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COMMUNICATIONS

COUPLED DEFECT LEVEL RECOMBINATION IN THE P—N JUNCTION

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The well known Shockley-Read-Hall (SRH) model considers emission and capture processes at defects exhibiting a single level or multiple non-coupled levels in the band gap of the semiconductor. The present paper generalizes the model to the case of two mutually coupled defect levels acting as trapping centres. If the intercenter transition is not considered, the model reduces to the case of two non-coupled levels treated by the SRH model.

K e y w o r d s: tunneling, coupled levels

1 THEORY

The paper considers the existence of lattice defects (electrically active traps) having two coupled defect levels (CDL) in the band gap of the semiconductor between which thermal exchange of free charge carriers takes place. The two coupled capture centres are denoted by indices a and b with corresponding energies E_t^a and E_t^b. We assume that the deep level E_t^a lies above E_t^b. The well-known SRH model does not consider this case. The commercially available simulator of electron devices and structures DESSIS already contains a CDL recombination model [1, 2] which is, however, relatively complicated.

Our CDL model considers ten exchange processes of free charge carriers between the capture centres and the conduction and valence bands. These processes are schematically shown in Fig. 1.

Each of the ten exchange processes (five capture and five emission processes) is characterized by its escape time. If the unknown occupation probability of a trapping centre is divided by the escape time of a capture process, or the probability of non-occupation by the escape time of an emission process, one obtains the frequency of the particular exchange process. The frequencies of exchange processes allow to build two equations with two unknown variables, the occupation probabilities of centres a and b. Their solution leads to a quadratic equation yielding finally the occupation probabilities. Then, in terms of the ten escape times and of the evaluated occupation probabilities of centres a and b one can correctly define the SRH and CDL recombination rates contained in the continuity equations [3]. The quasi-static continuity equations for electrons and holes can be written as

$$\frac{1}{q}\frac{\mathrm{d}J_{\mathrm{D}}^{e}(x)}{\mathrm{d}x} = U_{\mathrm{SRH}}(x) + U_{\mathrm{CDL}}^{e}(x)\,, \tag{1}$$

$$-\frac{1}{q}\frac{\mathrm{d}J_{\mathrm{D}}^{h}(x)}{\mathrm{d}x} = U_{\mathrm{SRH}} + U_{\mathrm{CDL}}^{h}(x)\,, \tag{2}$$

where J represents the current density, U stands for the generation-recombination rates, x is the coordinate, q is the electron charge and the indices have their obvious meanings.

In our model, the standard SRH electron and hole generation-recombination rates are given as

$$U_{\mathrm{SRH}} = \Big\{\Big(\frac{\tau_{\mathrm{S}}^{a}}{\tau_{\mathrm{Re}}^{a}\tau_{\mathrm{Rh}}^{a}} - \frac{\tau_{\mathrm{S}}^{a}}{\tau_{\mathrm{Ge}}^{a}\tau_{\mathrm{Gh}}^{a}}\Big) + \Big(\frac{\tau_{\mathrm{S}}^{b}}{\tau_{\mathrm{Re}}^{b}\tau_{\mathrm{Rh}}^{b}} - \frac{\tau_{\mathrm{S}}^{b}}{\tau_{\mathrm{Ge}}^{b}\tau_{\mathrm{Gh}}^{b}}\Big)\frac{N_t}{2}\,, \tag{3}$$

where N_t is the density of traps and the capture and emission escape times are defined as

$$\frac{1}{\tau_{\mathrm{Re}}^{a,b}(x)} = v_{\mathrm{th}}^{e}\sigma_{e}^{a.b}n(x)\,, \tag{4}$$

$$\frac{1}{\tau_{\mathrm{Rh}}^{a,b}(x)} = v_{\mathrm{th}}^{h}\sigma_{h}^{a.b}p(x)\,, \tag{5}$$

$$\frac{1}{\tau_{\mathrm{Ge}}^{a,b}} = v_{\mathrm{th}}^{e}\sigma_{e}^{a,b}N_C\exp\big(-\frac{E_t^{a,b}}{kT}\,, \tag{6}$$

$$\frac{1}{\tau_{\mathrm{Gh}}^{a,b}} = v_{\mathrm{th}}^{h}\sigma_{h}^{a,b}N_V\exp\big(-\frac{E_g - E_t^{a,b}}{kT}\,. \tag{7}$$

Here, the thermal electron and hole velocities are $v_{\mathrm{th}}^{e,h} = \sqrt{3kT/m_{e,h}^{*}}$, $\sigma_e^{a,b}$ and $\sigma_h^{a,b}$ are electron and hole capture

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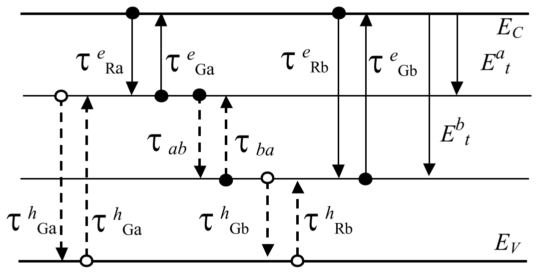

Fig. 1. Ten exchange processes involved in the CDL model. Energies E_t^a and E_t^b are taken with respect to the conduction band.

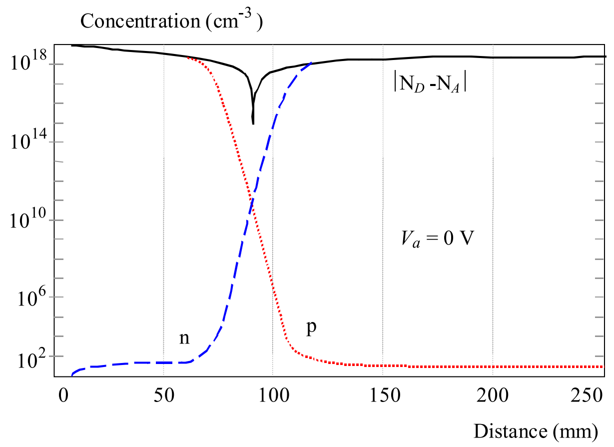

Fig. 2. Concentration profile of simulated PN diode

cross-sections belonging to capture levels a and b, $n(x)$ and $p(x)$ are actual densities of electrons and holes.

The sums of the reciprocal values of the capture and emission escape times are denoted as

$$\frac{1}{\tau_S^{a,b}} = \frac{1}{\tau_{\mathrm{Re}}^{a,b}} + \frac{1}{\tau_{\mathrm{Ge}}^{a,b}} + \frac{1}{\tau_{\mathrm{Gh}}^{a,b}} + \frac{1}{\tau_{\mathrm{Rh}}^{a,b}}\,, \tag{8}$$

$$\frac{1}{\tau_{\mathrm{ReGh}}^{a,b}} = \frac{1}{\tau_{\mathrm{Re}}^{a,b}} + \frac{1}{\tau_{\mathrm{Gh}}^{a,b}}\,. \tag{9}$$

On separating the SRH model, the remaining part is the CDL electron and hole recombination model that can be expressed in terms of its CDL generation-recombination rates

$$U_{\mathrm{CDL}}^e(x) = \Big\{\frac{1}{\tau_{\mathrm{Re}}^a} + F_{\mathrm{CDL}}^a\Big(\frac{1}{\tau_{\mathrm{Re}}^a} + \frac{1}{\tau_{\mathrm{Ge}}^a}\Big) + \frac{1}{\tau_{\mathrm{Re}}^b} + F_{\mathrm{CDL}}^b\Big(\frac{1}{\tau_{\mathrm{Re}}^b} + \frac{1}{\tau_{\mathrm{Ge}}^b}\Big)\Big\}\frac{N_t}{2}\,, \tag{10}$$

$$U_{\mathrm{CDL}}^h(x) = \Big\{\frac{1}{\tau_{\mathrm{Gh}}^a} + F_{\mathrm{CDL}}^a\Big(\frac{1}{\tau_{\mathrm{Rh}}^a} + \frac{1}{\tau_{\mathrm{Gh}}^a}\Big) + \frac{1}{\tau_{\mathrm{Gh}}^b} + F_{\mathrm{CDL}}^b\Big(\frac{1}{\tau_{\mathrm{Rh}}^b} + \frac{1}{\tau_{\mathrm{Gh}}^b}\Big)\Big\}\frac{N_t}{2}\,, \tag{11}$$

where the coupling functions F_{CDL}^a and F_{CDL}^b are

$$F_{\mathrm{CDL}}^a = r_{ab}(1 \mp D_a) - \frac{\tau_S^a}{\tau_{\mathrm{ReGh}}^b} \pm D_a\tau_S^a\Big(\frac{1}{\tau_{\mathrm{ReGh}}^a} + \frac{1}{\tau_{\mathrm{ReGh}}^b}\Big), \tag{12}$$

$$F_{\mathrm{CDL}}^b = -r_{ab}(1 \mp D_b) - \frac{\tau_S^b}{\tau_{\mathrm{ReGh}}^a} \pm D_b\tau_S^b\Big(\frac{1}{\tau_{\mathrm{ReGh}}^a} + \frac{1}{\tau_{\mathrm{ReGh}}^b}\Big). \tag{13}$$

Functions r_{ab} and r_{ba} are the coupling parameters of the trap levels E_t^a and E_t^b expressed as

$$r_{ab} = \frac{\frac{\tau_{ab}}{\tau_S^b} + \frac{\tau_S^a}{\tau_S^b} + \exp\big(-\frac{E_t^b - E_t^a}{kT/2}\big)}{1 - \exp\big(-\frac{E_t^b - E_t^a}{kT/2}\big)}\,, \tag{14}$$

$$r_{ba} = \frac{\frac{\tau_{ab}}{\tau_S^a} + 1 + \frac{\tau_S^b}{\tau_S^a}\exp\big(-\frac{E_t^b - E_t^a}{kT/2}\big)}{1 - \exp\big(-\frac{E_t^b - E_t^a}{kT/2}\big)}\,, \tag{15}$$

where τ_{ab} is the coupled escape time defined as

$$\frac{1}{\tau_{ab}} = \Big(v_{\mathrm{th}}^e\frac{\sigma_e^a\sigma_e^b}{\sigma_e^a + \sigma_e^b} + v_{\mathrm{th}}^h\frac{\sigma_h^a\sigma_h^b}{\sigma_h^a + \sigma_h^b}\Big)N_t\,. \tag{16}$$

Coefficients of the quadratic equations A_a, A_b, B_a, B_b, C_a and C_b are given by

$$A_a = \frac{\tau_S^b}{\tau_S^a}\frac{1}{\tau_{ab}}\Big(1 - \exp\frac{E_t^a - E_t^b}{kT/2}\Big), \tag{17}$$

$$A_b = -\frac{\tau_S^a}{\tau_S^b}\frac{1}{\tau_{ab}}\Big(1 - \exp\frac{E_t^a - E_t^b}{kT/2}\Big), \tag{18}$$

$$B_a = \frac{1}{\tau_S^a} + \frac{1}{\tau_{ab}} + \frac{\tau_S^b}{\tau_S^a}\frac{1}{\tau_{ab}}\exp\frac{E_t^a - E_t^b}{kT/2} - \frac{\tau_S^b}{\tau_{ab}}\Big(1 - \exp\frac{E_t^a - E_t^b}{kT/2}\Big)\Big(\frac{1}{\tau_{\mathrm{Re}}^a} + \frac{1}{\tau_{\mathrm{Gh}}^a} + \frac{1}{\tau_{\mathrm{Re}}^b} + \frac{1}{\tau_{\mathrm{Gh}}^b}\Big), \tag{19}$$

$$B_b = \frac{1}{\tau_S^b} + \frac{1}{\tau_{ab}}\exp\frac{E_t^a - E_t^b}{kT/2} + \frac{\tau_S^a}{\tau_S^b}\frac{1}{\tau_{ab}} + \frac{\tau_S^a}{\tau_{ab}}\Big(1 - \exp\frac{E_t^a - E_t^b}{kT/2}\Big)\Big(\frac{1}{\tau_{\mathrm{Re}}^a} + \frac{1}{\tau_{\mathrm{Gh}}^a} + \frac{1}{\tau_{\mathrm{Re}}^b} + \frac{1}{\tau_{\mathrm{Gh}}^b}\Big), \tag{20}$$

$$C_a = -\Big\{\frac{1}{\tau_{\mathrm{Re}}^a} + \frac{1}{\tau_{\mathrm{Gh}}^a} + \frac{\tau_S^b}{\tau_{ab}}\Big(\frac{1}{\tau_{\mathrm{Re}}^a} + \frac{1}{\tau_{\mathrm{Gh}}^a} + \frac{1}{\tau_{\mathrm{Re}}^b} + \frac{1}{\tau_{\mathrm{Gh}}^b}\Big)\exp\frac{E_t^a - E_t^b}{kT/2}\Big\}, \tag{21}$$

$$C_b = -\Big\{\frac{1}{\tau_{\mathrm{Re}}^b} + \frac{1}{\tau_{\mathrm{Gh}}^b} + \frac{\tau_S^b}{\tau_{ab}}\Big(\frac{1}{\tau_{\mathrm{Re}}^a} + \frac{1}{\tau_{\mathrm{Gh}}^a} + \frac{1}{\tau_{\mathrm{Re}}^b} + \frac{1}{\tau_{\mathrm{Gh}}^b}\Big)\Big\} \tag{22}$$

and the discriminants of the quadratic equations are

$$D_{a,b} = \sqrt{1 - \frac{4A_{a,b}C_{a,b}}{B_{a,b}^2}}\,. \tag{23}$$

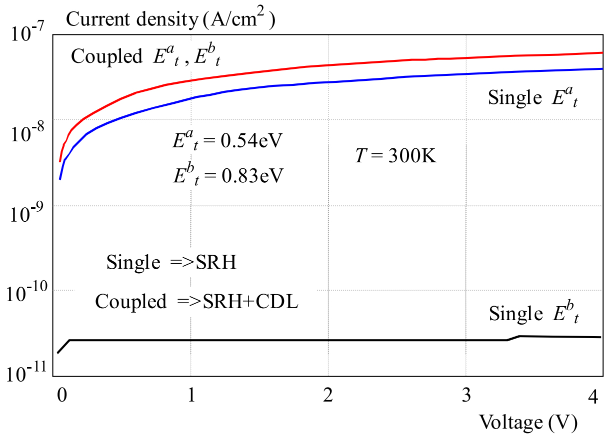

Fig. 3. Comparison of our CDL model with single SRH model of a PN diode contaminated by gold

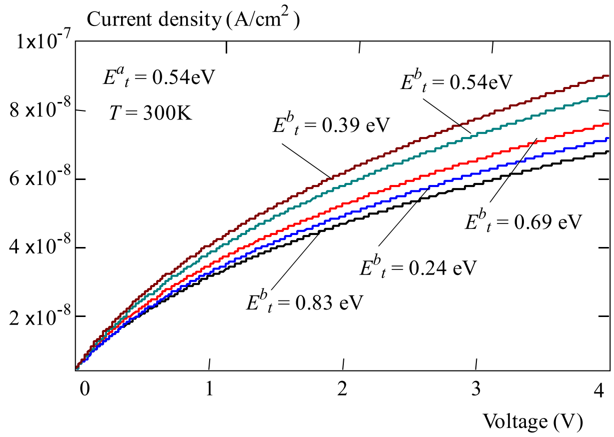

Fig. 4. Reverse I-V characteristics with CDL effect with $E_t^a = 0.55$ eV and various E_t^b

As long as we do not consider tunnelling of free charge carriers between the trap centres and the conduction or valence band, thus the trap assisted tunnelling, it must hold $U_{\rm CDL}^e \equiv U_{\rm CDL}^e$. This identity expresses the fact that the change in the amount of electrons in the conduction band due to generation and recombination is the same as the change in the amount of holes in the valence band. This is why it is enough to compute one generation-recombination rate only, either $U_{\rm CDL}^e$ or $U_{\rm CDL}^h$, trying to minimize the rounding error. It should be noted that the formulae for $U_{\rm CDL}^e$ and $U_{\rm CDL}^h$ hold only if $E_t^a \neq E_t^b$.

2 SIMULATION RESULTS

The new CDL recombination model was employed to simulate a PN diode prepared on a (111)-oriented phosphorous-doped silicon substrate ($N_D = 2.5 \times 10^{18}{\rm cm}^{-3}$) by boron diffusion from an infinite source with surface concentration $N_A = 10^{19}{\rm cm}^{-3}$. The concentration profile $|N_D - N_A|$ of the simulated PN diode in thermodynamic equilibrium along with distributions of free electrons and holes are shown in Fig. 2.

Figure 3 displays the simulated reverse $I-V$ curve of the PN diode contaminated by gold which forms two bands of traps, one of acceptor type with a distance of $E_t^a = 0.54$ eV from the conduction band edge, and one of donor type with its peak lying at a distance of $E_t^b = 0.83$ eV from the conduction band edge, with the same effective cross sections $\sigma_{e,h}^{a,b} = 5 \times 10^{-15}{\rm cm}^2$. The concentration of gold was assumed to be $N_t = 5 \times 10^{14}{\rm cm}^{-3}$. Simulations reveal that if the CDL effect is not considered, the donor level E_t^b has no effect upon the $I-V$ curves of the PN diode. However, if we assume coupling between the deep levels E_t^a and E_t^b, the impact of the donor level E_t^b is significant.

Figure 4 shows the reverse $I-V$ characteristics taking into account the CDL effect, with effective cross section $\sigma_{e,h}^{a,b} = 5 \times 10^{-15}{\rm cm}^2$, constant $E_t^a = 0.55$ eV and various $E_t^b = 0.83$, 0.69, 0.54, 0.39 and 0.24 eV.

3 CONCLUSION

As mentioned previously, the presented model assumes $E_t^a \neq E_t^b$. The extreme case, when $E_t^a \cong E_t^b$, results in $U_{\rm CDL}^e = U_{\rm CDL}^e = U_{\rm SRH}$. In other words, the right side of continuity equations (1) and (2) reduces to $U_{\rm SRH} + U_{\rm CDL} \cong 2U_{\rm SRH}$. In the other extreme case, when $E_t^a - E_t^b \cong E_g$, thus when the distance between the trap levels E_t^a and E_t^b is big and approaches the band gap E_g, the contributions of both SRH capture and emission as well as of the CDL effect are negligible, $U_{\rm SRH} + U_{\rm CDL} \cong 0$. It is obvious that the CDL effects has a stronger influence in wide gap semiconductors, particularly if dopants or defects exhibit more than two coupled levels in the forbidden band. A more accurate model that is currently under development takes into account that the levels are broadened into band of traps due to multiphonon excitation.

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