Derivation interface traps

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1 Shockley-Read-Hall recombination expansion

Shockley-Read-Hall recombination can be derived by stating that the 4 processes that can occur from a trap must follow detailed balance. the 4 processes are electron trapping and detrapping and hole trapping and detrapping. It's theoretical framework was first published by Shockley and Read [2]. For a regular trap we have 4 processes

$$R_n^{SRH} = C_n^{SRH} \cdot n \cdot N_t \cdot (1 - f_t) \tag{1}$$
$$R_p^{SRH} = C_p^{SRH} \cdot p \cdot N_t \cdot f_t \tag{2}$$
$$G_n^{SRH} = C_n^{SRH} \cdot n_t \cdot N_t f_t \tag{3}$$
$$G_p^{SRH} = C_p^{SRH} \cdot p_t \cdot N_t (1 - f_t), \tag{4}$$

where Eq. 1 is equation 2.5 as published by Shockley and Read [2] and Eq. 2 are the capture rates for electrons and holes respectively and Eq. 3 and Eq. 4 are the emission rates for electrons and holes, N_t is the density of traps, n and p are the electron and hole densities, n_t and p_t are electron and hole densities when the quasi Fermi level matches he trap energy.

In the case of interface traps we would like to make them accessable from bothe the left and the right side of the interface. This leads to a doubling of the number of rates, as we now have every generation and recombination

term from the left or the right side of the interface. This leads to

$$R_{n^+} = C_{cn+} \cdot n^+ \cdot N_t \cdot (1 - f_t) = a^+ \cdot (1 - f_t) \tag{5}$$
$$R_{n^-} = C_{cn-} \cdot n^- \cdot N_t \cdot (1 - f_t) = a^- \cdot (1 - f_t) \tag{6}$$
$$R_{p^+} = C_{cp+} \cdot p^+ \cdot N_t \cdot f_t = b^+ \cdot f_t \tag{7}$$
$$R_{p^-} = C_{cp-} \cdot p^- \cdot N_t \cdot f_t = b^- \cdot f_t \tag{8}$$
$$G_{n^+} = C_{en+} \cdot n_t^+ \cdot N_t \cdot f_t = c^+ \cdot f_t \tag{9}$$
$$G_{n^-} = C_{en-} \cdot n_t^- \cdot N_t \cdot f_t = c^- \cdot f_t \tag{10}$$
$$G_{p^+} = C_{ep+} \cdot p_t^+ \cdot N_t \cdot (1 - f_t) = d^+ \cdot (1 - f_t) \tag{11}$$
$$G_{p^-} = C_{ep-} \cdot p_t^- \cdot N_t \cdot (1 - f_t) = d^- \cdot (1 - f_t), \tag{12}$$

where the left and right side of the interface are denoted by $+$ and $-$. As in the regular case, generation and recombination rates for electrons and holes must be equal which yields

$$R^{SRH} = R_{n^+} + R_{n^-} - G_{n^+} - G_{n^-} = R_{p^+} + R_{p^-} - G_{p^+} - G_{p^-} \tag{13}$$
$$(a^+ + a^- + d^+ + d^-) \cdot (1 - f_t) = (b^+ + b^- + c^+ + c^-) \cdot f_t \tag{14}$$

This means that for f_t we find

$$f_t = \frac{a^+ + a^- + d^+ + d^-}{a^+ + a^- + b^+ + b^- + c^+ + c^- + d^+ + d^-} \tag{15}$$

and for $1 - f_t$ we find

$$1 - f_t = \frac{b^+ + b^- + c^+ + c^-}{a^+ + a^- + b^+ + b^- + c^+ + c^- + d^+ + d^-}.$$

To get to discretised continuity equations we now need to assign positions on the grid to $n_{(t)}^{+/-}$ and $p_{(t)}^{+/-}$. As we are dealing with an interface the logical choice is to take i on the grid point before the interface position and $+$ as the gridpoint after the interface position. At the gridpoints left and right of the interface we can then evaluate the net generation rate U_i^{int} on grid point i by adding the terms for the relevant bands, so for the net generation of electrons we get

$$\Gamma_n^i = G_{n_i} - R_{n_i} \tag{16}$$
$$= c^i \cdot f_t - a^i \cdot (1 - f_t) \tag{17}$$
$$= \frac{c^i \cdot \sum_{j=i-1}^{i+1} (a^j + d^j) - a^i \cdot \sum_{j=i-1}^{i+1} (b^j + c^j)}{\sum_{j=i-1}^{i+1} (a^j + b^j + c^j + d^j)}. \tag{18}$$

Note that this works only if we state that there has to be a minimum of 3 gridpoint bewteen 2 interfaces (which are between the grid), as we need one of the 3 terms in the sums of equation 21 to equal zero. This will work if one of the three points does not contain interface traps.

For holes we get

$$\Gamma_p^i = G_{p_i} - R_{p_i} \tag{19}$$
$$= d^i \cdot (1 - f_t) - b^i \cdot f_t \tag{20}$$
$$= \frac{d^i \cdot \sum_{j=i-1}^{i+1}(b^j + c^j) - b^i \cdot \sum_{j=i-1}^{i+1}(a^j + d^j)}{\sum_{j=i-1}^{i+1}(a^j + b^j + c^j + d^j)}. \tag{21}$$

The continuity equation for electrons is then given by

$$\begin{aligned} &\mu_{ni+1/2}\Big(\frac{V_{i+1} - V_i}{V_t}\Big)h_{i-1}n_{i+1} \\ -\Big[\mu_{ni+1/2}\Big(\frac{V_i - V_{i+1}}{V_t}\Big)h_{i-1} &+ \mu_{ni-1/2}\Big(\frac{V_i - V_{i-1}}{V_t}\Big)h_i\Big]n_i \\ &+\mu_{ni-1/2}\Big(\frac{V_{i-1} - V_i}{V_t}\Big)h_i n_{i-1} \\ &= -\frac{\Gamma_n^i L^2 h_i h_{i-1}(h_i + h_{i-1})}{2}. \end{aligned} \tag{22}$$

Note that Γ_n^i is the net generation, or minux net recombination, at grid point i. This means that all generation and recombination processes enter the continuity equation via this term. For sake of simplicity, we will introduce only interface recombination and generation in this term here, as other recombination processes can simply be added. The interface recombination term is not linear in charge carrier density. Especially since the amount of recombination may vary wildly when the charge carrier density changes, it is wise to linearize the recombination term in charge carrier density. To linearize we use a Taylor series, where we have to account for the fact that we have to add the partial derivatives to the charge carrier densities at gridpoints $i-1$, i, and $i+1$. For our Taylor expansion of net interface generation rate Γ_{int}^n this gives us

$$\Gamma_n^i(\vec{n}) \approx \Gamma_n^i(\vec{n}_{old}) + \sum_{j=i-1}^{i+1} \frac{\partial \Gamma_n^i(\vec{n}_{old})}{\partial n_j}(n^j - n_{old}^j),$$

where $\vec{n}_{old}$ are the electron densities from the previous iteration, which are known and $\vec{n}$ are the electron densities to be calculated.

The three partial derivatives are

$$\frac{\partial \Gamma_n^i}{\partial n^{i-1}} = \frac{c^i a'^{i-1}\big(\sum_{j=i-1}^{i+1}(a^j+b^j+c^j+d^j)-a^{i-1}\big)}{\big(\sum_{j=i-1}^{i+1}(a^j+b^j+c^j+d^j)\big)^2} - \frac{a^{i-1}\big(c^i(a^i+a^{i+1}+\sum_{j=i-1}^{i+1}d^j)-a^i\sum_{j=i-1}^{i+1}(b^j+c^j)\big)}{\big(\sum_{j=i-1}^{i+1}(a^j+b^j+c^j+d^j)\big)^2} \tag{23}$$

$$\frac{\partial \Gamma_n^i}{\partial n^{i}} = \frac{a'^i\big(c^i-\sum_{j=i-1}^{i+1}(b^j+c^j)\big)\big(\sum_{j=i-1}^{i+1}(a^j+b^j+c^j+d^j)-a^i\big)\big)}{\big(\sum_{j=i-1}^{i+1}(a^j+b^j+c^j+d^j)\big)^2} - \frac{a'^i c^i\big(a^{i-1}+a^{i+1}+\sum_{j=i-1}^{i+1}d^j\big)}{\big(\sum_{j=i-1}^{i+1}(a^j+b^j+c^j+d^j)\big)^2} \tag{24}$$

$$\frac{\partial \Gamma_n^i}{\partial n^{i+1}} = \frac{c^i a'^{i+1}\big(\sum_{j=i-1}^{i+1}(a^j+b^j+c^j+d^j)-a^{i+1}\big)}{\big(\sum_{j=i-1}^{i+1}(a^j+b^j+c^j+d^j)\big)^2} - \frac{a^{i+1}\big(c^i(a^i+a^{i-1}+\sum_{j=i-1}^{i+1}d^j)-a^i\sum_{j=i-1}^{i+1}(b^j+c^j)\big)}{\big(\sum_{j=i-1}^{i+1}(a^j+b^j+c^j+d^j)\big)^2} \tag{25}$$

Inserting the Taylor approximation of recombination term Γ_n^i in equation 22 gives us

$$\begin{aligned}
&\Big(\mu_{ni+1/2}B\Big(\frac{V_{i+1}-V_i}{V_t}\Big)h_{i-1}+\frac{\partial\Gamma_n^i(\vec{n}_{old})}{\partial n^{i+1}}\frac{1}{2}L^2h_ih_{i-1}(h_i+h_{i-1})\Big)n_{i+1}\\
&\quad-\Big[\mu_{ni+1/2}B\Big(\frac{V_i-V_{i+1}}{V_t}\Big)h_{i-1}+\mu_{ni-1/2}B\Big(\frac{V_i-V_{i-1}}{V_t}\Big)h_i\\
&\quad-\frac{\partial\Gamma_n^i(\vec{n}_{old})}{\partial n^{i}}\frac{1}{2}L^2h_ih_{i-1}(h_i+h_{i-1})\Big]n_i\\
&+\Big(\mu_{ni-1/2}B\Big(\frac{V_{i-1}-V_i}{V_t}\Big)h_i+\frac{\partial\Gamma_n^i(\vec{n}_{old})}{\partial n^{i-1}}\frac{1}{2}L^2h_ih_{i-1}(h_i+h_{i-1})\Big)n_{i-1}\\
&=-\big(G_i+\Gamma_n^i(\vec{n}_{old})-\sum_{j=i-1}^{i+1}(\frac{\partial\Gamma_n^i(\vec{n}_{old})}{\partial n_j}n_{old}^j)\big)\frac{1}{2}L^2h_ih_{i-1}(h_i+h_{i-1}),
\end{aligned} \tag{26}$$

as the continuity equation for electrons. Because of electron-hole symetry, exchanging all n and p labels and in the shorthand notation the a and b, and c and d labels we can get the continuity equation for holes.

2 Poisson's equation

We start with Eq. (6.1-24) in Selberherr [1]

$$\frac{\frac{V_{i+1}-V_i}{h_i} - \frac{V_i-V_{i-1}}{h_{i-1}}}{h_i + h_{i-1}} = \frac{q}{2\varepsilon}(n_i - p_i - C_i), \tag{27}$$

where V_i is the potential at $x = x_i$, n_i, p_i are the electron and hole densities at x_i, resp., and C_i is an additional charge at x_i, e.g., trapped charge. The symbol λ in Selberherr has the meaning $\lambda^2 = \frac{q}{\varepsilon}$. In Selberherr, the grid spacing is defined as $h_i = x_{i+1} - x_i$, however, in the program it is defined as $h_i = (x_{i+1} - x_i)/L$, therefore Eq. 27 becomes

$$\frac{V_{i+1}h_{i-1} - h_{i-1}V_i - h_iV_i + h_iV_{i-1}}{h_ih_{i-1}L} = (h_i + h_{i-1})L\frac{q}{2\varepsilon}(n_i - p_i - C_i). \tag{28}$$

The goal is to arrive at a set of linear equations suitable for solving with a standard matrix algorithm. To do this, an initial guess is made for V_i, and with this guess a correction is calculated, which is subsequently added to V_i. In this way we arrive at a new (better) guess for V_i. This procedure is repeated until the (infinity) norm of the correction term is smaller than a certain tolerance (tolPois in the program).

Substituting V_i with $V_i + \delta V_i$, where δV_i is a small correction to the original V_i, we get

$$\begin{aligned}\frac{\delta V_{i+1}h_{i-1} - h_{i-1}\delta V_i - h_i\delta V_i + h_i\delta V_{i-1}}{h_ih_{i-1}L} \\ = (h_i + h_{i-1})L\frac{q}{2\varepsilon}(n_i - p_i - C_i) \\ -\big(\frac{V_{i+1}h_{i-1} - h_{i-1}V_i - h_iV_i + h_iV_{i-1}}{h_ih_{i-1}L}\big).\end{aligned} \tag{29}$$

Correction δV_i is what is actually solved for in SIMsalabim.

The charged particle densities actually vary with the potential, so keeping them at the right hand side negatively influences convergence. Therefore we need to linearize the particle densities in terms of the potential. Inserting interface traps gives us

$$\begin{aligned}\frac{\delta V_{i+1}h_{i-1} - h_{i-1}\delta V_i - h_i\delta V_i + h_i\delta V_{i-1}}{h_ih_{i-1}L} = \\ (h_i + h_{i-1})L\frac{q}{2\varepsilon}(n_i - p_i - (q_{et} - f_{ti})N_{ti}) \\ -\big(\frac{V_{i+1}h_{i-1} - h_{i-1}V_i - h_iV_i + h_iV_{i-1}}{h_ih_{i-1}L}\big),\end{aligned} \tag{30}$$

where q_{et} is the charge of empty interface traps (traps that do not contain an electron) and f_{ti} is the fraction of filled interface traps from Eq. 15. We can linearize the electrons, holes and interface traps separately to δV_i. Since f_{ti} depends on both n and p, we can linearize the charges in the Poisson equation by expressing n and p in terms of the potential. Doing so gives us

$$n = n_{int} \exp\Big(\frac{V_i + \delta V_i}{V_t}\Big) \exp\Big(-\frac{\phi_n}{V_t}\Big) \tag{31}$$

$$p = n_{int} \exp\Big(-\frac{V_i + \delta V_i}{V_t}\Big) \exp\Big(+\frac{\phi_p}{V_t}\Big). \tag{32}$$

Now we can substitute n and p to get a first order Taylor expansion of trap occupancy f_{ti} around $\delta V = 0$ given by

$$f_{ti}(\vec{V} + \delta\vec{V}) \approx f_{ti}(\vec{V}) + \sum_{j=1}^{N} \frac{\partial f_{ti}(\vec{V})}{\partial V_j} \delta V.$$

Now we need to find the partial derivatives of f_{ti} with respect to the potential. We get a partial derivative of the form

$$\begin{aligned} \frac{\partial}{\partial x}\Big(\frac{d\exp\big(\frac{a+x}{b}\big) + c}{d\exp\big(\frac{a+x}{b}\big) + g\exp\big(\frac{-a-x}{b}\big) + f}\Big) = \\ \frac{d\exp\big(\frac{a+x}{b}\big)}{b\big(d\exp\big(\frac{a+x}{b}\big) + g\exp\big(\frac{-a-x}{b}\big) + f\big)} \\ -\frac{\big(d\exp\big(\frac{a+x}{b}\big) + c\big)\big(d\exp\big(\frac{a+x}{b}\big) - g\exp\big(\frac{-a-x}{b}\big)\big)}{b\big(d\exp\big(\frac{a+x}{b}\big) + g\exp\big(\frac{-a-x}{b}\big) + f\big)^2}. \end{aligned} \tag{33}$$

Taking the partial derivatives and substituting back the charge carrier densities, while using the shorthand notation from Eq. 5 to 12 we get

$$\begin{aligned} \frac{\partial f_{ti}(n,p)}{\partial V_{i-1}} &= \frac{a^{i-1}}{V_t\big(\sum_{j=i-1}^{i+1}(a^j + b^j + c^j + d^j)\big)} - \frac{\sum_{j=i-1}^{i+1}(a^j + d^j)(a^{i-1} - b^{i-1})}{V_t\big(\sum_{j=i-1}^{i+1}(a^j + b^j + c^j + d^j)\big)^2} \\ \frac{\partial f_{ti}(n,p)}{\partial V_{i}} &= \frac{a^{i}}{V_t\big(\sum_{j=i-1}^{i+1}(a^j + b^j + c^j + d^j)\big)} - \frac{\sum_{j=i-1}^{i+1}(a^j + d^j)(a^{i} - b^{i})}{V_t\big(\sum_{j=i-1}^{i+1}(a^j + b^j + c^j + d^j)\big)^2} \\ \frac{\partial f_{ti}(n,p)}{\partial V_{i+1}} &= \frac{a^{i+1}}{V_t\big(\sum_{j=i-1}^{i+1}(a^j + b^j + c^j + d^j)\big)} - \frac{\sum_{j=i-1}^{i+1}(a^j + d^j)(a^{i+1} - b^{i+1})}{V_t\big(\sum_{j=i-1}^{i+1}(a^j + b^j + c^j + d^j)\big)^2}. \end{aligned} \tag{34}$$

We can now write the Poisson equation as

$$\begin{aligned}
&\Big(\frac{h_{i-1}}{h_i h_{i-1} L} + (h_i + h_{i-1}) L \frac{q}{2\varepsilon} \frac{\partial f_{ti}(n,p)}{\partial V_{i+1}}\Big) \delta V_{i+1} \\
-&\Big(\frac{(h_{i-1} + h_i)}{h_i h_{i-1} L} - (h_i + h_{i-1}) L \frac{q}{2\varepsilon} \frac{\partial f_{ti}(n,p)}{\partial V_i}\Big) \delta V_i \\
+&\Big(\frac{h_i}{h_i h_{i-1} L} + (h_i + h_{i-1}) L \frac{q}{2\varepsilon} \frac{\partial f_{ti}(n,p)}{\partial V_{i+1}}\Big) \delta V_{i-1} \\
&= (h_i + h_{i-1}) L \frac{q}{2\varepsilon} (n_i - p_i - (q_{tie} - f_{tio}) \frac{N_t}{2}) \\
&\quad -\big(\frac{V_{i+1} h_{i-1} - h_{i-1} V_i - h_i V_i + h_i V_{i-1}}{h_i h_{i-1} L}\big). \qquad (35)
\end{aligned}$$

References

[1] S. Selberherr, *Analysis and Simulation of Semiconductor Devices*, Springer-Verlag, Wien, **1984** (cit. on p. 5).

[2] W. Shockley, W. T. Read, *Phys. Rev.* **1952**, *87*, 835–842 (cit. on p. 1).