doped Si and GaAs. Using the method suggested by these authors we have determined the values of Fermi level in  $p$  Si and  $p$  GaAs from the luminescence data at low temperatures and converted the Fermi levels to room temperature assuming that the effective density of states, though modified due to heavy doping (see Section 2), still varies at  $T^{1.5}$ . The error involved in this procedure for converting the Fermi level from low temperature to room temperature is not known; it will be negligible if the band is still approximately parabolic with a new higher value of effective density of states. We have used the luminescence data of Refs [30,37,38,39,40 and 41] for heavily doped  $p$  GaAs and Refs[20,35,36 and 53] for heavily doped  $p$  Si for this purpose. The values of Fermi level determined in this manner are shown in Fig. 8 for  $p$  Si, and in Fig. 9 for  $p$  GaAs. Values of Fermi level calculated by the conventional procedure, i.e. by using eqn (8) at a few doping concentrations are also shown for comparison. All values shown in Figs 7–9 are at room temperature.

The reduction in Fermi level implies that in  $p$  type semiconductors the rigid band model on which our theory is based becomes poor at high doping concentrations. The distortion does not seem to affect the

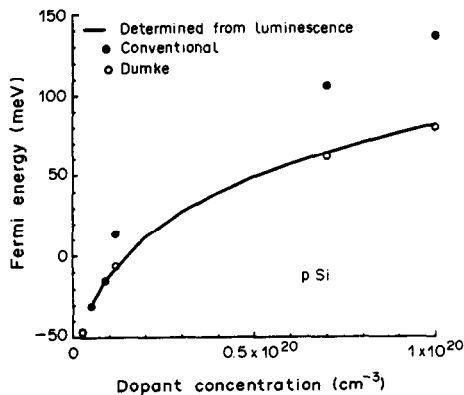


Fig. 8. Fermi energies (measured from the valence band edge) of heavily doped  $p$  Si determined from the luminescence measurements are displayed. Values quoted by Dumke[34] from his luminescence measurements are also given. Values calculated using eqn (8) at a few values of doping concentrations, designated as conventional, are shown for comparison.

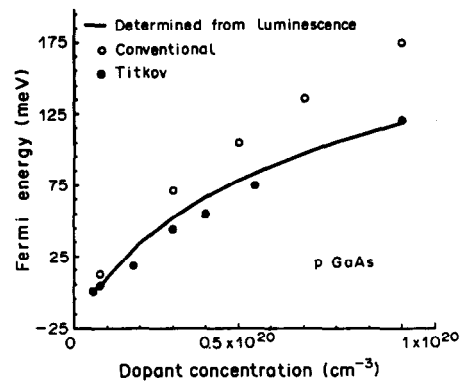


Fig. 9. Fermi energies (measured from the valence band edge) of heavily doped  $p$  GaAs determined from the luminescence measurements are displayed. Values quoted by Titkov *et al.*[42] derived from his luminescence measurements are also given. Values calculated using eqn (8) at a few values of doping concentrations, designated as conventional, are shown for comparison.

BGN but affects  $E_F$  and apparent BGN considerably. Pending an *ab initio* calculation of the band structure of heavily doped  $p$  semiconductors, it is best to use observed  $E_F$  for determining apparent BGN.

#### 4.3. Temperature correction

We face yet another difficulty in calculating the apparent BGN which can be compared with device measurements. The high density theories that we have used are strictly valid only at very low temperatures. Since the device measurements are normally made at room temperature, we need the value of BGN at room temperature. As we mentioned earlier, several authors[20,22] have attempted to determine the difference in BGN at low and at room temperatures. Since calculations at room temperature are involved and the difference being calculated is small, reliable values of the temperature correction can not be obtained. We will use a value between 0 and 20 meV for this correction[20,22]. We will adopt the following procedure. After applying the Fermi Dirac correction to BGN to obtain apparent BGN, we will increase the value of the apparent BGN at  $N = 1 \times 10^{20} \text{ cm}^{-3}$  in Si and at the highest doping used in the experiment in  $p$  GaAs by adding a small quantity up to 20 meV to bring it in agreement with the experimental value. We choose these doping concentrations because our theory is expected to be most accurate at the highest doping concentrations. The correction is constant at all doping concentrations, i.e. the curve as a whole is shifted upwards by this small amount. After applying this correction if we find that the fit of the whole experimental data (i.e. including the lower dopings) with the theory is satisfactory, the theory should be regarded as adequate for calculating apparent BGN and for interpreting device experiments.

#### 4.4. Apparent BGN in $p$ GaAs and in $n$ and $p$ Si

The calculation of apparent BGN is now straightforward. (We will not discuss  $n$  and  $p$  Ge and  $n$  GaAs

in this section because of lack of interest in these materials for devices. No experimental data on apparent BGN exists for these materials.) For every doping concentration, the Fermi level is first determined from Figs 8 and 9 for  $p$  Si and  $p$  GaAs and calculated using eqn (8) (with  $N_V$  replaced by  $N_C$ ), for  $n$  Si. The corresponding Fermi Dirac correction is then read from Fig. 7. Apparent BGN is now calculated using eqns (22) and (23). As explained earlier, a small constant temperature correction up to 20 meV is added to the calculated values of apparent BGN so as to bring the data at the highest concentration in agreement with the observed value at this concentration. The agreement of theory and experimental data at other doping concentrations is then examined. The results for  $p$  GaAs,  $p$  Si and  $n$  Si are shown in Figs 10–12. The three cases are briefly discussed below.

For  $p$  GaAs, a temperature correction of 12 meV is added to the calculated values of apparent BGN before they are plotted in Fig. 10. The theoretical results of Bennett and Lowney[14] are also shown. It is seen that the agreement of our theory with the data of Lundstrom and co-workers is quite satisfactory. The reason for the large discrepancy between the data of Tiwari *et al.* and Lundstrom *et al.* is not clear (we have not shown some of the data of Tiwari *et al.* at larger dopings which has very high values). The theoretical values support strongly the experimental data of Lundstrom *et al.* Lundstrom's data should be reliable since it has been taken by him and his different co-workers over the last 4 or 5 yr. The scatter seen in the data is inherent in such measurements. The thin solid straight line is the numerical fit given by:

$$\text{BGN}(\text{meV}) = 8.6 \ln \frac{N_A}{1.13 \times 10^{16}}.$$

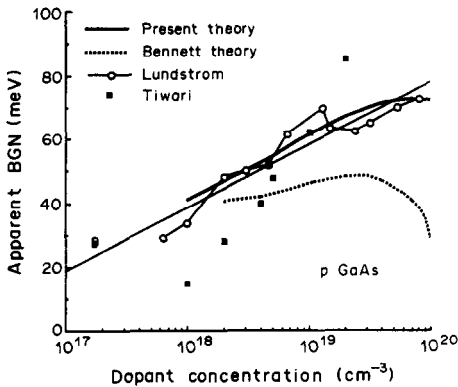


Fig. 10. The calculated and experimental values of apparent BGN in heavily doped  $p$  type GaAs are shown. The result of our theory agrees closely with the experimental values of Lundstrom coworkers[24,26,29]. The values of Tiwari and Wright[30] appear to be too high for larger doping concentrations. The theoretical results of Bennett and Lowney[24] are also given for comparison. The best log numerical fit to the data is shown by the straight line plot.

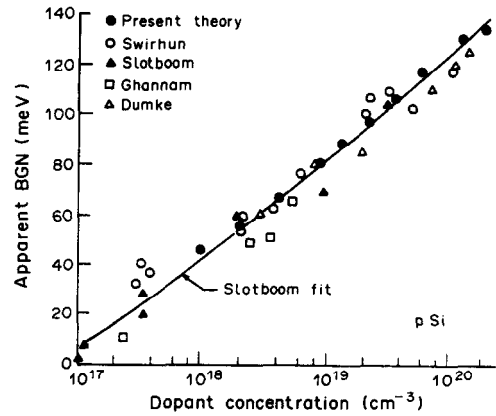


Fig. 11. The calculated and experimental values of apparent BGN in heavily doped  $p$  type Si are shown. The solid circles calculated using the simple expression derived in this paper agree closely with the Slotboom fit extended to higher dopings by Dumke[34] and by Swirhun *et al.*[47] and with all the experimental data. The experimental data are taken from Refs[34] and[47].

The result of our theory for  $p$  Si, including a temperature correction of 17 meV, are given in Fig. 11. We have shown the experimental data of Slotboom, of Ghanam and of Swirhun *et al.* taken from Ref.[45] and of Dumke and Tang from Ref.[32] (Tang's data is quoted only at low doping concentrations to avoid crowding of the figure, at high doping concentrations, it agrees with Dumke's values). Our calculated results are in very good agreement with all the experimental data and in almost exact agreement with the Slotboom fit extended by Dumke[35] and Swirhun *et al.*[47] to higher concentrations.

The case of  $n$  Si shown in Fig. 12 is less satisfactory. Here we found an optimum temperature correction to be rather small, about 5 meV. The spread in

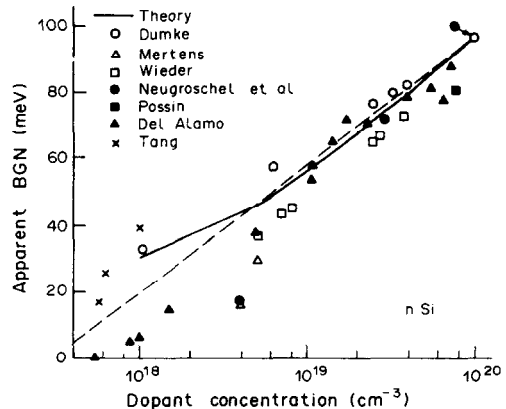


Fig. 12. The calculated and experimental values of apparent BGN in heavily doped  $n$  type silicon are shown. The data of Tang and of Dumke are taken from Ref.[35] and the remaining data from Ref.[21]. The curve based on our theory agrees well with the experimental data at higher dopings. There is a large discrepancy in the data obtained by different workers at lower doping concentrations.

the experimental data points is much larger than in the case of *p* Si. At low concentrations it is as much as 30 meV. The results of our theory agree with the experimental data at high doping concentration. A comparison of Figs 11 and 12 shows that apparent BGN of *n* Si is significantly smaller than the BGN in *p* Si. The results of the theory of Berggren and Sernelius[13], which is probably the most complete theory at present, are even higher than our results. It is suggested that fresh measurements of apparent BGN at low doping concentrations should be made in *n* Si.

The discrepancy between theoretical and experimental values of  $E_F$  for *p* semiconductor suggests that all interactions have not been properly taken into account in calculating the BGN in the rigid parabolic band approximation for *p* semiconductors. In view of this the fitted curves in Figs 10 and 11 should not be regarded as being theoretical in the strict sense. They are useful however in interpreting experiments and designing devices.

#### 4.5. A method to predict the BGN and apparent BGN of semiconductors at low doping concentrations

A numerical fit shows that in the high density limit BGN can be represented by:

$$\text{BGN} = \text{constant } N^{1/3} \quad (24)$$

quite accurately. Many authors observed that the experimental data can be fitted quite accurately by this law and this led to the belief that the exchange energy shift, eqn (7), is the sole cause of the BGN. The  $N^{1/3}$  law has no physical meaning, it is the result of the fact that the many-body shifts increase sub-linearly with  $N^{1/3}$  and the impurity interaction shifts super-linearly; when added together, they vary linearly with  $N^{1/3}$  to a very good approximation. The high density theories predict that BGN goes to zero slowly as  $N$  goes to zero but experiments show that BGN decreases rapidly at lower concentrations and becomes zero at about  $1 \times 10^{16}$ – $3 \times 10^{17} \text{ cm}^{-3}$ . The high density theories break down at doping concentrations of  $1 \times 10^{18} \text{ cm}^{-3}$  or lower. At these concentrations they give much higher values of BGN and apparent BGN.

An examination of Figs 10–12 shows that at high doping concentrations, apparent BGN can be fitted with a logarithmic law, similar to that of a Slotboom fit, to a good approximation. Note however that at very high doping concentrations, the apparent BGN plot starts curving down, see Fig. 10 for *p* GaAs. If we avoid this region of very high concentrations, fit a  $\log(N)$  law and extrapolate it to lower doping concentrations, we can get approximately the apparent BGN (or BGN, since the apparent and real physical BGN approach one another at low dopings where non-degenerate statistics apply) at lower doping concentrations. This seems to be the case at least for the three semiconductors considered in Figs 10–12. The  $\log(N)$  law has no physical meaning

and will not hold if higher concentrations are included in the plot.

#### 5. BGN IN HEAVILY DOPED $\text{Ge}_x\text{Si}_{1-x}$ ALLOYS AND STRAINED LAYERS

Heavily doped *p*  $\text{Ge}_x\text{Si}_{1-x}$  strained layers have become very important for applications in Double Heterostructure Bipolar Transistors[54]. For high Ge fractions, the critical thickness of the strained layers is small and two dimensional effects become important. We are interested however, in thicker layers for  $x < 0.3$ , which are important for heterostructure transistors and in which the density of state function is still three dimensional. We use eqn (12) to calculate the BGN and apparent BGN of  $\text{Ge}_x\text{Si}_{1-x}$  alloys and strained layers. For  $x < 0.3$ , the conduction band of the alloy is Si like [55], and the value of  $m_c$  is the same as for Si, i.e. 0.33. For  $m_h$  and  $\epsilon$  we use a linear interpolation:  $m_h(x) = 0.59(1 - 0.41x)$  and  $\epsilon(x) = 11.4(1 + 0.35x)$  between the values for Si and Ge.

For  $x < 0.3$ , we can expand the coefficients in eqn (12) in powers of  $x$  and obtain a simple expression for the BGN of the *p* type  $\text{Ge}_x\text{Si}_{1-x}$  alloy:

$$\begin{aligned} \Delta E_g(x) = & 11.07(1 - 0.35x) \left( \frac{N}{10^{18}} \right)^{1/3} \\ & + 15.17(1 - 0.54x) \left( \frac{N}{10^{18}} \right)^{1/4} \\ & + 5.07(1 + 0.18x) \left( \frac{N}{10^{18}} \right)^{1/2} \quad (25) \end{aligned}$$

The maximum error in BGN due to neglecting higher powers of  $x$  in eqn (12) is about 2.5% at  $x = 0.3$ . As  $x$  decreases, the error decreases rapidly and becomes negligible for  $x < 0.25$ . Expression (25) reduces to that applicable to *p* Si for  $x = 0$ . The values calculated using this equation are compared with the *p* Si values in Table 3 for  $x = 0.3$ . We can use the same procedure for *n* type alloys. The values for strained layers[56] are discussed next.

The effect of strain in the  $\text{Ge}_x\text{Si}_{1-x}$  layers grown on (100)-Si is to split the six conduction minima into four lower valleys and two upper valleys; and to split the heavy hole and the light hole edges such that the heavy hole band moves into the gap and the light hole band moves away from the gap of the unperturbed crystal. The splitting of the valence band edges weakens considerably the coupling between the heavy hole and the light hole bands and reduces the value of  $N_b$  and increases the value of BGN. When the

Table 3. Values for  $\text{BGN} = \Delta E_g$  in meV for *p* Si and *p*  $\text{Ge}_{0.3}\text{Si}_{0.7}$  bulk alloy and strained layers for three values of doping concentration,  $N$

	$N = 1 \times 10^{18} \text{ cm}^{-3}$	$N = 1 \times 10^{19} \text{ cm}^{-3}$	$N = 1 \times 10^{20} \text{ cm}^{-3}$
<i>p</i> $\text{Ge}_{0.3}\text{Si}_{0.7}$	28	61	140
<i>p</i> Si	31	67	150
<i>p</i> $\text{Ge}_{0.3}\text{Si}_{0.7}$	31	69	162
Strained layers			

separation between the two valence bands becomes large, the value of  $N_b$  becomes unity. People[55] has calculated the energy separation of the two bands as a function of  $x$ . For  $x = 0.3$ , the separation is roughly 60 meV. At this value of separation the interaction between the two bands cannot be neglected completely. We suggest that a somewhat reduced effective value of  $N_b$ , say 1.5, may be used for the strained layers of  $p$  type alloy in eqn (12). There is some experimental evidence that this value is reasonable. Jain *et al.*[57] have analyzed the low temperature luminescence spectra of B and P doped Si in two different types of specimens. In one case, the samples were conventional bulk doped crystals; in the other they were MBE doped layers grown on pure (100) Si. Since lattice constants of doped layers are smaller than those of the pure Si substrate, the MBE Si:B layers are under bi-axial tensile strain. Jain *et al.*[57] were able to explain the observed shift in the luminescence spectra by assuming a weakening of the coupling between the two valence bands in the case of the B doped Si MBE layers which is equivalent to reducing  $N_b$  in our formulation. We assume that other parameters in eqn (12) are not affected by the strain. The calculated values of the BGN in the  $\text{Ge}_x\text{Si}_{1-x}$  strained layers using the reduced values of  $N_b$  in eqn (14) and for  $x = 0.3$  are shown in Table 3. It is seen that the values are considerably enhanced on straining the alloy layer. In fact they are now slightly larger than the values for  $p$  Si at  $1 \times 10^{20} \text{ cm}^{-3}$  doping.

The structure of the conduction band of the  $n$  type  $\text{Ge}_x\text{Si}_{1-x}$  strained layers is simple[55] and in this case it is easier to assign a value to  $N_b$  in the strained layers. For sufficiently large strain, it is 4 for layers under compression and 2 for layers under tensile strain[55]. The BGN can be calculated quite easily using the above method and taking  $N_b$  equal to 4 or 2 as the case may be[see also 56]. For small values of strain, the carriers are present in the lower as well as the upper bands. The distribution of carriers in the lower bands and the upper bands must be calculated first; the BGN of each band can then be calculated depending on the relative concentration of carriers in each band.

As we saw earlier, a precise knowledge of the Fermi level is required to convert BGN into apparent BGN which, for the alloys and the strained layers, is not available. We note however that reducing the value of  $N_b$  will increase the value of the Fermi level and of the Fermi Dirac correction. This reduces the value of apparent BGN by a larger amount in the strained layers. The value of apparent BGN becomes very close to that for  $p$  Si. At the present time, it is therefore best to use Slotboom's  $p$  Si values of apparent BGN for  $p$  type  $\text{GeSi}$  strained layers also for small Ge fractions. Note however that the BGN of  $p \text{ Ge}_x\text{Si}_{1-x}$  bulk alloys is significantly different from that of  $p$  Si. Also the BGN values in  $n$  type  $\text{Ge}_x\text{Si}_{1-x}$  alloys and  $n$  type  $\text{Ge}_x\text{Si}_{1-x}$  strained layers are very different[56].

## 6. SIMPLE EXPRESSIONS FOR APPARENT BGN FOR USE IN COMPUTER SIMULATION

We give below the fitted expressions for apparent BGN which represent best the experimental data and are consistent with the theory at this time. It is best to represent the apparent BGN in the form originally given by Slotboom and De Graaf[48] for  $p$  Si:

apparent BGN (meV)

$$= K_1 \left\{ \ln \frac{N}{K_2} + \left[ \left( \ln \frac{N}{K_2} \right)^2 \right] + 0.5 \right\}^{1/2} \quad (26)$$

where  $N$  is the  $p$  or  $n$  type dopant concentration in  $\text{cm}^{-3}$ .

For  $p$  Si and for  $p \text{ Ge}_x\text{Si}_{1-x}$  strained layers up to  $x = 0.3$ , Slotboom–Dumke–Swirhun fit:

$$K_1 = 9.0 \text{ and } K_2 = 10^{17} \text{ cm}^{-3}. \quad (27a)$$

For  $n$  Si, the present work:

$$K_1 = 8.5 \text{ and } K_2 = 3.5 \times 10^{17} \text{ cm}^{-3}. \quad (27b)$$

For  $p$  GaAs, the present work and Ref.[24]:

$$K_1 = 4.5 \text{ and } K_2 = 1.7 \times 10^{16} \text{ cm}^{-3}. \quad (28)$$

Equations (27a) and (27b) are valid up to  $N = 1 \times 10^{20} \text{ cm}^{-3}$  and eqn (28), up to  $N_A = 7 \times 10^{19} \text{ cm}^{-3}$ . At higher concentrations, apparent BGN starts decreasing with the increase of  $N$ .

## 7. FINAL REMARKS AND SUMMARY OF IMPORTANT RESULTS

(1) We have given a simple expression to calculate the BGN for all semiconductors. For simple isotropic bands, this equation is universal and needs the knowledge only of the effective Rydberg  $R$  and effective Bohr radius  $a$  for the semiconductor whose BGN is to be calculated.

(2) For real semiconductors, corrections due to multi-bands, due to anisotropy of the bands and due to interaction between the bands are introduced. For  $n$  type semiconductors, the expressions do not need any further modification. However, the structure of the valence band is more complex and it is found necessary to model it with two equivalent bands in the valence bands. Strong experimental and theoretical evidence to support this suggestion is given.

(3) For  $n$  Si,  $n$  Ge and  $n$  and  $p$  GaAs, the BGN calculated using this expression is in excellent agreement with the BGN calculated by other authors using more complicated procedure. For  $p$  Si and  $p$  Ge ours are the first theoretical calculations of BGN.

(4) The theoretical values predicted by this expression are in very good agreement with the experimental values of BGN derived from luminescence measurements for all semiconductors considered except  $p$  Ge for which we did not find any experimental data.

(5) We have found that the observed Fermi levels for  $p$  Si and for  $p$  GaAs are considerably

smaller than those calculated using the known value of density of states. Using the observed values of Fermi levels for *p* semiconductors and temperature corrections of up to 20 meV, the calculated values of apparent BGN for *p* semiconductors are in very good agreement with the results of device measurements. For *n* Si the agreement is very good at higher dopings. At lower doping concentrations, the scatter in the experimental values is very large.

(6) A new interesting paper has recently appeared on the temperature variation of effective masses in Si by Green[58]. After a very careful analysis, Green came to the conclusion that the effective mass of holes at low temperatures has the conventional value similar to what we have used, but it increases more rapidly with temperature than is implied in the work of Barber[33]. We have shown that the observed Fermi level at low temperatures requires that the value of the effective density of states be increased. Since the careful work of Green shows that the effective mass cannot be changed at low temperatures, his work further supports our introduction of the factor  $N_b$  in eqn (12).

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