Physica B 405 (2010) 1139–1149

Contents lists available at ScienceDirect

Physica B

journal homepage: www.elsevier.com/locate/physb

Bandgap changes in excited intrinsic (heavily doped) Si and Ge semiconductors

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ARTICLE INFO

Article history:
Received 14 May 2009
Received in revised form
26 October 2009
Accepted 3 November 2009

Keywords:
Si
Ge
SiGe
Intrinsic bandgap
Fermi energy
Bandgap narrowing
Optical bandgap
Electrical bandgap

ABSTRACT

Our results for the bandgap changes in highly excited intrinsic (heavily doped-HD) Si (Ge) for any majority-carrier density N and temperature T have been investigated and expressed in terms of (i) the bandgap narrowing (BGN > 0) due to many-body carrier–carrier interactions and screening effect on carrier-impurity (or electron–hole) potential energies, (ii) the bandgap widening (BGW < 0) due to the effects of Fermi Dirac statistics, and (iii) the apparent BGN defined by ABGN ≡ BGN+BGW < BGN. Since those ABGN and BGN can be extracted from respective electical-and-optical measurements, this relation thus suggests a conjunction between electrical-and-optical bandgaps (EBG-and-OBG). Then, our results for BGN, ABGN, OBG, and EBG have been computed and also compared with other theoretical and experimental ones, giving rise to a satisfactory description of both electrical-and-optical data in those materials. Furthermore, in the p-type HD base of $Si_{1-x}Ge_x$ hetero bipolar transistors for $x \leq 0.3$, using a same assumption taken by Eberhardt and Kasper (EK) [Mater. Sci. Eng. B 89 (2002) 93–96], we have obtained the results for ABGN and EBG, which are found to be in good accordance with the respective EK-ones.

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1. Introduction

The bandgap changes in excited intrinsic (EI)-and-heavily doped (HD) Si and Ge semiconductors at temperatures T, are given in the following relation, in which the apparent bandgap narrowing (ABGN) [1,2], $\Delta E_{g,A} > 0$, may be expressed in terms of (i) the intrinsic carrier concentration, n_i, and the effective intrinsic carrier concentration, $n_{i,e}$, and (ii) the bandgap narrowing (BGN) due to many-body interactions, $\Delta E_g > 0$, and the bandgap widening (BGW) due to the effects of Fermi–Dirac statistics, $\Delta E_{g,FD} < 0$, as

$$\Delta E_{g,A} = 2k_BT \times \mathrm{Ln}(n_{i,e}/n_i) = \Delta E_g + \Delta E_{g,FD}, \quad (1)$$

where k_B is Boltzmann's constant, and the BGW is defined by

$$\Delta E_{g,FD} \equiv k_BT \times \mathrm{Ln}(N/N_{c(v)}) - E_F. \quad (2)$$

It should be noted that relation (1) gives rise to a conjunction between BGN and ABGN or optical-and-electrical phenomena occurring in those materials [2].

In Eq. (2), E_F is the penetration of the Fermi energy level into the majority band, N is the density of electron–hole (e–h) pairs defined in EI Si(Ge) or the total impurity density in HD Si(Ge) assuming that all the impurities are ionized even at 0 K, and $N_{c(v)}$ means the conduction (valence)-band density of states (DOS) defined by [3]

$$N_{c(v)} \equiv [g_s g_{c(v)}](m_{dc(v)} k_B T/2\pi\hbar^2)^{3/2} = 2.540933 \times 10^{19} [m^*_{dc(v)} T/300]^{3/2}\,(\mathrm{cm}^{-3}), \quad (3)$$

where $\hbar \equiv h/2\pi$, h being Planck's constant, $m_{dc(v)}$ is the DOS effective mass found in each conduction (valence) band to free electron mass m_o, g_s=2 is the spin degeneracy factor defined with spin up and spin down, $g_{c(v),Si} = 6(2)$ [4] and $g_{c(v),Ge} = 4(1)$[4–6] are the average numbers of equivalent conduction (valence)-band edges in the n(p)-type Si and Ge, respectively, and finally $m^*_{dc(v)} \equiv g^{2/3}_{c(v)} m_{dc(v)}$ means the DOS effective mass in such materials. Thus, in this Eq. (3), $N_{c(v)}$ is expressed as functions of $m_{dc(v)}, g_{c(v)}$ and T.

Moreover, in Eq. (1), the intrinsic carrier concentration is defined by

$$n_i \equiv \sqrt{N_c N_v} \exp(-E_{g,I}/2k_BT), \quad (4)$$

where $E_{gI}(T)$ is the intrinsic bandgap.

It should be noted in Eqs. (1) and (2) that in the EI Si (Ge) one has $\Delta E_g = \Delta E_{gn} + \Delta E_{gp}$ and E_F=E_{Fn}+E_{Fn} and in the n(p)-type HD

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doi:10.1016/j.physb.2009.11.016

Si(Ge), ΔE_g and E_F are simply replaced by $\Delta E_{gn(p)}$ and $E_{Fn(p)}$, respectively.

In those semiconductors, the photoluminescence (PL) spectra consist of a number of different lines arising from electrons and holes recombining from states such as free excitons, excitons bound to impurities, and electron–hole condensate [7–10]. Here, we are primarily concerned with free-exciton and condensate emission. Since Si(Ge) are indirect bandgap semiconductors, radiative recombination may be accompanied by phonon emission; the PL spectra thus consist in general of phonon replicas involving the momentum-conserving transverse-acoustic(optical) TA(O)phonon with respective energy $E_{p,TA(O)}$ or longitudinal-acoustic(optical) LA(O) with respective energy $E_{p,LA(O)}$. The effective bandgaps of given phonon-mode replicas are defined as follows.

First of all, the low-energy threshold or reduced bandgap, $E_g' \equiv E_g - E_p$, is defined by

$$E_g' \equiv E_{gI} - \Delta E_g, \tag{5}$$

which is the difference between the bottom (top) of perturbed conduction (valence)-band edges. Then, the high-energy cutoff, equivalent chemical potential or optical bandgap (OBG) energy, $E_{g,O}' = E_{g,O} - E_p = E_g' + E_F$, is determined by

$$E_{g,O}' = E_{gI} - \Delta E_g = E_F = E_{gI} + \mu, \tag{6}$$

where $\mu \equiv -\Delta E_g + E_F$ is the chemical potential defined in the EI Si (Ge) and in the n(p)-type HD Si (Ge) μ is simply replaced by $\mu_{n(p)} \equiv -\Delta E_{gn(p)} + E_{Fn(p)}$.

Further, the free exciton low-energy threshold, $E_{gx}' \equiv E_{gx} - E_p$, is defined by

$$E_{gx}' \equiv E_{gI} - E_x - E_p, \tag{7}$$

where E_x is the exciton Rydberg. Here, in the EI Si (Ge) at very low temperatures one, respectively, has $E_x = 12.87(2.65)$ meV, $E_{gI}(T=0) = 1170(743.7)$ meV and data of free exciton low-enery threshold $E_{gx}' = 1096.9(712.9)$ meV [10]. Therefore, the values of phonon energy are found to be $E_{p(TO);Si} = 60.23$ (meV) and $E_{p(LA);Ge} = 26.548$ (meV).

Then, from Eqs. (1), (2), and (6), if denoting the electrical bandgap (EBG) in the n(p)-type HD Si (Ge) by $E_{gn(p),E}' \equiv E_{gn(p),E} - E_p = E_{gI} - \Delta E_{gn(p),A}$, where $\Delta E_{gn(p),A}$ is defined in Eq. (1), the above conjunction (1) can now be rewritten by the one between the OBG and EBG as

$$E_{g,O}' = E_{g,E}' + k_B T \times \mathrm{Ln}(N/N_{c(v)}). \tag{8}$$

Note that in Eq. (8), if replacing $\Delta E_{g,A}$ by its empirical form, extracted from electrical measurements in n-and-p types Si doped with $N \le 10^{20}\,\mathrm{cm}^{-3}$, by Klaassen et al. [1], assuming that the ABGN obtained in the N-type Si is found to be equal to the one measured in the p-type Si,

$$\Delta E_{g,A(Si)}^{KSG}(N) = 6.92 \times \left[\mathrm{Ln}\left(\frac{N}{1.3 \times 10^{17}\,\mathrm{cm}^{-3}}\right) + \sqrt{\mathrm{Ln}^2}\left(\frac{N}{1.3 \times 10^{17}\,\mathrm{cm}^{-3}}\right) + 0.5\right], \tag{9}$$

the OBG can then be determined and denoted by $E_{g,O}^{(KSG)'}$.

In summary, as seen in Eqs. (1) and (2), there are three fundamental parameters to be determine such as the intrinsic carrier concentration n_i, the Fermi energy E_F, and the BGN: ΔE_g, from which other ones can also be determined and computed.

The aim of the present paper is to investigate the accurate results for these parameters, and also compare those with existing data and other theoretical (or empirical) results, giving rise to a satisfactory description of both optical-and-electrical data observed in EI-and-HD Si (Ge) at any N and T.

2. Intrinsic carrier concentration

As seen in Eqs. (3)–(7), the intrinsic carrier concentration $E_{gI}(T)$ depends not only on the intrinsic bandgap $E_{gI}(T)$ but also on the DOS effective masses $m_{dc(v)}^* \equiv g_{c(v)}^{2/3} m_{dc(v)}$ defined in Eq. (3). In order to evaluate n_i we thus need to know those values of $E_{gI}(T)$ and $m_{dc(v)}^*$, which are chosen as follows.

First of all, we use here accurate approximate forms for intrinsic bandgap $E_{gI}(T)$ in meV at any T, which were recently investigated by Pässler [11], taking into account not only the change in the crystal volume with T resulting from the lattice expansion but also the electron–phonon interaction at constant volume, for the Si as

$$E_{gI,Si}(T) = 1170 - 72[(1 + [2T/446]^{2.2011})1/2.2011 - 1] \tag{10}$$

and for the Ge by

$$E_{gI,Ge}(T) = 743.7 - 52[(1 + [2T/253]^{2.2726})^{1/2.2726} - 1]. \tag{11}$$

Then, m_{dc}^* is expressed here in terms of $E_{gI}(T)$, and longitudinal and transverse effective masses to free electron mass m_o, associated with the ellipsoidal constant energy surfaces in the Si as [3,9]

$$m_{dc}^*(T) = 6^{2/3} \times \left[0.9163 \times \left(0.1905 \times \frac{E_{gI}(T=0)}{E_{gI}(T)}\right)^2\right]^{1/3}, \tag{12}$$

where $E_{gI}(T)$ is determined by Eq. (10), and similarly in the Ge by

$$m_{dc}^*(T) = 4^{2/3} \times \left[1.580 \times \left(0.082 \times \frac{E_{gI}(T=0)}{E_{gI}(T)}\right)^2\right]^{1/3}, \tag{13}$$

where $E_{gI}(T)$ is determined in Eq. (11).

Further, we will use the approximate form for m_{dv}^* in the Si obtained by Lang et al. [12], using the exact calculation including the full nonspherical-and-nonparabolic nature of the valence band structure, as

$$m_{dv}^*(T) = \left(\frac{0.443587 + 3.609528 \times 10^{-3} \times T + 1.173515 \times 10^{-6} \times T^3 + 3.025581 \times 10^{-7} \times T^4}{1 + 4.683382 \times 10^{-3} \times T + 2.286895 \times 10^{-4} \times T^2 + 7.469271 \times 10^{-7} \times T^3 + 1.727481 \times 10^{-9} \times T^4}\right)^{2/3}, \tag{14}$$

and m_{dv}^* in the Ge [3,9] can be expressed in terms of ligh hole (heavy hole) effective masses of the valence bands, spin–orbit split-off energy and the first Kohn–Luttinger parameter [13], as

$$m_{dv}^*(T) = (0.34^{3/2} + 0.042^{3/2} + 13.4^{-3/2} \times e^{-3 \times 296\,\mathrm{meV}/2k_BT})^{2.3}. \tag{15}$$

In the Si, the values of $E_{gI}(T)$, $m_{dc}^*(T)$, and $m_{dv}^*(T)$, calculated for any T using Eqs. (10), (12), and (14), respectively, are tabulated in Table 1, in which we also include the respective data given by Green [3] to calculate the relative errors (RE) defined by RE $\equiv$ 1−(Result/Data) and expressed in %.

Table 1 indicates that our chosen results are accurate to within 0.11% for $E_{gI}(T)$, 0.48% for$m_{dc}^*(T)$ and 2.65% for $m_{dv}^*(T)$, giving us some confidence in our above analytic forms for those structure–band parameters at any T.

Then, from those accurate structure–band parameters of the Si given in Table 1, our values of $n_i(T)$ at any T are computed using

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