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Modelling heavy doping effects for low temperature device simulations

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Abstract: A new temperature dependent apparent bandgap narrowing model, appropriate for low temperature device simulations is proposed. The model is based on the decomposition of apparent bandgap narrowing in equilibrium into different contributions at 300K and on the theoretical temperature dependence of each phenomenon. Specific heavy doping effects that can be important at low temperatures are discussed. Temperature dependence of apparent bandgap narrowing in equilibrium is more significant at high concentration of ionized impurities, where apparent bandgap narrowing decreases with decreasing temperature, as a consequence of temperature dependent degeneracy.

1. INTRODUCTION

Heavily doped regions exist in almost every silicon device operating at low temperatures. Increased interest in low-temperature operation of semiconductor devices requires for improved simulation tools, appropriate for low-temperature device modelling. For the purposes of device modelling, heavy doping effects are almost universally described with apparent bandgap narrowing in equilibrium ΔG_0 or closely related effective intrinsic concentration in equilibrium n_{ieff0} . The relatively straightforward empirical validation of ΔG_0 and its simplicity are the most important reasons for the popularity of this approach. As shown in [1,2], ΔG_0 consists of two main contributions: - actual bandgap narrowing in equilibrium ΔE_{g0} as a consequence of actual band distortion influencing steady-state transport of minority carriers (shift of band edges, formation of band tails and other distortion mechanisms), and - degeneracy in equilibrium ΔE_{FD0} as a result of the invalidity of Boltzmann statistics in the high doping regime:

$$p_0 n_0 = n_{ieff0}^2 = n_{i0}^2 \exp\left(\frac{\Delta G_0}{kT}\right) = n_{i0}^2 \exp\left(\frac{\Delta E_{g0} + \Delta E_{FD0}}{kT}\right) \quad (1)$$

During the past two decades, a lot of experimental and theoretical work studying doping dependence of ΔG_0 at room temperature has been done [3,4,5]. The authors in [3] illuminated the theory underlying the electrical characterization of heavily doped regions and the assumptions necessary for extraction of ΔG_0 . In contrast with room temperature work, little theoretical and experimental work concerning ΔG_0 at low temperatures has been performed. However, two approaches related to the modelling of ΔG_0 at low temperatures are most frequently in use: - the apparent bandgap narrowing is considered as temperature independent, and - pure theoretical models with their temperature dependence are employed. The purpose of this work is to present a new temperature dependent apparent bandgap narrowing model, appropriate for device simulations. The derivation is based on critical analysis of different phenomena involved in ΔG_0 at room temperature, and the theoretical prediction of the

temperature dependence of each phenomenon. We found that apparent bandgap narrowing is a strong function of temperature, especially in p -type silicon at high concentration of impurities.

2. APPARENT BANDGAP NARROWING AT 300K

For the purposes of analysis, a heavily doped N^+ region in quasi-equilibrium was considered. The validity of Boltzmann statistics for minority carriers was assumed. By means of the rigid band model [1], the equilibrium carrier concentrations can be described with (2) and (3):

$$n_0 = N_C \frac{2}{\sqrt{\pi}} F_{1/2} \left(\frac{E_F - E_{C0}}{kT} \right), \quad (2)$$

$$p_0 = N_V \exp \left(\frac{E_{V0} - E_F}{kT} \right), \quad (3)$$

where N_C and N_V are effective densities of states in conduction and the valence band, respectively; $F_{1/2}$ is Fermi-Dirac integral of order 1/2, and E_{C0} and E_{V0} are conduction and valence band edges, respectively. The actual bandgap narrowing is determined by the position of the band edges, and degeneracy is included in the Fermi-Dirac integral. Taking into account (1), (2), (3), together with the space charge neutrality assumption [6], the following relationship can be obtained:

$$N_D^* = N_C \frac{2}{\sqrt{\pi}} F_{1/2} \left(\frac{E_{V0} - E_{C0}}{kT} - \ln \left(\frac{n_{i0}^2 \exp \left(\frac{\Delta G_0}{kT} \right)}{N_V N_D^*} \right) \right). \quad (4)$$

If we further consider the relation between intrinsic carrier concentration in equilibrium n_{i0} and bandgap in the absence of heavy doping effects E_{g0}^0 ($n_{i0}^2 = N_C N_V \exp(-E_{g0}^0/kT)$), and take into account the inverse Fermi function of order 1/2 ($G_{1/2}(2\pi^{-1/2}F_{1/2}(x)) = x$), the following expressions for ΔE_{g0} (5) and ΔE_{FD0} (6) can be derived:

$$\Delta E_{g0}(N_D^*, T) = \Delta G_0(N_D^*, T) + kT G_{1/2} \left(\frac{N_D^*}{N_C(T)} \right) - kT \ln \left(\frac{N_D^*}{N_C(T)} \right), \quad (5)$$

$$\Delta E_{FD0}(N_D^*, T) = -kT G_{1/2} \left(\frac{N_D^*}{N_C(T)} \right) + kT \ln \left(\frac{N_D^*}{N_C(T)} \right). \quad (6)$$

Analogous expressions can be derived for heavily doped P^+ regions as well. If the concentration of ionized impurities is known - at room temperature total ionization of impurities can be assumed - ΔE_{g0} and ΔE_{FD0} can be recalculated from any ΔG_0 data.

Our analysis was based on the experimental ΔG_0 data given in [4] (data from many authors recalculated for the unified mobility model) and [5]. The values for N_C , N_V and E_{g0}^0 were taken from [7]. $G_{1/2}$ was approximated according to [8]. Since most of the experimental procedures need the value of n_{i0} to render ΔG_0 [4], the experimental data were first recalculated to be consistent with our set of N_C , N_V and E_{g0}^0 according to the procedure described in [4]. ΔE_{g0} data obtained from recalculated ΔG_0 data are presented in Fig.1. Good agreement between p - and n -type data is retained due to similar degeneracies in p - type and n - type silicon at room temperatures.

The shift of band edges was assumed to be the dominant mechanism present in the actual bandgap

narrowing. Therefore, the theoretical model for band edge shifts was used in order to find a fit for ΔE_{g0} data. Although different dependencies for gap shift in p - and n -type of silicon are proposed by theoretical models, we neglected this difference because of good agreement between existing n - and p -type experimental data, and because of the small quantity of p -type data at doping concentrations higher than 10^{19} cm^{-3} . Complete ΔE_{g0} data were in best agreement with the model presented in [9] describing the doping dependence of ΔE_{g0} in n -type silicon. The authors in [9] found $N^{1/2}$ dependence at low doping concentrations and $N^{1/4}$ dependence at high doping concentrations, with transition point around $2 \cdot 10^{18} \text{ cm}^{-3}$. ΔE_{g0} data were therefore fitted with (7)

$$\Delta E_{g0} = \left((a_{300} N^{1/2})^{-c} + (b_{300} N^{1/4})^{-c} \right)^{-1/c} \quad (7)$$

where N is ionized donor or acceptor concentration [cm^{-3}], and a_{300} , b_{300} and c are fitting parameters (c determines the sharpness of transition between two dependencies). The best fit obtained with $a_{300} = 4.373 \cdot 10^{-11} [\text{eV cm}^{3/2}]$, $b_{300} = 1.272 \cdot 10^{-6} [\text{eV cm}^{3/4}]$ and $c=4$ is presented in Fig.1. Optical measurements of gap narrowing [2] were found to be in good agreement both with electrically obtained experimental data and with the theory (Fig.1), confirming the assumption of rigid shrinkage as a dominant actual bandgap narrowing mechanism.

Finally, by combining theoretical expressions for degeneracy (6) and experiment-based fit for actual bandgap narrowing (7), the apparent bandgap narrowing is obtained. Detailed discussion concerning analysis of apparent bandgap narrowing at 300K and comparison with other approaches and models is given in [10].

Fig.1: Doping dependence of actual bandgap narrowing. All symbols except ▼ correspond to the actual bandgap narrowing obtained from experimental apparent bandgap narrowing data: ◆ is taken from [5], all others are taken from [4] (notation is the same as in [4]). All data except ◆ and ▲ were recalculated for this work n_{i0} . ▼ represents optical data taken from [2]. The solid line represents the best fit for actual bandgap narrowing based on electrical data (eq. (7)).

3. TEMPERATURE DEPENDENCIES OF ΔE_{g0} , ΔE_{FD0} and ΔG_0

3.1 Temperature dependence of ΔE_{g0}

To find the temperature dependence of ΔE_{g0} , the theoretically predicted temperature dependence of rigid gap shrinkage was considered. As suggested in [9], the $n^{1/4}$ part of the ΔE_{g0} curve describing

actual bandgap narrowing in the high doping concentration regime is temperature independent. By contrast, the low concentration portion of ΔE_{g0} curve is temperature dependent; according to [9] it exhibits $T^{1/2}$ temperature dependence. These theoretical results are in reasonable agreement with temperature dependence of optical data [2], reported for 20K and recalculated for 300K. Therefore, to obtain the temperature dependent expression for ΔE_{g0} , a_{300} term in (7) is replaced with $a(T)$ ($a(T)=a_{300}(T/300)^{-1/2}$). The results are presented in Fig.2.

Fig.2: Temperature and ionized doping dependence of actual bandgap narrowing, calculated according to (7).

3.2 Temperature dependence of ΔE_{FD0}

The temperature dependence of conduction and valence band degeneracy was calculated according to (6) and its counterpart for *p*-type silicon. Temperature dependencies of N_c and N_v were taken from [7]. The results are presented in Fig.3. It is obvious that degeneracy is much more temperature dependent than actual bandgap narrowing, especially in *p*-type silicon.

Fig.3: Temperature and ionized doping dependence of degeneracy, obtained from (6).

3.3 Temperature dependence of ΔG_0

The temperature dependence of apparent bandgap narrowing was obtained as a sum of temperature dependent actual bandgap narrowing and temperature dependent degeneracy. The results are presented in Fig.4. The temperature dependence of ΔG_0 in the low ionized impurity concentration regime is a consequence of the temperature dependency of ΔE_{g0} . This temperature dependence is not significant and can be neglected in comparison with temperature dependence at high concentration of ionized impurities ($>10^{18} \text{ cm}^{-3}$), which is a consequence of temperature dependent degeneracy. The temperature dependence is more pronounced in *p*-type silicon.

Fig.4: Temperature and doping dependence of apparent bandgap narrowing obtained by combining temperature and doping dependence of actual bandgap narrowing and degeneracy.

4. DISCUSSION

In order to verify the results obtained, it is necessary to compare our model with existing experimental data and with models used by other authors. Some apparent bandgap narrowing data measured at different temperatures are available in the limited temperature and doping range ($T > 150\text{K}$, $N = 2 \cdot 10^{19} \text{ cm}^{-3}$, $1.4 \cdot 10^{20} \text{ cm}^{-3}$) [4,5], and indicate the temperature independence of apparent bandgap narrowing. Our results are in reasonable agreement with this conclusion for a given temperature range. Comparison with other models is not straightforward, due to the lack of the work on modelling low temperature apparent bandgap narrowing, and due to frequent misuse of apparent bandgap narrowing in carrier concentration and transport equations (it is often neglected that degeneracy is embedded in ΔG_0).

It is worth mentioning that our temperature dependent model for ΔG_0 is an extension of the room temperature model to low temperatures. In other words, the definite validity of the model is restricted to the conditions valid in heavily doped emitters under low-level injection. In this case, use of ionized impurity concentration as an independent variable is straightforward. The model cannot be used in nonequilibrium carrier concentration and transport equation without generalization of actual bandgap narrowing - it is impossible to extract an arbitrary nonequilibrium value of actual bandgap narrowing from an equilibrium *pn* product. Although appropriate for most practical conditions, this generalization is not valid in the high-level injection regime. Concentration of minority carriers, comparable to the concentration of majority carriers, is in disagreement with the assumptions employed through the derivation of our model and the assumptions employed through the derivation of the theoretical model for rigid band shrinkage [9]. The problem of high-level injection and related heavy doping effects at low temperatures has been discussed in [11]. In order to account for different apparent bandgap narrowing, resulting from high-level injection of minority carriers from the emitter to the base of an advanced bipolar transistor operating at low temperatures, the authors in [11] introduced the injection-induced bandgap

narrowing.

Another uncertainty concerning extension of the room temperature apparent bandgap narrowing to low temperatures is related to minority carriers in the band tails, which are unimportant at room temperature. As apparent bandgap narrowing in equilibrium is a consequence of minority carrier transport [3], it can account for mobile minority carriers only. Since minority carriers in the tails are considered to be immobile, and their concentration is low compared to the concentration of mobile minority carriers at room temperature [12], they do not contribute to the apparent bandgap narrowing. As shown in [12], the portion of minority carriers in the tails in relation to those in the delocalized states increases rapidly with decreasing temperature. Although our low temperature apparent bandgap narrowing does not account for minority carriers in the tails, it is not yet clearly understood what the influence is of the high portion of minority carriers in the tails on minority carrier transport (apparent bandgap narrowing is primarily the minority carrier transport parameter).

Recent work [13] emphasizes the importance of non-parabolicity in the p -type of silicon, modelled by doping dependence of effective mass. Non-parabolicity of the valence band negates the use of the rigid band model [1], complicating the inclusion of heavy doping effects in device modelling. Nevertheless, if the doping and temperature dependence of effective densities of states is known, the derivation of the apparent bandgap narrowing model can also be done for the non-rigid band model.

The uncertainties described emphasize the necessity for more theoretical and experimental work related to heavy doping effects at low temperatures. Moreover, they prove the adequacy of the proposed approach to the low temperature apparent bandgap narrowing, splitting the apparent bandgap narrowing into contributions of different physical origin.

5. CONCLUSIONS

A new approach to the temperature dependence of apparent bandgap narrowing in equilibrium is presented, based on the decomposition of ΔG_0 into different contributions at 300K and on the theoretical temperature dependence of each phenomenon. ΔG_0 exhibits strong temperature dependence in the high doping regime, as a consequence of temperature dependent degeneracy. Due to the lack of adequate experimental data, verification of the model in the wide range of temperatures and doping concentrations is not yet possible. Although it is clear that the model presented cannot account for every heavy doping phenomenon that can be important at low temperatures, the authors believe that an improved model for heavy doping phenomena at low temperatures is proposed, which is appropriate for low temperature device simulations.

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