Journal of Electron Devices, Vol. 8, 2010, pp. 293-299

© JED [ISSN: 1682 -3427]

Journal of Electron Devices
www.jeldev.org

A New and Simple Model for Plasma- and Doping-Induced Band Gap Narrowing

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Received 30 Sptember 2010, Accepted 18 October 2010

Abstract

In this paper, we present a new and simple model for the band gap narrowing (BGN) that could be applied to any semiconductor material and implemented easily in device simulators. We here apply the model to Silicon. The model is based on treating the problem considering the Coulombic forces between carriers. The model has the ability to describe any type of BGN; including plasma- and doping-induced BGN. Moreover, the model takes the temperature effects into account; an issue that is not covered well in literature. Comparisons between the model simulation results and available measurements are done showing very good agreement.

Keywords

Ambipolar Diffusion Equation (ADE), Device Simulation, Finite Difference Method (FDM), Modeling, Matlab, Parameter Extraction.

1. INTRODUCTION

Medium and highly doped semiconductor materials specially Silicon are widely used in device technology. Strange enough, the experimental values of the basic physical parameters at such doping levels, even in silicon, as well as their theoretical verification are up to now under discussion. The band gap narrowing (BGN) is one of the most important physical parameters encountered at medium and high dopings.

Earlier theoretical approaches to BGN were typically restricted to the $T = 0$ K limit. Mahan [1] performed a Hartree-Fock variational calculation of the ground state energy of the electron-donor system in n-type silicon valid up to concentrations of 10^{20} cm^{-3} assuming that the donors are distributed on a regular *fcc* sublattice. He obtained closed form expressions for Si and Ge. Jain and Roulston [2] treated the problem by the same approach as Mahan and extended the applicability of the expressions to include Si, Ge, and GaAs. Lindefelt [3] proposed models that constitute an extension of the theory of Jain and Roulston taking into account the three different electron effective mass components associated with hexagonal lattices and obtained expressions for BGN applicable to n-type and p-type 3C–, 4H–, 6H–SiC, and Si. Berggren and Sernelius [4] derived the self-energy of the electron-donor interaction from second-order perturbation theory for a random system of impurities. They included a random-phase approximation (RPA) dielectric screening in their $T = 0$ K calculation. Schenk [5] derived an analytical model for Si from a non-self-consistent finite-temperature full RPA formalism. The theoretical results of this model could be applied for finite temperatures rather than 0 K limit.

2. Optical, Rigid, and Apparent BGN

The rigid band gap energy is defined as the difference between the minimum of the conduction band and the maximum of the valence band. On the other hand, the optical band gap energy is the same as the rigid band gap if the Fermi level (E_F) is below

the edges of the bands (E_C and E_V). When the Fermi level moves above the conduction band edge (the case of n-type) or below the valance band edge (the case of p-type) or when the quasi Fermi levels move above the two edges (the case of highly excited semiconductors), then the optical band gap energy is greater than the rigid one by the amount of the increase of the Fermi levels. This could be seen from Figure 1.

According to Figure 1, the optical BGN is:

$$\begin{aligned} \Delta E_g^{op} &= E_{gi} - E_{g,optical} = \Delta E_g^{rigid} - \Delta E_F \\ &\equiv \Delta E_g - \Delta E_F \end{aligned} \quad (1)$$

where E_{qi} is the energy gap of an intrinsic material at thermal equilibrium, and ΔE_F could be evaluated (for n-type) as:

$$\Delta E_F = kT\left[F_{1/2}^{-1}\left(\frac{n}{N_C}\right)\right] \quad (2)$$

where n is the electron concentration, N_C is the effective density of states in the conduction band, T is the temperature, and k is Boltzmann's constant. The apparent BGN is calculated using Maxwell-Boltzmann (MB) statistics. The difference between the apparent and the rigid BGN is very complicated. It is usually assumed that:

$$\Delta E_g^{app} = \Delta E_g + \Delta E_g^{FD} \quad (3)$$

where ΔE_g^{FD} is a correction factor that could be written as:

$$\Delta E_g^{FD} = kT\left[F_{1/2}^{-1}\left(\frac{n}{N_C}\right) - \ln\left(\frac{n}{N_C}\right)\right] \quad (4)$$

Actually, the relation given in Eq. (3) is not that simple. There are other effects not included. In [6], it was shown that the apparent or electrical BGN is related to the rigid BGN by the equation:

$$\Delta E_g^{app} = \Delta E_g + \theta_n + \theta_p \quad (5)$$

where θ_n and θ_p are complicated functions including the density of states effect, the degeneracy effect, and the non-parabolicity effect. The degeneracy effect is included in Eq. (3) and could be calculated using Eq. (4). The density of states effect is a complicated effect and there is no closed form for it. In [6], they calculated this effect and found that it is very important because it may exceed the degeneracy effect. The non-parabolicity effect is calculated and found to be negligible. In our model, to relate the apparent (electrical) BGN to the rigid BGN we use Eq. (5) with the same approach as in [6].

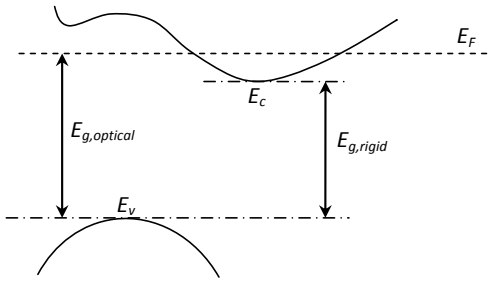
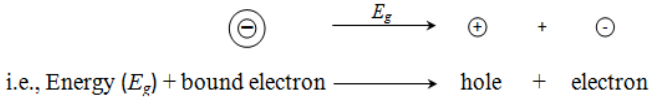


Figure 1 The difference between the rigid and optical band gap energy for n-type doping silicon.

3. Proposed BGN Model

The proposed model presented here was first introduced by Zekry [7]. We here take the main assumptions of the model and extend its approach and validity. We include Fermi-Dirac (FD) statistics in calculating the carrier concentration instead of MB statistics. Also, we include the effect of temperature through the modeling of incomplete ionization.

By definition, the energy gap is the minimum energy required to free an electron from its weakest valence bond such that it will be available for conduction in the crystal. In this process, the initial state of the electron corresponds to the top energy level in the valence band while its final state corresponds to the energy level in the bottom of the conduction band. In both states, the electron has no kinetic energy. Therefore, in principle, an amount of work which equals the rigid energy gap is required to separate an electron against the electrostatic attraction force of its partner hole to certain distance in the crystal, i.e. the separation energy of an electron-hole pair. This process could be described by the chemical reaction:



When the separation distance between the electron and its complementary hole increases, one has to spend more energy to separate them against the attraction force between the pair. As a result, the energy gap will be reduced as the distance between the electron and hole decreases. In a semiconductor material, when the concentration of electrons or of holes or both together is raised because of doping, heating or any other disturbance, the separation distance of an electron-hole pair will become smaller and consequently BGN occurs.

The BGN is normally measured by taking an intrinsic material at the same temperature as a reference for the material of interest. Consider the electron-hole pairs present in electrically polarizable medium with a relative dielectric constant ε_r and applying Coulomb's law on both materials (the material of interest with a certain doping and the intrinsic material), we can express the difference in the work done for electron-hole pair separations i.e., the difference in the energy gap ΔE_g^{rigid} as follows [7]:

$$\Delta E_g^{rigid} \equiv \Delta E_g = \frac{q}{4\pi\varepsilon_o\varepsilon_r}\left(\frac{1}{a_{he}} - \frac{1}{a_i}\right) \tag{6}$$

where a_{he} and a_i are the separation distances of an electron-hole pair in the material of interest and its reference intrinsic material.

It is important to note that our picture of the BGN is a microscopic picture rather than a macroscopic one. Also, the expression introduced in Eq. (6) could be used for any type of semiconductor at any doping level and any injection level. In general, the band gap will contract with increasing mobile carrier concentration and this reduction is the direct consequence of the electrostatic interaction between electrons in the conduction band and the holes in the valence band. We will see some applications in the following sections.

3.1 BGN in Highly-Excited Intrinsic Silicon

In this application, there are no impurities and the reduction of the energy gap will be due to electrons and holes only. Assume that we have an intrinsic semiconductor material in which equal concentrations of electrons and holes are generated by illuminating it with light of a suitable wavelength. In this material, the average spacing a_{he} between an electron and hole amounts to one half of the average distance between two consequent electrons as shown in Figure 2 [7]. So, we can write:

$$a_{he} = \frac{1}{2}a_{ee} \tag{7}$$

where the electron-electron spacing a_{ee} is related to the electron concentration n in the material by the relation:

$$a_{ee} = \frac{1}{n^{1/3}} \tag{8}$$

Substituting Eq. (7) and Eq. (8) into Eq. (6), we can get the rigid BGN for the highly excited intrinsic semiconductor:

$$\Delta E_g = \frac{2q}{4\pi\varepsilon_o\varepsilon_r}\left(n^{1/3} - n_{io}^{1/3}\right) \tag{9}$$

For high excitation, $n >> n_{io}$, then Eq. (9) reduces to:

$$\Delta E_g = \frac{q}{2\pi\varepsilon_o\varepsilon_r}\left(n^{1/3}\right) \tag{10}$$

For silicon material: $\varepsilon_r = 11.7$, then we can write the rigid BGN for highly excited Si material in eV as:

$$\Delta E_g \approx 2.46\times10^{-8}\, n^{1/3} \tag{11}$$

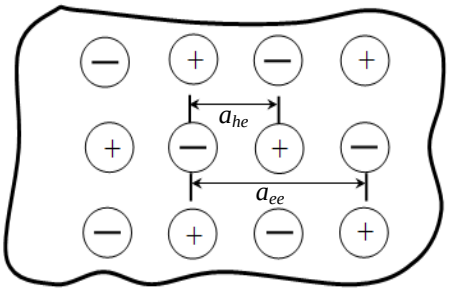


Figure 2 Average geometrical order of electrons and holes in highly excited intrinsic semiconductors.

Nilsson and Svantesson [8] observed the decay of the spectral distribution of the recombination radiation from intrinsic silicon after strongly exciting it by Q-switched ruby laser. The authors found that the reduction in the energy gap is given by the empirical formula:

$$\Delta E_g^{recombination} \approx 2.4\times10^{-8} n^{1/3} \quad (12)$$

The BGN obtained by recombination is approximately the rigid BGN, as electrons are recombined from the lowest energies of the conduction band with holes from the highest energies of the valence band. Comparing the results, we can see a good agreement with our proposed theoretical value.

3.2 BGN in Highly-Excited Doped Silicon

High-density electron-hole plasmas occur frequently in semiconductor devices such that in the lightly-doped region of the PIN diode subjected to high currents [9]. Both experimental and theoretical studies indicate that BGN effects due to dense electron-hole plasma begin to occur in silicon for an electron-hole concentration of about 10^{17} cm^{-3} which is achievable in silicon devices under highly excited electrical or optical conditions [10]. The BGN effect here is well known in literature by the name: plasma-induced band gap narrowing (PIBGN).

For highly-excited materials, $n = p >>$ doping level. So, we can assume the same distribution of electrons and holes as in the case of the intrinsic material because of the equal existence of holes and electrons. Then, we can apply the same equation handled in the previous section (Eq. (11)).

Considering other theoretical approaches, Persson *et al.* proposed a method which is based on zero-temperature formalism within the RPA [11]. Electron-electron, hole-hole, electron-hole, electron-optical phonon and hole-optical phonon interactions have been taken into account. The calculations are based on band structure data from a relativistic, full-potential band structure calculation. Their solution to find the rigid BGN for Si could be parameterized by the following equation:

$$\Delta E_g = -0.53\left(\frac{n}{10^{18}}\right)^{1/3} + 29.13\left(\frac{n}{10^{18}}\right)^{1/4} \quad (13)$$

Another model was proposed by Lowney [12], which is based on the many-body theory, extends the result of Abram *et al.* [13] originally obtained at zero temperature to room temperature.

Using our model, and changing the electron-hole concentration, we can find the rigid BGN and then calculate the optical BGN. A comparison between our results and the model of Persson *et al.* is demonstrated in Figure 3. The figure shows that our simple approach is capable in tracing the phenomenon compared to a very complicated approach.

There are not enough experimental data to compare with. Only the experimental results extracted from bipolar transistor measurements found in [9] are available. Figure 4 shows the original data of [9] along with our model, Lowney, and Persson *et al.* models.

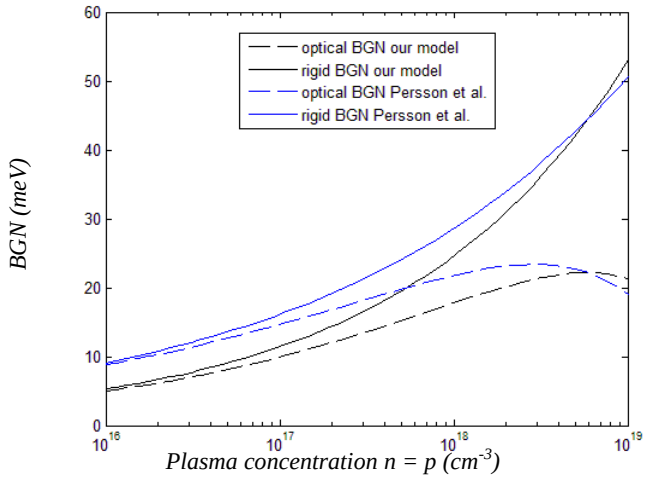


Figure 3 Comparison of rigid and optical BGN between our model and the model by Persson *et al.*

When experimental results are compared to any theoretical models, they give higher values than expected. Lowney [12] pointed to experimental uncertainties as causing difficulty for interpreting experimental data accurately.

We point out some key factors that should be considered in reevaluating the experimental data such that to decrease the discrepancy between theory and experiment. Actually, the effect of the intrinsic concentration value n_{io} is critical in manipulating the experimental results. Prior to

1990, n_{io} = 1.45×10^{10} cm^{-3} was commonly used for silicon, leading to significant deviations between the theoretically predicted and the measured behavior of devices [14]. A value of n_{io} = 1×10^{10} cm^{-3} was experimentally confirmed by Sproul and Green [15], which is a widely accepted value for silicon nowadays. The results given in [9] were interpreted using a value of n_{io} = 1.45×10^{10} cm^{-3} and thus we can't accept these results as they are. Another correction should be done for the density of states effect. Degeneracy effect was taken into consideration.

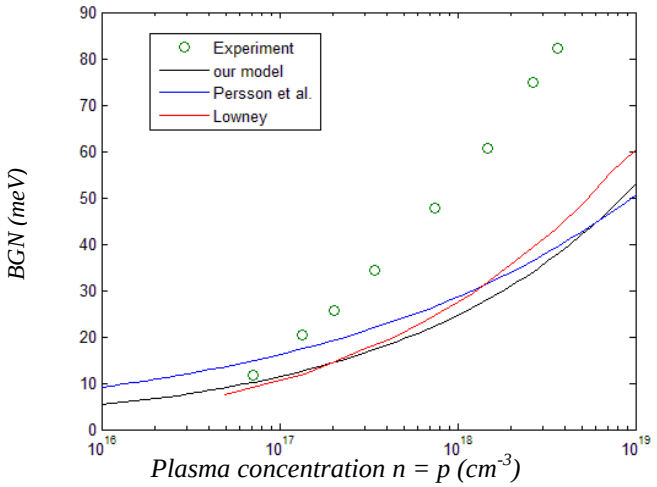


Figure 4 Comparison of rigid BGN between our model, Persson *et al.*, and Lowney models, along with the experimental data by Neugroschel *et al.*

3.3 BGN in Highly-Doped Silicon

Consider an n-type semiconductor with doping concentration N_D, the electron concentration n at thermal equilibrium is much higher than that of holes p. Since electrons are homogeneously distributed in the material, they could be considered to form a three dimensional matrix with an equal spacing a_{ee} in the three dimensions as shown in Figure 5. The holes occupy the center of some cubes as they will exist in equilibrium in these sites. Therefore, the electron-hole spacing a_{he} amounts to one half the diagonal of the cube as depicted in Figure 5, i.e.

$$a_{he} = \frac{\sqrt{3}}{2} a_{ee} \tag{14}$$

The electron-electron spacing a_{ee} can be expressed by the relation:

$$a_{ee} = \frac{1}{n^{1/3}} \tag{15}$$

Combining Eq. (14), (15), and (6) we get the rigid BGN as a function of the majority carrier concentration:

$$\Delta E_g = \frac{q}{2\sqrt{3}\pi\varepsilon_o\varepsilon_r}\left(n^{1/3} - n_{io}^{1/3}\right) \tag{16}$$

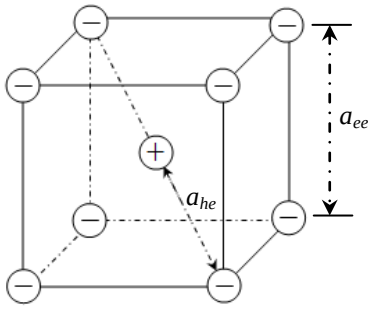


Figure 5 Electrons and holes average distribution in n-type semiconductor.

For Si: ε_r = 11.7, and for high doping $n >> n_{io}$, then Eq. (16) reduces approximately to:

$$\Delta E_g \approx 1.42\times10^{-8} n^{1/3} \tag{17}$$

which is the rigid BGN for n-type Si. For a p-type semiconductor, the above relation holds except that n is replaced by p.

To calculate the BGN based on our approach, we first evaluate the majority carrier concentration at the specified doping level and at a given temperature. This could be found by (for n-type):

$$n \approx N_D^+ = N_C F_{1/2}\left(\frac{E_F - E_C}{kT}\right) \tag{18}$$

N_D^+ could be calculated by a most recent expression for the incomplete ionization given by the Altermatt parameterization method [16].

Now, we will compare some experimental results with our model results. Also, we will compare with some theoretical theories to see the differences between our model and other models. First, consider

some optical absorption measurements as in [17] and [18]. In [17], the fundamental band gap (which gives the rigid band gap) was extracted at different temperatures T = 300, 85, and 35 K (P in Si). In [18], the rigid BGN was also extracted at T = 300 and 4 K (As in Si).

Figure 6 shows the measurements of Balakanski *et al.* [17] at T = 300 K along with our model results. Also shown some theoretically-based models: Jain *et al.* [2], Persson *et al.* [19], and Schenk [5]. The figure indicates that our model is capable in tracing the behavior of the BGN with doping either for low or high dopings while some theoretical models overestimate the BGN at high and/or low dopings.

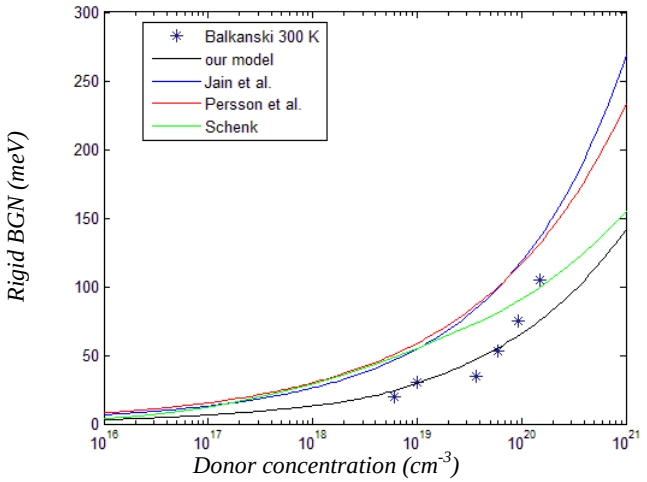


Figure 6 Comparison of rigid BGN models with experimental data for n-type Si at T = 300 K.

Figure 7 shows the measurements of Schmid [18] at T = 4 K along with our model results. Also shown some theoretically-based models previously indicated. We notice that the other theoretical models don't account for the temperature variations, because complete ionization is assumed. In all theoretical models to date, the BGN is calculated according to the doping concentration level. On the other side, in our model, we account for the incomplete ionization, as the BGN is calculated according to the majority carrier concentration.

Considering the electrical measurements, the rigid BGN ΔE_g values cannot be generally compared to the experimental electrical BGN data. This is so because the electrical BGN values were extracted from transport measurements, and are thus influenced by the transport model employed. In particular, MB statistics and the ideal density-of-states (DOS) of silicon were used [14]. We have reported the relation between the rigid and apparent BGN in Eq. (5). For instance, the difference between the electrical and rigid BGN is about 10 meV at a doping of 9.64×10^{19} cm^{-3} due to $\theta_n + \theta_p$ effect according to [8].

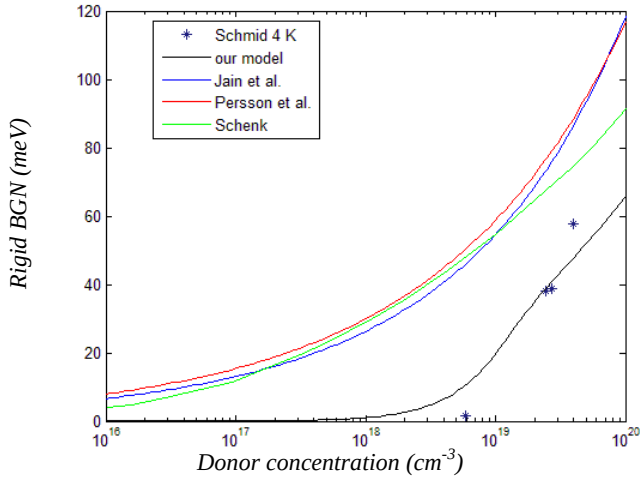


Figure 7 Comparison of rigid BGN models with experimental data for n-type Si at T = 4 K.

In Figure 8 we compare our results for the apparent BGN with that reported by del Alamo *et al.* (at T = 292 K) [20] and Weider [21] along with Persson *et al.*, Jain *et al.*, and Schenk rigid models. The results show good agreement between experiments and our model although its simplicity.

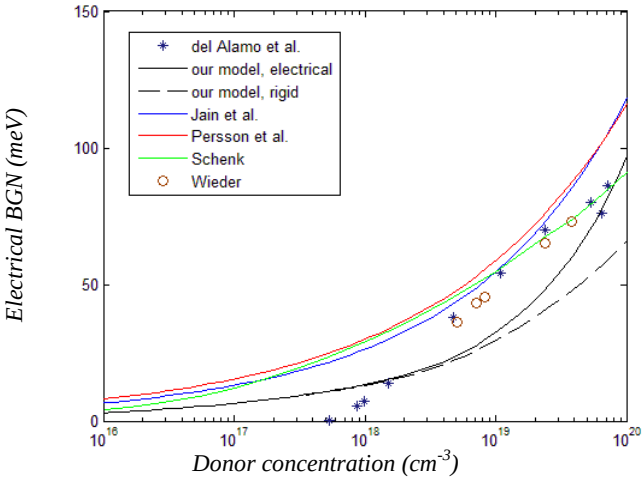


Figure 8 Comparison of electrical BGN from experiments and theoretical models with our model.

We emphasize that all experimental data should be corrected to include the effect of decreasing n_{io} because most of experimental data was interpreted for high value of it. Also, when calculating the p-n product like in [20], they assumed complete ionization which is not true even at room temperature. Actually, when including the later effect we see that the BGN calculated should be revised and decreased at least by an average value of about 5 meV for donor concentration in the range of 5×10^{18} to 2×10^{19} cm^{-3}.

4. Conclusions

In this paper, we presented a simple model for the BGN based on some basic physical concepts. The model gives a generalized approach for the BGN occurred at any doping level and could be applied to any semiconductor material. In this model, we proved that the BGN depends mainly on the majority carrier concentration. Plasma- and doping-induced BGN could be found by the same approach instead of treating them by different approaches as assumed in literature. We compared the model results by the available experiments at different temperatures and good agreement was found. More effort will be directed to applying the model considering other semiconductor materials.

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