



# **New dielectric constant, due to the impurity size effect, and determined by an effective Bohr model, affecting strongly the Mott criterion in the metal-insulator transition and the optical band gap in degenerate (Si, GaAs, InP)-semiconductors**

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## **Abstract**

In the n(p)-type degenerate semiconductors, our expression for the relative static dielectric constant,  $\epsilon(r_{d(a)})$ , is determined by an effective Bohr model,  $r_{d(a)}$  being the donor (acceptor) d(a)-radius, suggesting that, for an increasing  $r_{d(a)}$ , both  $\epsilon(r_{d(a)})$  and the effective Bohr radius  $a_B(r_{d(a)})$ , due to such the impurity size effect, decrease ( $\searrow$ ), according to the increase ( $\nearrow$ ) in:

(i) the effective d(a)-ionization energy  $E_{d(a)}(r_{d(a)})$  in absolute values,

(ii) the effective band gap  $E_{gn(gp)}(r_{d(a)})$ , and also

(iii) the critical density  $N_{CDn(CDp)}(r_{d(a)}, 0.25 \leq y \leq 1)$  in the MIT,

as those showed in Tables 2-4, for the n(p)-type (Si, GaAs, InP)-semiconductors, in which the empirical parameter  $y$  has been chosen as:  $y=0.25$  and  $0.271$ . One notes here that  $y=0.25$  was given

in the Mott criterion:  $a_B \times N_{CD}^{1/3} \approx y = 0.25$ . Further, if denoting the d(a)-density by  $N$ , the physical condition given for such degenerate semiconductors (or for the metallic phase) is found to be given by:  $N \geq N_{CDn(CDp)}$ . Then, in such the important physical condition, our numerical results of optical band gap (OBG), due to the effects of impurity size and heavy doping, are also investigated and given in Tables 6-8.

In summary, our new expression for  $\epsilon(r_{d(a)})$ , due to such an impurity size effect, strongly affects  $a_B(r_{d(a)})$ ,  $N_{CDn(CDp)}(r_{d(a)}, y)$ , and the OBG, obtained in the n(p)-type (Si, GaAs, InP)- degenerate semiconductors.

**Keywords:** effects of impurity size and heavy doping; degenerate semiconductors; static dielectric constant; critical density in metal-insulator transition; optical band gap

## 1. Introduction

In the present paper, using an effective Bohr model given in the n(p)-type semiconductors, we determine the relative static dielectric constant  $\epsilon(r_{d(a)})$ , expressed as a function of the donor (acceptor) d(a)-radius, accordingg thus to the impurity effect. As showed in Tables (2-4, 6-8), this function  $\epsilon(r_{d(a)})$  strongly affects the numerical results, obtained for: (i) the effective Bohr radius  $a_B(r_{d(a)})$ , (ii) the effective d(a)-ionization energy  $E_{d(a)}(r_{d(a)})$  in absolutes values, (iii) the effective band gap  $E_{gn(gp)}(r_{d(a)})$ , (iv) the critical density  $N_{CDn(CDp)}(r_{d(a)}, y = 0.25(0.271))$  in the metal-insulator transition (**MIT**), and finally (v) the optical band gap (**OBG**),  $E_{gn1(gp1)}(r_{d(a)}, N, y = 0.25(0.271))$ ,  $N$  being the d(a)-density [1-9]. It should be noted that:

- (i) the value:  $y=0.25$  was given in the Mott criterion [1] as:  $a_B \times N_{CD}^{1/3} \approx y = 0.25$ ,
- (ii) Pergament [2] used this Mott criterion to obtain, with  $a_B = 1.77$  nm, the value of  $N_{CD} = 2.8 \times 10^{18} \text{cm}^{-3}$  for vanadium dioxides  $\text{VO}_2$ , and
- (iii) Edwards and others [3] proposed  $y \geq 0.38$ , explaining the transition to the metallic state for Cs, Rb and H-elements.

In Section 2, the numerical results of energy-band-structure parameters, characteristic of the n(p)-type intrinsic (Si, GaAs, InP)-crystals [4, 8] will be presented in Table 1. Then, our expression for  $\epsilon(r_{d(a)})$  will be determined in Section 3. Therefore, in Section 4, our expressions for

$N_{\text{CDn(CDp)}}(r_{\text{d(a)}}, y)$  and the OBG will be investigated. Then, in Section 5, our numerical results, obtained for  $N_{\text{CDn(CDp)}}(r_{\text{d(a)}}, y = 0.25(0.271))$  and  $E_{\text{gn1(gp1)}}(r_{\text{d(a)}}, N, y = 0.25(0.271))$  will be presented, as those given in Tables (2-4, 6-8). Finally, some important concluding remarks will be given in Section 6.

## 2. Energy-band-structure parameters given in the n(p)-type (Si, GaAs, InP)-semiconductors

First of all, we present the values of the parameters, characteristic of the n(p)-type (Si, GaAs, InP)-semiconductors such as [4, 8]: the effective average numbers of equivalent conduction (valence)-band edge,  $g_{\text{c(v)}}$ , the relative static dielectric constant,  $\epsilon_0(r_{\text{do(ao)}}) \equiv \epsilon_0$ , the relative effective electron (hole) mass in conduction (valence) bands,  $(m_{\text{c(v)}}/m_0)$ ,  $m_0$  being the free electron mass, and the intrinsic band gap,  $E_{\text{go}}(r_{\text{do(ao)}})$ . Further, in those semiconductors, the Bohr radius respectively yields:

$$a_{\text{Bno(Bpo)}} \equiv \frac{\epsilon_0 \times \hbar^2}{(m_{\text{c(v)}}/m_0) \times e^2} = 0.53 \times 10^{-8} \text{ cm} \times \frac{\epsilon_0}{(m_{\text{c(v)}}/m_0)}, \quad (1)$$

the do(ao)-ionization energy is given by:

$$E_{\text{do(ao)}} \equiv \frac{e^4 \times m_{\text{c(v)}}}{2\epsilon_0^2 \times \hbar^2} = \frac{13600 \times (m_{\text{c(v)}}/m_0)}{\epsilon_0^2} \text{ meV}, \quad (2)$$

and for a do(ao)-volume  $V_{\text{do(ao)}} = (4\pi/3) \times (r_{\text{do(ao)}})^3$ , the isothermal bulk modulus is determined respectively for n(p)-type Si, GaAs, InP)-crystals, as:

$$B_{\text{n(p)}} \equiv \frac{E_{\text{do(ao)}}}{V_{\text{do(ao)}}}. \quad (3)$$

Furthermore, in the n(p)-type (Si, GaAs, and InP)-doped semiconductors, the critical density (CD) in the metal-insulator transition (MIT) was proposed by Mott [1], as:

$$N_{\text{CDno(CDpo)}}(r_{\text{do(ao)}}, y = 0.25) \equiv \left( \frac{y}{a_{\text{Bno(Bpo)}}} \right)^3 = 6.7168 \times 10^{24} \text{ cm}^{-3} \times \left( \frac{y \times (m_{\text{c(v)}}/m_0)}{\epsilon_0} \right)^3, \quad (4)$$

noting that the physical condition, used to define the MIT, can be found to be given by:

$$(\text{Insulator})N \leq N_{\text{CDno(CDpo)}}(r_{\text{do(ao)}}, y) \leq N \text{ (Metal or degenerate semiconductors)}, \text{ for } 0.25 \leq y < 1. \quad (5)$$

Then, the values of those parameters, characteristic of the n(p)-type (Si, GaAs, InP)-semiconductors are given in the following Table 1, from which we can choose the value of  $y$  so that

there is an agreement between our numerical results and the experimental ones. For example, in the n(p)-Si crystal, the best choice is  $y=0.271$ , according to such an agreement.

**Table 1.** The parameters, characteristic of the n(p)-type (Si, GaAs, InP)- semiconductors [4], and others are obtained, using Equations (1-4), for  $y = 0.25$  and  $0.271$ , suggesting that in the n(p)-type Si, the obtained values of  $N_{CDno(CDpo)}(r_{do(ao)}, y = 0.271) \cong 3 (4.44) \times 10^{18} \text{ cm}^{-3}$ , in good accordance with those given in literature. Here, its values for  $0.25 \leq y \leq 1$  are also given, for a coparison.

Semiconductors	Si	GaAs	InP
$\varepsilon_{c(v)}$ [4]	6 (2)	1 (1)	1 (1)
$r_{do(ao)}$ in nm [4]	$r_{do(ao)} \equiv r_{Si} = 0.117$	$r_{do(ao)} \equiv r_{As(Ga)} = 0.118 (0.126)$	$r_{do(ao)} \equiv r_{P(In)} = 0.110 (0.144)$
$\varepsilon_0$ [4]	$11.4 \pm 0.3$	$13.13 \pm 0.3$	$12.37 \pm 0.3$
$m_{c(v)}/m_0$	$0.3216 (0.3664)$ [8]	$0.066 (\frac{0.082+0.5}{2} = 0.291)$ [4]	$0.073 (\frac{0.078+0.4}{2} = 0.239)$ [4]
$E_{g0}$ in eV [4]	1.17	1.52	1.42
$a_{Bno(Bpo)}$ in nm	1.88 (1.65)	10.54 (2.39)	8.98 (2.74)
$E_{do(ao)}$ in meV	33.7 (38.3)	5.2 (23)	6.49 (21.24)
$B_{n(p)}$ in $10^8 (N/m^2)$	8.04 (9.16)	1.212 (4.389)	1.86 (2.72)
$N_{CDno(CDpo)}(r_{do(ao)}, y = 0.25)$ in $10^{16} \text{ cm}^{-3}$	235.63 (348.5)	1.33 (114.3)	2.16 (7.57)
$N_{CDno(CDpo)}(r_{do(ao)}, y = 0.271)$ in $10^{16} \text{ cm}^{-3}$	300.15 (443.8)	1.70 (145.5)	2.75 (96.4)
$N_{CDno(CDpo)}(r_{do(ao)}, y = 0.38)$ in $10^{18} \text{ cm}^{-3}$	8.27 (12.24)	0.047 (4.01)	0.076 (2.66)
$N_{CDno(CDpo)}(r_{do(ao)}, y = 0.50)$ in $10^{18} \text{ cm}^{-3}$	18.85 (27.88)	0.011 (9.14)	0.17 (6.06)
$N_{CDno(CDpo)}(r_{do(ao)}, y = 1)$ in $10^{18} \text{ cm}^{-3}$	150.8 (223.01)	0.85 (73.12)	1.38 (48.45)

Those numerical values given in this Table 1 will be used to determine various physical quantities, investigated in the following.

### 3. Our expression for $\varepsilon(r_{d(a)})$ , due to the impurity size effect

In the [d(a)-semiconductors]-systems at  $T=0$  K, since  $r_{d(a)}$ , given in tetrahedral covalent bonds, is usually either larger or smaller than  $r_{do(ao)}$ , a local mechanical strain (or deformation potential energy) is induced, according to a compression (dilation) for  $r_{d(a)} > r_{do(ao)}$  ( $r_{d(a)} < r_{do(ao)}$ ), respectively, due to the d(a)-size effect [5]. Then, we have shown [5] that this  $r_{d(a)}$ -effect affects the

changes in all the energy-band-structure parameters, expressed in terms of the relative static dielectric constant  $\varepsilon(r_{d(a)})$ .

Now, at  $r_{d(a)} = r_{do(ao)}$ , the boundary conditions are found to be, for the impurity-atom volume  $V$ ,  $V_{do(ao)} = (4\pi/3) \times (r_{do(ro)})^3$ , the pressure  $p$ ,  $p_o = 0$ , and the deformation potential energy or the strain energy  $\sigma$ ,  $\sigma_o = 0$ , according the absence of the impurity size effect.

Further, the two important equations [5], needed to determine the  $\sigma$ -variation  $\Delta\sigma \equiv \sigma - \sigma_o = \sigma$ , are defined by:

$$\frac{dp}{dV} \equiv -\frac{B_{n(p)}}{V} \text{ and } p \equiv -\frac{d\sigma}{dV}, \text{ giving: } \frac{d}{dV}\left(\frac{d\sigma}{dV}\right) = \frac{B_{n(p)}}{V}, \quad (6)$$

where the isothermal bulk modulus  $B_{n(p)}$  is determined in Eq. (3).

Then, in the  $n(p)$ -type doped semiconductors, by an integration, from Equations (2, 3, 6), one gets in the Bohr model:

$$(\Delta\sigma)_{n(p)} = B_{n(p)} \times (V - V_{do(ao)}) \times \ln\left(\frac{V}{V_{do(ao)}}\right) = E_{do(ao)} \times \left[ \left(\frac{r_{d(a)}}{r_{do(ao)}}\right)^3 - 1 \right] \times \ln\left(\frac{r_{d(a)}}{r_{do(ao)}}\right)^3 \geq 0. \quad (7)$$

Furthermore, at  $T=0K$ , we also shown [5] that, as  $r_{d(a)} > r_{do(ao)}$  ( $r_{d(a)} < r_{do(ao)}$ ), the compression (dilatation) corresponding the repulsive (attractive) force increases (decreases) the energy gap  $E_{gn(gp)}(r_{d(a)})$  and the effective donor(acceptor)-ionization energy  $E_{d(a)}(r_{d(a)})$  in absolute values, obtained in such an effective Bohr model, being represented by:  $\pm (\Delta\sigma)_{n(p)}$ , respectively. That gives:

$$E_{gn(gp)} - E_{go} = E_{d(a)} - E_{do(ao)} = E_{do(ao)} \times \left[ \left(\frac{\varepsilon_o}{\varepsilon(r_{d(a)})}\right)^2 - 1 \right] = + (\Delta\sigma)_{n(p)}, \text{ for } r_{d(a)} \geq r_{do(ao)}, \text{ and}$$

$$E_{gn(gp)} - E_{go} = E_{d(a)} - E_{do(ao)} = E_{do(ao)} \times \left[ \left(\frac{\varepsilon_o}{\varepsilon(r_{d(a)})}\right)^2 - 1 \right] = - (\Delta\sigma)_{n(p)}, \text{ for } r_{d(a)} \leq r_{do(ao)}. \quad (8)$$

Then, from Equations (7, 8), we obtain:

$$\varepsilon(r_{d(a)}) = \frac{\varepsilon_o}{\sqrt{1 + \left[\left(\frac{r_{d(a)}}{r_{do(ao)}}\right)^3 - 1\right] \times \ln\left(\frac{r_{d(a)}}{r_{do(ao)}}\right)^3}} \leq \varepsilon_o, \text{ for } r_{d(a)} \geq r_{do(ao)}, \text{ and}$$

$$\varepsilon(r_{d(a)}) = \frac{\varepsilon_o}{\sqrt{1 - \left[\left(\frac{r_{d(a)}}{r_{do(ao)}}\right)^3 - 1\right] \times \ln\left(\frac{r_{d(a)}}{r_{do(ao)}}\right)^3}} \geq \varepsilon_o, \text{ for } r_{d(a)} \leq r_{do(ao)}, \quad (9)$$

being an essential result of the present paper.

As a result, using Eq. (9), the expressions given in Equations (1, 2, 8) become effective as:

$$a_{\text{Bn(Bp)}}(r_{\text{d(a)}}) = 0.53 \times 10^{-8} \text{ cm} \times \frac{\varepsilon(r_{\text{d(a)}})}{(m_{\text{c(v)}}/m_0)}, \quad (10)$$

$$E_{\text{d(a)}}(r_{\text{d(a)}}) = E_{\text{do(ao)}} \times \left( \frac{\varepsilon_0}{\varepsilon(r_{\text{d(a)}})} \right)^2 = \frac{13600 \times (m_{\text{c(v)}}/m_0)}{\varepsilon_0^2} \text{ meV} \times \left( \frac{\varepsilon_0}{\varepsilon(r_{\text{d(a)}})} \right)^2, \text{ and} \quad (11)$$

$$E_{\text{gn(gp)}}(r_{\text{d(a)}}) = E_{\text{go}} + E_{\text{do(ao)}} \times \left( \frac{\varepsilon_0}{\varepsilon(r_{\text{d(a)}})} \right)^2 = E_{\text{go}} + \frac{13600 \times (m_{\text{c(v)}}/m_0)}{\varepsilon_0^2} \text{ meV} \times \left( \frac{\varepsilon_0}{\varepsilon(r_{\text{d(a)}})} \right)^2. \quad (12)$$

Here, in the n(p)-type (Si, GaAs, InP)-semiconductors, the important values of  $(m_{\text{c(v)}}/m_0)$ ,  $\varepsilon_0$  and  $E_{\text{go}}$  are given in Table 1 [4, 8].

#### 4. Our expressions for the critical density in the MIT and optical band gap

Here, replacing  $\varepsilon_0$  by  $\varepsilon(r_{\text{d(a)}})$ , obtained in Eq. (9), into Eq. (4), our expression for the critical density in the MIT is now determined by:

$$N_{\text{CDn(NDp)}}(r_{\text{d(a)}}, y) \equiv \left( \frac{y}{a_{\text{Bn(Bp)}}(r_{\text{d(a)}})} \right)^3 = 6.7168 \times 10^{24} \text{ cm}^{-3} \times \left( \frac{y \times (m_{\text{c(v)}}/m_0)}{\varepsilon(r_{\text{d(a)}})} \right)^3, \text{ for } 0.25 \leq y < 1. \quad (13)$$

Then, in the n(p)-type (Si, GaAs, InP)- semiconductors, all the numerical results for energy-band-structure parameters and  $N_{\text{CDn(CDp)}}[r_{\text{d(a)}}, y = 0.25(0.271)]$ , expressed as functions of  $r_{\text{d(a)}}$ -radius, are calculated, using Equations (9, 10, 11, 12, 13), and given respectively in following Tables 2, 3 and 4.

**Table 2.** In the n(p)-type Si, in which  $(m_{\text{c(v)}}/m_0) = 0.3216$  (0.3664) [4], all the numerical results for the energy-band-structure parameters and  $N_{\text{CDn(CDp)}}[r_{\text{d(a)}}, y = 0.25(0.271)]$ , expressed as functions of  $r_{\text{d(a)}}$ -radius, are respectively obtained, using Equations (9, 10, 11, 12, 13), suggesting that, with an increasing  $r_{\text{d(a)}}$ , both  $\varepsilon(r_{\text{d(a)}})$  and  $a_{\text{Bn(Bp)}}(r_{\text{d(a)}})$  decrease, while  $E_{\text{d(a)}}(r_{\text{d(a)}})$ ,  $E_{\text{gn(gp)}}(r_{\text{d(a)}})$  and  $N_{\text{CDn(CDp)}}[r_{\text{d(a)}}, y = 0.25(0.271)]$  increase.

Donor	P	$r_{\text{do}}$	As	Te	Sb	Sn
$r_{\text{d}}$ (nm) [4] ↗	0.110	0.117	0.118	0.132	0.136	0.140
$\varepsilon(r_{\text{d}})$ ↘	11.58	11.4	11.396	10.59	10.16	9.69
$a_{\text{Bn}}(r_{\text{d}})$ in nm ↘	1.91	1.88	1.878	1.75	1.67	1.59
$E_{\text{d}}(r_{\text{d}})$ in meV ↗	32.6	33.7	33.71	39	42.3	46.6
$E_{\text{gn}}(r_{\text{d}})$ in meV ↗	1168.9	1170	1170.02	1175.31	1178.67	1182.9
$N_{\text{CDn}}[r_{\text{d}}, y = 0.25(0.271)]$ in $10^{18} \text{ cm}^{-3}$ ↗	2.25(2.86)	2.36(3.0)	2.3601(3.004)	2.94(3.74)	3.32(4.23)	3.84(4.89)

  

Acceptor	B	$r_{\text{ao}}$	Ga	Al	Mg	In
$r_{\text{a}}$ (nm) [4] ↗	0.088	0.117	0.126	0.126	0.140	0.144
$\varepsilon(r_{\text{a}})$ ↘	15.98	11.4	11.1	11.1	9.69	9.19

$a_{\text{BP}}(r_a)$ in nm $\searrow$	2.31	1.65	1.60	1.60	1.40	1.33
$E_a(r_a)$ in meV $\nearrow$	19.5	38.3	40.5	40.5	53.1	59
$E_{\text{gp}}(r_a)$ in meV $\nearrow$	1151.2	1170	1172.1	1172.1	1184.7	1190.6
$N_{\text{CDP}}[r_a, y = 0.25(0.271)]$ $\nearrow$ in $10^{18} \text{ cm}^{-3}$	1.27(1.61)	3.48( <b>4.44</b> )	3.78( <b>4.81</b> )	3.78( <b>4.81</b> )	<b>5.67(7.23)</b>	<b>6.65(8.47)</b>

**Table 3.** In the n(p)-type GaAs, in which  $(m_{c(v)}/m_o) = 0.066 (0.291)$  [4], all the numerical results for the energy-band-structure parameters and  $N_{\text{CDn(CDP)}}[r_{\text{d(a)}}, y = 0.25(0.271)]$ , expressed as functions of  $r_{\text{d(a)}}$ -radius, are obtained respectively, by using Equations (9, 10, 11, 12, 13), suggesting that, with an increasing  $r_{\text{d(a)}}$ , both  $\varepsilon(0.271)$  and  $a_{\text{Bn(Bp)}}(r_{\text{d(a)}})$  decrease, while  $E_{\text{d(a)}}(r_{\text{d(a)}})$ ,  $E_{\text{gn(gp)}}(r_{\text{d(a)}})$  and  $N_{\text{CDn(CDP)}}[r_{\text{d(a)}}, y = 0.25(0.271)]$  increase.

Donor		P	As	Te	Sb	Sn
$r_d$ (nm) [4] $\nearrow$		0.110	0.118	0.132	0.136	0.140
$\varepsilon(r_d)$ $\searrow$		13.4	13.13	12.33	11.86	11.33
$a_{\text{Bn}}(r_d)$ in nm $\searrow$		10.76	10.54	9.90	9.52	9.10
$E_d(r_d)$ in meV $\nearrow$		5.0	5.2	5.91	6.38	7.00
$E_{\text{gn}}(r_d)$ in meV $\nearrow$		1519.8	1520	1520.7	1521.2	1521.8
$N_{\text{CDn}}[r_d, y = 0.25(0.271)]$ $\nearrow$ in $10^{16} \text{ cm}^{-3}$		1.25(1.60)	1.33(1.70)	1.61(2.05)	1.81(2.30)	2.08(2.64)
Acceptor		B	Ga	Al	Mg	In
$r_a$ (nm) [4] $\nearrow$		0.088	0.126	0.126	0.140	0.144
$\varepsilon(r_a)$ $\searrow$		24.38	13.13	13.13	12.42	11.99
$a_{\text{BP}}(r_a)$ in nm $\searrow$		4.44	2.39	2.39	2.26	2.18
$E_a(r_a)$ in meV $\nearrow$		6.66	23	23	25.7	27.5
$E_{\text{gp}}(r_a)$ in meV $\nearrow$		1503.7	1520	1520	1522.7	1524.5
$N_{\text{CDP}}[r_a, y = 0.25(0.271)]$ $\nearrow$ in $10^{17} \text{ cm}^{-3}$		1.78(10.41)	11.43(14.55)	11.43(14.55)	13.50(17.19)	15.00(19.07)

**Table 4.** In the n(p)-type InP, in which  $(m_{c(v)}/m_o) = 0.073 (0.239)$  [4], all the numerical results for the energy-band-structure parameters and  $N_{\text{CDn(CDP)}}[r_{\text{d(a)}}, y = 0.25(0.271)]$ , expressed as functions of  $r_{\text{d(a)}}$ -radius, are obtained respectively, by using Equations (9, 10, 11, 12, 13), suggesting that, with an increasing (decreasing)  $r_{\text{d(a)}}$ , both  $\varepsilon(r_{\text{d(a)}})$  and  $a_{\text{Bn(Bp)}}(r_{\text{d(a)}})$  decrease (increase), while  $E_{\text{d(a)}}(r_{\text{d(a)}})$ ,  $E_{\text{gn(gp)}}(r_{\text{d(a)}})$  and  $N_{\text{CDn(CDP)}}[r_{\text{d(a)}}, y = 0.25(0.271)]$  increase (decrease), respectively.

Donor		$d_o \equiv \text{P}$	As	Te	Sb	Sn
$r_d$ (nm) [4] $\nearrow$		0.110	0.118	0.132	0.136	0.140
$\varepsilon(r_d)$ $\searrow$		12.37	12.07	10.46	9.88	9.30
$a_{\text{Bn}}(r_d)$ in nm $\searrow$		8.98	8.77	7.59	7.17	6.75

$E_d(r_d)$ in meV ↗	6.49	6.81	9.07	10.16	11.47
$E_{gn}(r_d)$ in meV ↗	1420	1420.3	1422.58	1423.67	1424.98
$N_{CDn}[r_d, y = 0.25(0.271)]$ ↗ in $10^{16} \text{ cm}^{-3}$	2.16(2.75)	2.32(2.95)	3.57(4.54)	4.23(5.39)	5.07(6.46)

Acceptor	$a_0 \equiv \text{In}$	Mg	Al	Ga
$r_a$ (nm) [4] ↘	0.144	0.140	0.126	0.126
$\epsilon(r_a)$ ↗	12.37	12.41	13.28	13.28
$a_{BP}(r_a)$ in nm ↗	2.74	2.75	2.94	2.94
$E_a(r_a)$ in meV ↘	21.24	21.10	18.43	18.43
$E_{gp}(r_a)$ in meV ↘	1420	1419.8	1417.2	1417.2
$N_{CDp}(r_a)$ in $10^{17} \text{ cm}^{-3}$ ↘	7.57(9.64)	7.49(9.54)	6.12(7.79)	6.12(7.79)

In Table 2, it should be concluded that for the n-type Si semiconductor, our obtained numerical results,

$$N_{CDn}[r_P(r_{do}), y = 0.271] = 2.86 (3) \times 10^{18} \text{ cm}^{-3},$$

are found to be in good agreement with the corresponding experimental ones, given in the literature [4]. Further, one note that they strongly depend on the used values of  $m_c/m_o$ ,  $\epsilon_o$  and  $r_P(r_{do})$ , being taken in Refs. [4, 8], and also on the chosen value of the parameter  $y$ .

Finally, in the n(p)-type heavily doped (Si, GaAs, and InP)-crystals at very low temperature, the optical band gap can be determined by:

$$E_{gn1(gp1)}(N, r_{d(a)}) \equiv E_{gn(gp)}(r_{d(a)}) - \Delta E_{gn(gp)}(N, r_{d(a)}) + E_{Fn(Fp)}(N), \quad (14)$$

where  $E_{gn(gp)}(r_{d(a)})$  is determined in Eq. (12), the Fermi energy  $E_{Fn(Fp)}(N, T)$  [6], expressed as functions of d(a)-density  $N$  and temperature  $T$ , and the band gap narrowing  $\Delta E_{gn(gp)}(N, r_{d(a)})$  [7], are determined respectively in Equations (A2, B4, B5) of the appendix A and B.

Now, in the n-type heavily doped Si, the numerical results of  $E_{gn1}(N, r_d)$ , are calculated by using Eq. (14), for  $(m_c/m_o) = 0.3216$  [8]. Then, they can be compared with  $E_{gn1}$  – data, obtained by Wagner and Alamo [9], as observed in the following Table 5, giving rise to a reasonable maximal relative deviation, obtained in absolute value,  $|\text{MRD}|=3.19\%$ .

**Table 5.** In n-type P-Si system, in which  $E_{gn}(r_P) = 1.1689$  eV, as that given in Table 2, and for  $(m_c/m_o) = 0.3216$ , the numerical results of  $E_{gn1}(N, r_P)$  are obtained, using Eq. (14) and also compared with  $E_{gn1}$  – data [9], giving the relative deviations in absolute values  $|\text{RD}|$ .

$N$ in $10^{18} \text{ cm}^{-3}$	4	8.5	15	50	80	150
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$E_{Fn}(N)$ in meV	8.65	14.3	20.9	46.6	63.7	96.9
$\Delta E_{gn}(N, r_p)$ in meV	33.9	46.9	60	102.6	126.9	169.1
$E_{gn1}(N, r_p)$ in eV	1.1437	1.1364	1.1298	1.113	1.1058	1.0968
$E_{gn1} - \text{data}$ (eV)	1.138	1.133	1.129	1.131	1.132	1.133
$ \text{RD} $ in (%)	0.5	0.3	0.07	1.59	2.31	<b>3.19</b>

So, in the n(p)-type (Si, GaAs, InP)-degenerate semiconductors, and for the physical condition:  $N \geq N_{CDn(CDp)}[r_{d(a)}, y = 0.25 (0.271)]$ , and with use of the numerical values of all the parameters given in Table 1, we obtain the numerical results of  $E_{gn1(gp1)}(N, r_{d(a)})$ , using Eq. (14), as those given in following Tables 6, 7 and 8.

**Table 6.** Using the physical condition,  $N \geq N_{CDn(CDp)}[r_{d(a)}, y = 0.25(0.271)]$ , the values of OBG,  $E_{gn1(gp1)}(N, r_{d(a)})$ , calculated using Eq. (14) for the n(p)-type degenerate Si-semiconductor are obtained, as functions of  $N$  and  $r_{d(a)}$ .

$N$ in $10^{18} \text{ cm}^{-3}$	4	8.5	15	50	80	150
In <b>P-Si</b> crystal, where $\epsilon(r_p) = 11.58$ and $E_{gn}(r_p) = 1.1689$ eV						
$E_{gn1}(N, r_p)$ (eV)	1.144	1.136	1.130	1.113	1.106	1.097
In <b>As-Si</b> crystal, where $\epsilon(r_{As}) = 11.396$ and $E_{gn}(r_{As}) = 1.17002$ eV						
$E_{gn1}(N, r_{As})$ (eV)	1.1443	1.137	1.130	1.113	1.106	1.096
In <b>Te-Si</b> crystal, where $\epsilon(r_{Te}) = 10.595$ and $E_{gn}(r_{Te}) = 1.1753$ eV						
$E_{gn1}(N, r_{Te})$ (eV)	1.148	1.140	1.132	1.113	1.105	1.093
In <b>Sb-Si</b> crystal, where $\epsilon(r_{Sb}) = 10.17$ and $E_{gn}(r_{Sb}) = 1.179$ eV						
$E_{gn1}(N, r_{Sb})$ (eV)	1.150	1.142	1.134	1.114	1.104	1.092
In <b>Sn-Si</b> crystal, where $\epsilon(r_{Sn}) = 9.69$ and $E_{gn}(r_{Sn}) = 1.183$ eV						
$E_{gn1}(N, r_{Sn})$ (eV)	1.153	1.144	1.136	1.114	1.104	1.091
$N$ in $10^{18} \text{ cm}^{-3}$	4	8.5	15	50	80	150
In <b>B-Si</b> crystal, where $\epsilon(r_B) = 15.98$ and $E_{gn}(r_B) = 1.1512$ eV						
$E_{gp1}(N, r_B)$ (eV)	1.148	1.151	1.156	1.180	1.199	1.237
In <b>Ga-Si</b> crystal, where $\epsilon(r_{Ga}) = 11.097$ and $E_{gn}(r_{Ga}) = 1.1721$ eV						
$E_{gp1}(N, r_{Ga})$ (eV)	1.163	1.164	1.167	1.185	1.200	1.232
In <b>Mg-Si</b> crystal, where $\epsilon(r_{Mg}) = 9.69$ and $E_{gn}(r_{Mg}) = 1.185$ eV						
$E_{gp1}(N, r_{Mg})$ (eV)		1.173	1.175	1.190	1.203	1.234
In <b>In-Si</b> crystal, where $\epsilon(r_{In}) = 9.43$ and $E_{gn}(r_{In}) = 1.188$ eV						
$E_{gp1}(N, r_{In})$ (eV)		1.178	1.179	1.193	1.206	1.235

**Table 7.** Using the physical condition,  $N \geq N_{CDn(CDp)}[r_{d(a)}, y = 0.25(0.271)]$ , the values of OBG,  $E_{gn1(gp1)}(N, r_{d(a)})$ , calculated using Eq. (14) for the n(p)-type degenerate GaAs-semiconductor are obtained, as functions of  $N$  and  $r_{d(a)}$ .

$N$ in $10^{18} \text{ cm}^{-3}$	4	8.5	15	50	80	150
<b>In P-GaAs</b> crystal, where $\epsilon(r_p) = 13.40$ and $E_{gn}(r_p) = 1.5198 \text{ eV}$						
$E_{gn1}(N, r_p)$ (eV)	1.621	1.698	1.790	2.159	2.410	2.901
<b>In As- GaAs</b> crystal, where $\epsilon(r_{As}) = 13.13$ and $E_{gn}(r_{As}) = 1.5207 \text{ eV}$						
$E_{gn1}(N, r_{As})$ (eV)	1.620	1.697	1.789	2.158	2.409	2.898
<b>In Te- GaAs</b> crystal, where $\epsilon(r_{Te}) = 12.33$ and $E_{gn}(r_{Te}) = 1.15207 \text{ eV}$						
$E_{gn1}(N, r_{Te})$ (eV)	1.619	1.696	1.787	2.154	2.403	2.892
<b>In Sb- GaAs</b> crystal, where $\epsilon(r_{Sb}) = 11.86$ and $E_{gn}(r_{Sb}) = 1.1512 \text{ eV}$						
$E_{gn1}(N, r_{Sb})$ (eV)	1.618	1.694	1.785	2.151	2.400	2.887
<b>In Sn- GaAs</b> crystal, where $\epsilon(r_{Sn}) = 11.33$ and $E_{gn}(r_{Sn}) = 1.5218 \text{ eV}$						
$E_{gn1}(N, r_{Sn})$ (eV)	1.617	1.693	1.784	2.148	2.396	2.882
$N$ in $10^{18} \text{ cm}^{-3}$	4	8.5	15	50	80	150
<b>In B- GaAs</b> crystal, where $\epsilon(r_B) = 24.38$ and $E_{gn}(r_B) = 1.5037 \text{ eV}$						
$E_{gp1}(N, r_B)$ (eV)	1.519	1.533	1.550	1.622	1.671	1.770
<b>In Ga- GaAs</b> crystal, where $\epsilon(r_{Ga}) = 13.13$ and $E_{gn}(r_{Ga}) = 1.520 \text{ eV}$						
$E_{gp1}(N, r_{Ga})$ (eV)	1.527	1.538	1.553	1.615	1.660	1.749
<b>In Mg- GaAs</b> crystal, where $\epsilon(r_{Mg}) = 12.42$ and $E_{gn}(r_{Mg}) = 1.5227 \text{ eV}$						
$E_{gp1}(N, r_{Mg})$ (eV)	1.529	1.540	1.554	1.615	1.659	1.748
<b>In In- GaAs</b> crystal, where $\epsilon(r_{In}) = 11.99$ and $E_{gn}(r_{In}) = 1.5245 \text{ eV}$						
$E_{gp1}(N, r_{Mg})$ (eV)	1.530	1.541	1.555	1.615	1.659	1.747

**Table 8.** Using the physical condition,  $N \geq N_{CDn(CDp)}[r_{d(a)}, y = 0.25(0.271)]$ , the values of OBG,  $E_{gn1(gp1)}(N, r_{d(a)})$ , calculated using Eq. (14) for the n(p)-type degenerate InP-semiconductor are obtained, as functions of  $N$  and  $r_{d(a)}$ .

$N$ in $10^{18} \text{ cm}^{-3}$	4	8.5	15	50	80	150
<b>In P-InP</b> crystal, where $\epsilon(r_p) = 12.37$ and $E_{gn}(r_p) = 1.420 \text{ eV}$						
$E_{gn1}(N, r_p)$ (eV)	1.513	1.582	1.664	1.994	2.218	2.657
<b>In As- InP</b> crystal, where $\epsilon(r_{As}) = 12.07$ and $E_{gn}(r_{As}) = 1.4203 \text{ eV}$						
$E_{gn1}(N, r_{As})$ (eV)	1.513	1.581	1.663	1.992	2.216	2.655
<b>In Te- InP</b> crystal, where $\epsilon(r_{Te}) = 10.46$ and $E_{gn}(r_{Te}) = 1.4226 \text{ eV}$						
$E_{gn1}(N, r_{Te})$ (eV)	1.513	1.580	1.660	1.985	2.207	2.641
<b>In Sb- InP</b> crystal, where $\epsilon(r_{Sb}) = 9.88$ and $E_{gn}(r_{Sb}) = 1.4237 \text{ eV}$						
$E_{gn1}(N, r_{Sb})$ (eV)	1.513	1.579	1.659	1.982	2.203	2.636
<b>In Sn- InP</b> crystal, where $\epsilon(r_{Sn}) = 9.30$ and $E_{gn}(r_{Sn}) = 1.4250 \text{ eV}$						
$E_{gn1}(N, r_{Sn})$ (eV)	1.513	1.579	1.658	1.979	2.199	2.630
$N$ in $10^{18} \text{ cm}^{-3}$	4	8.5	15	50	80	150
<b>In Ga- InP</b> crystal, where $\epsilon(r_{Ga}) = 13.28$ and $E_{gn}(r_{Ga}) = 1.4172 \text{ eV}$						

$E_{gp1}(N, r_{Ga})$ (eV)	1.432	1.448	1.468	1.551	1.610	1.727
In <b>Mg- InP</b> crystal, where $\epsilon(r_{Mg}) = 12.41$ and $E_{gn}(r_{Mg}) = 1.4198$ eV						
$E_{gp1}(N, r_{Mg})$ (eV)	1.433	1.449	1.468	1.551	1.609	1.725
In <b>In- InP</b> crystal, where $\epsilon(r_{In}) = 12.37$ and $E_{gn}(r_{In}) = 1.420$ eV						
$E_{gp1}(N, r_{Mg})$ (eV)	1.434	1.449	1.469	1.551	1.609	1.725

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Finally, from the Tables 2, 3 and 4, we can justify the physical application condition (PAC):  $N \geq N_{CDn(CDp)}[r_{d(a)}, y = 0.25 (0.271)]$  imposed for our numerical results of  $E_{gn1(gp1)}(N, r_{d(a)})$ , being obtained in those Tables 6, 7 and 8, as follows.

(i) From the Tables 2 and 6, in various d(a)-Si systems, since  $N \geq 4 \times 10^{18} \text{ cm}^{-3} > N_{CDn(CDp)}[r_{d(a)}, y = 0.25(0.271)]$ , the PAC is justified, except, it is only satisfied,

-in the (Sb, Sn)-Si systems, respectively for:

$$N \geq 8.5 \times 10^{18} \text{ cm}^{-3} > N_{CDn}[r_{(Sb,Sn)}, y = 0.271] = (4.23, 4.89) \times 10^{18} \text{ cm}^{-3},$$

- in the (Mg, In)-Si systems, respectively for:

$$N \geq 8.5 \times 10^{18} \text{ cm}^{-3} > N_{CDp}[r_{(Mg,In)}, y = 0.25] = (5.67, 6.65) \times 10^{18} \text{ cm}^{-3}, \text{ and finally}$$

- in the (Ga, Mg, In)-Si systems, respectively for:

$$N \geq 8.5 \times 10^{18} \text{ cm}^{-3} > N_{CDp}[r_{(Ga,Mg,In)}, y = 0.271] = (4.81, 7.3, 8.47) \times 10^{18} \text{ cm}^{-3}.$$

(ii) However, from the Tables 2, 7 and 8, in all the d(a)-(GaAs, InP) systems, the PAC is well justified since

$$N \geq 4 \times 10^{18} \text{ cm}^{-3} > N_{CDn(CDp)}[r_{d(a)}, y = 0.25(0.271)].$$

## 5. Concluding remarks

By using an effective Bohr model given in the n(p)-type semiconductors, we have determined the relative static dielectric constant  $\epsilon(r_{d(a)})$ , expressed as a function of the d(a)-radius, according to the impurity size effect.

Then, as showed in Tables (2-4, 6-8), this function  $\varepsilon(r_{d(a)})$  strongly affects the numerical results for: (i) the effective Bohr radius  $a_B(r_{d(a)})$ , (ii) the effective d(a)-ionization energy  $E_{d(a)}(r_{d(a)})$  in absolute values, (iii) the effective band gap  $E_{gn(gp)}(r_{d(a)})$ , (iv) the effective critical density  $N_{CDn(CDp)}(r_{d(a)}, y = 0.25(0.271))$  in the MIT, and finally (v) the OBG,  $E_{gn1(gp1)}(r_{d(a)}, N, y = 0.25(0.271))$ . One notes here that:

- (i) the value:  $y=0.25$  was given in the Mott criterion [1] as:  $a_B \times N_{CD}^{1/3} \approx y = 0.25$ ,
- (ii) Pergament [2] used this Mott criterion to obtain the value of  $N_{CD}$  ( $= 2.8 \times 10^{18} \text{cm}^{-3}$ ) for  $\text{VO}_2$ , with  $a_B = 1.77 \text{ nm}$ ,
- (iii) Edwards and others [3] proposed  $y \geq 0.38$ , explaining the transition to the metallic state for Cs, Rb and H-elements.

One notes here that, in the n(p)-Si crystal, the best choice is found to be given by:  $y=0.271$ , according to an agreement between our numerical results of  $N_{CDn(CDp)} = 3(4.44) \times 10^{18} \text{cm}^{-3}$ , as given in Table 1, and the experimental ones given in the literature [4]. Further, other choice of  $y \in [0, 1]$  can be proposed, depending on the considered systems (or elements).

## Appendix

### Appendix A. Fermi Energy

In the n(p)-type (Si, GaAs, InP)-crystals, the Fermi energy  $E_{Fn}(-E_{Fp})$ , obtained for any T and donor (acceptor) density N, being investigated in our previous paper, with a precision of the order of  $2.11 \times 10^{-4}$  [6], is now summarized in the following.

First of all, we define the reduced electron density by:

$$u \equiv \frac{N}{N_{c(v)}}, N_c(T) = 2 \times g_c \times \left( \frac{m_c \times k_B T}{2\pi\hbar^2} \right)^{\frac{3}{2}} (\text{cm}^{-3}), N_v(T) = 2 \times g_v \times \left( \frac{m_v \times k_B T}{2\pi\hbar^2} \right)^{\frac{3}{2}} (\text{cm}^{-3}), \quad (\text{A1})$$

where  $N_{c(v)}$  is the conduction (valence)-band density of states, and the values of  $g_{c(v)}$  and  $m_{c(v)}$  are defined and given in Table 1. Then, the reduced Fermi energies in the n(p)-type semiconductor are determined respectively by [6]:

$$\frac{E_{Fn}(u)}{k_B T} \left( \frac{-E_{Fp}(u)}{k_B T} \right) = \frac{G(u) + Au^B F(u)}{1 + Au^B}, A = 0.0005372 \text{ and } B = 4.82842262. \quad (\text{A2})$$

Here,  $F(u) = au^{\frac{2}{3}} \left(1 + bu^{-\frac{4}{3}} + cu^{-\frac{8}{3}}\right)^{-\frac{2}{3}}$ , with  $a = [(3\sqrt{\pi}/4) \times u]^{2/3}$ ,  $b = \frac{1}{8} \left(\frac{\pi}{a}\right)^2$ ,  $c = \frac{62.3739855}{1920} \left(\frac{\pi}{a}\right)^4$ , and  $G(u) \simeq \text{Ln}(u) + 2^{-\frac{3}{2}} \times u \times e^{-du}$ ;  $d = 2^{3/2} \left[\frac{1}{\sqrt{27}} - \frac{3}{16}\right] > 0$ .

## Appendix B. Approximate forms for band gap narrowing (BGN)

First of all, in the n(p)-type doped (Si, GaAs, InP)-semiconductors, we define the effective Wigner-Seitz radius  $r_{\text{sn(sp)}}$ , characteristic of the interactions, by [7]

$$r_{\text{sn}} \equiv r_s(N, r_d) = 1.1723 \times 10^8 \times \left(\frac{g_c}{N}\right)^{1/3} \times \frac{m_c/m_0}{\varepsilon(r_d)} \quad (\text{B1})$$

and

$$r_{\text{sp}} \equiv r_s(N, r_a) = 1.1723 \times 10^8 \times \left(\frac{g_v}{N}\right)^{1/3} \times \frac{m_v/m_0}{\varepsilon(r_a)}, \quad (\text{B2})$$

where the values of  $g_{c(v)}$  and  $(m_{c(v)}/m_0)$  are defined and given in Table 1.

Therefore, the correlation energy of an effective electron gas,  $E_c(r_{\text{sn(sp)}})$ , is found to be given by [3]:

$$E_{\text{cn(cp)}}(r_{\text{sn(sp)}}) = \frac{-0.87553}{0.0908+r_{\text{sn(sp)}}} + \frac{0.87553}{0.0908+r_{\text{sn(sp)}}} + \frac{(2[1-\ln(2)]) \times \ln(r_{\text{sn(sp)}}) - 0.093288}{1+0.03847728 \times r_{\text{sn(sp)}}^{1.67378876}}. \quad (\text{B3})$$

Then, in the n-type heavily doped (Si, GaAs, InP)-semiconductors, in which the values of the dielectric  $\varepsilon_0$  of the intrinsic (Si, GaAs, InP)-semiconductors are given in Table 1, the BGN is determined by [7]:

$$\Delta E_{\text{gn}}(N, r_{\text{sn}}, r_d) \simeq a_1 \times \frac{\varepsilon_0}{\varepsilon(r_d)} \times N_r^{1/3} + a_2 \times \frac{\varepsilon_0}{\varepsilon(r_d)} \times N_r^{1/3} \times (2.503 \times [-E_c(r_{\text{sn}}) \times r_{\text{sn}}]) + a_3 \times \left[\frac{\varepsilon_0}{\varepsilon(r_d)}\right]^{5/4} \times \sqrt{\frac{m_v}{m_c}} \times N_r^{1/4} + a_4 \times \sqrt{\frac{\varepsilon_0}{\varepsilon(r_d)}} \times N_r^{1/2} \times 2 + a_5 \times \left[\frac{\varepsilon_0}{\varepsilon(r_d)}\right]^2 \times N_r^{1/6}, \quad N_r \equiv \left(\frac{N_d}{9.999 \times 10^{17} \text{ cm}^{-3}}\right), \quad (\text{B4})$$

where  $a_1 = 3.8 \times 10^{-3}(\text{eV})$ ,  $a_2 = 6.5 \times 10^{-4}(\text{eV})$ ,  $a_3 = 2.8 \times 10^{-3}(\text{eV})$ ,  $a_4 = 5.597 \times 10^{-3}(\text{eV})$  and  $a_5 = 8.1 \times 10^{-4}(\text{eV})$ , and in the p-type heavily doped ones, one has [7]:

$$\Delta E_{\text{gp}}(N, r_{\text{sp}}, r_a) \simeq a_1 \times \frac{\varepsilon_0}{\varepsilon(r_a)} \times N_r^{1/3} + a_2 \times \frac{\varepsilon_0}{\varepsilon(r_a)} \times N_r^{1/3} \times (2.503 \times [-E_c(r_{\text{sp}}) \times r_{\text{sp}}]) + a_3 \times \left[\frac{\varepsilon_0}{\varepsilon(r_a)}\right]^{5/4} \times \sqrt{\frac{m_c}{m_v}} \times N_r^{1/4} + 2a_4 \times \sqrt{\frac{\varepsilon_0}{\varepsilon(r_a)}} \times N_r^{1/2} + a_5 \times \left[\frac{\varepsilon_0}{\varepsilon(r_a)}\right]^2 \times N_r^{1/6}, \quad N_r \equiv \left(\frac{N_a}{9.999 \times 10^{17} \text{ cm}^{-3}}\right), \quad (\text{B5})$$

where  $a_1 = 3.15 \times 10^{-3}(\text{eV})$ ,  $a_2 = 5.41 \times 10^{-4}(\text{eV})$ ,  $a_3 = 2.32 \times 10^{-3}(\text{eV})$ ,  $a_4 = 4.12 \times 10^{-3}(\text{eV})$  and  $a_5 = 9.80 \times 10^{-5}(\text{eV})$ .

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