ON MODELING THE INTRINSIC NUMBER AND FERMI LEVELS FOR DEVICE AND PROCESS SIMULATION

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Abstract - We discuss three models describing carrier densities in highly doped silicon, which have been used for process and device simulation. We calculate n_{ie} for each of the models for various doping concentrations within temperature ranges interesting for device and process simulation. Our calculated results are compared to measurements. Furthermore we offer simple formulae for the calculated n_{ie}. We show how far the relation between the carrier densities and the Fermi levels can be described by the simple formulae of Boltzmann statistics when using a doping dependent effective intrinsic number.

1. The Models

Van Overstraeten's model (index "ov") is well described in /1/ and /2/; the formulae of Slotboom's model (index "sl") have been derived from /3/, and Mock's model (index "mo") is defined in /4/. The models for the relative masses and the bandgap have been taken from /7/ for the low temperature range (275 K to 400 K) and from /2/ for the high temperature range (800 C to 1200 C). The ionisation energies of the donors and acceptors are set to 0.044 eV. Furthermore, we assume total ionisation of the impurity atoms. For Slotboom's and Mock's models no limitations of the validity range have been published, whereas Van Overstraeten's model is only valid for $/N_D-N_A/ \gg 10^{17}cm^{-3}$.

2. The Calculation of the Intrinsic Number

We assume thermodynamic equilibrium and charge neutrality for the calculation of the effective intrinsic carrier densities $n_{ie}^2 := n*p$, i.e. $F=+F_n=-F_p$ and $n(F_n)-p(F_p) = N_D^+-N_A^-$. n, p and F are evaluated by Newton iterations in F for Van Overstraeten's model. Slotboom's and Mock's models have to be solved by an Aitken fixpoint iteration in λ (screening length) and Newton iterations in F. The Newton and Aitken iteration and the programs to evaluate $n(F_n)$ are derived from /8/. The intrinsic number is calculated for n-doped silicon. We calculate n_{ie} as a function of the doping difference and take N_A as a parameter to get a survey of n_{ie} in lightly and heavily doped silicon with as well as without compensation.

3. Results

Fig.1, 2 and 3 show the effective intrinsic number for 300 K, Fig.4, 5 and 6 for 1000 C. In some figures $n_{ie,ov}$ is evaluated for doping differences less than $10^{17}cm^{-3}$ in order to compare the models more easily. Fig.7, 8 and 9 show the temperature dependence of n_{ie}. The parameter in Fig.1 to 9 is the doping concentration of the acceptors. The plotted lines have numbers which indicate the value of N_A with respect to the following table.

1.....$10^{10}cm^{-3}$	2.....$10^{16}cm^{-3}$	3...$3.16*10^{16}cm^{-3}$
4.....$10^{18}cm^{-3}$	5...$3.16*10^{19}cm^{-3}$	6.....$10^{19}cm^{-3}$
7...$3.16*10^{20}cm^{-3}$	8.....$10^{20}cm^{-3}$	9...$3.16*10^{21}cm^{-3}$
10.....$10^{21}cm^{-3}$	11...$3.16*10^{20}cm$	12.....$10^{21}cm^{-3}$
13...$3.16*10^{21}cm$		

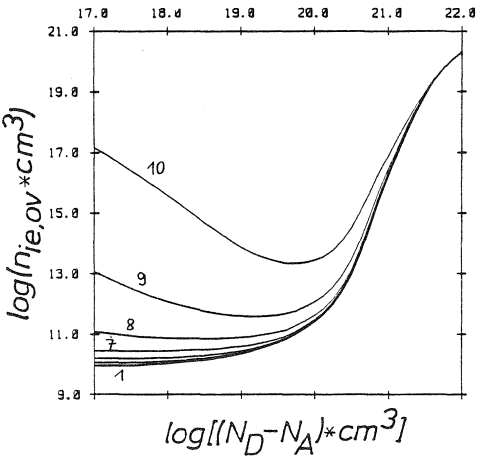

Fig.1: $n_{ie,ov}$, T=300 K

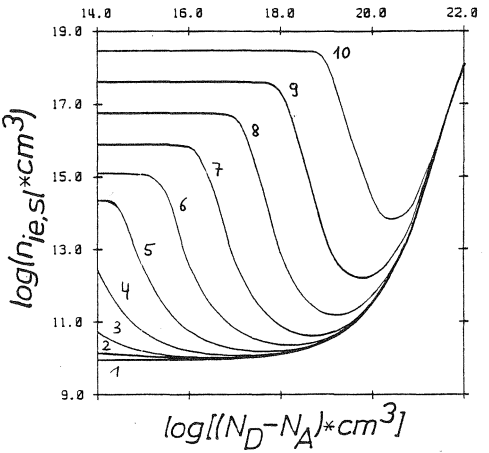

Fig.2: $n_{ie,sl}$, T=300 K

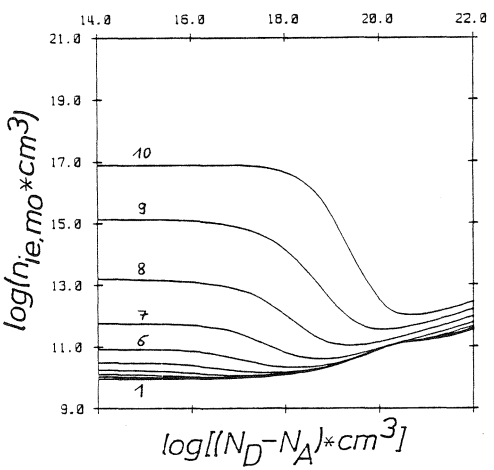

Fig.3: $n_{ie,mo}$, T=300 K

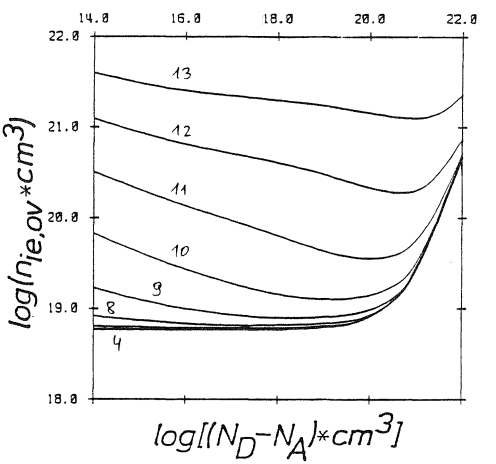

Fig.4: $n_{ie,ov}$, T=1000 C

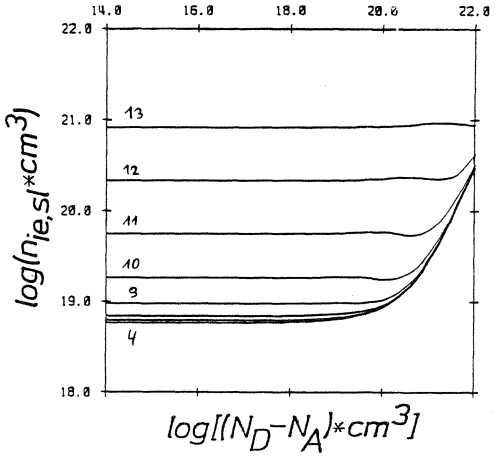

Fig.5: $n_{ie,sl}$, T=1000 C

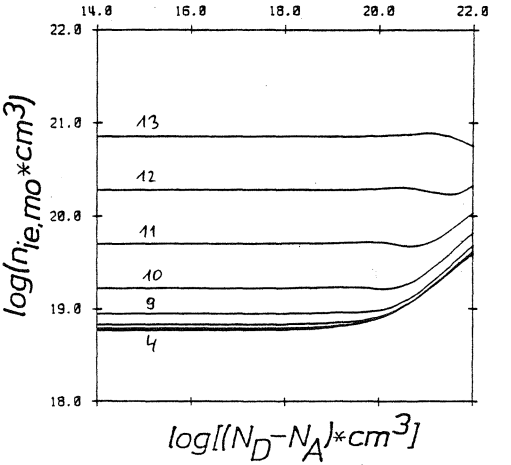

Fig.6: $n_{ie,mo}$, T=1000 C

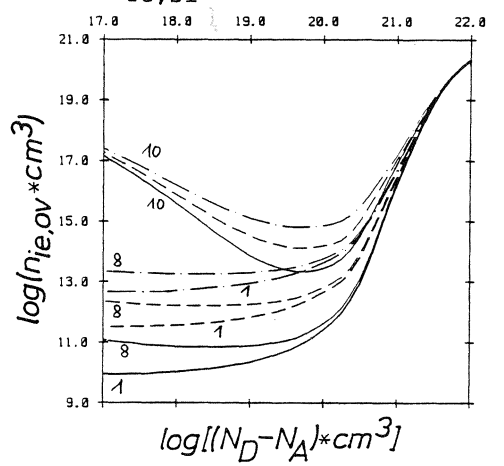

Fig.7: $n_{ie,ov}(N_A,T)$

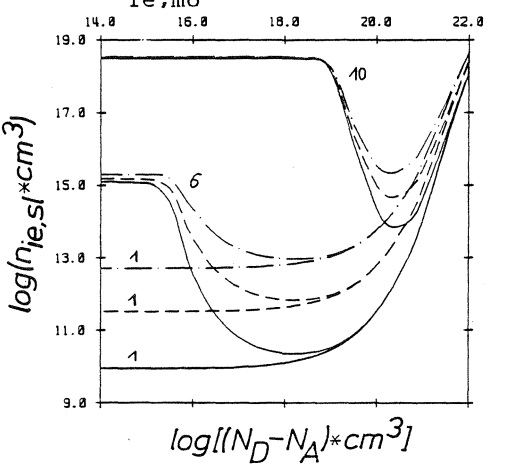

Fig.8: $n_{ie,sl}(N_A,T)$

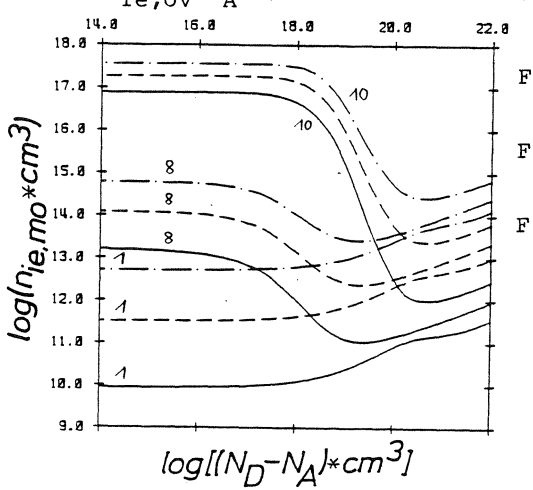

Fig.9: $n_{ie,mo}(N_A,T)$

Fig.7 $n_{ie,ov}(N_A=10^{10}cm^{-3},10^{19}cm^{-3},10^{20}cm^{-3})$

Fig.8 $n_{ie,sl}(N_A=10^{10}cm^{-3},10^{18}cm^{-3},10^{20}cm^{-3})$

Fig.9 $n_{ie,mo}(N_A=10^{10}cm^{-3},10^{19}cm^{-3},10^{20}cm^{-3})$

Parameter: N_A

——— T=300K

– – – – T=350K

—·—·— T=400K

4. Comparison of our calculations to measured results

In /5/ values of $(n_{ie}/n_{ie0})^2$ are derived from measurements of the collector current in a p-n-p bipolar transistor. Fig.10 shows the measured values and our calculated values for the three theories. Similar measurements and calculations have been published in /6/ for a n-p-n transistor.

The three models do not differ very much for uncompensated material up to doping rates of $5*10^{19}cm^{-3}$. As the measured values do not favour one of the models we cannot conclude which of the theories describes the effective intrinsic number best.

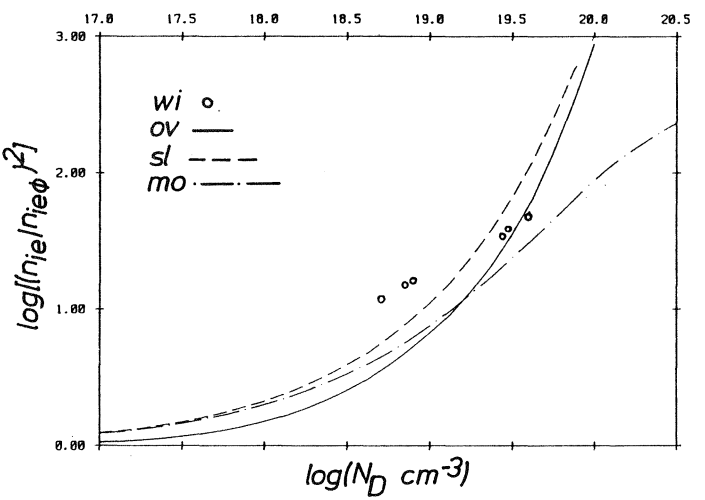

Fig.1, 2 and 3 show that the intrinsic numbers of the three models differ widely for compensated silicon. Therefore only measurements of n_{ie} in compensated silicon can possibly decide if one of the models is able to describe the intrinsic number in highly doped silicon.

Fig.10: Calculated and measured values of $(n_{ie}/n_{ie0})^2$

5. Formulae for the effective intrinsic number

For uncompensated material we offer temperature and doping dependent formulae for all three theories. The basis of these approximations are calculated values for a temperature range from 275 K to 400 K with a step width of 25 K and for doping concentrations within the validity range with a step factor of 3.16. The coefficients a1, a2 and a3 are derived by a least squares fit of the calculated values of n_{ie}. We describe n_{ie} as

$$n_{ie} = \exp(a1(T)+a2(T)*(N_D/10^{17}cm^{-3})**a3(T))$$

The optimal coefficients are
for Van Overstraeten's model ($10^{15}cm^{-3} < N_D < 10^{21}cm^{-3}$)

$$a1(T) = -1.97986*10^{+1} + 2.01089*10^{-1}*T - 1.96269*10^{-4}*T^2$$
$$a2(T) = +2.38838*10^{-1} - 9.57814*10^{-4}*T + 1.07551*10^{-6}*T^2$$
$$a3(T) = +5.10190*10^{-1} + 5.75190*10^{-4}*T - 7.01029*10^{-7}*T^2,$$

for Slotboom's model ($10^{12}cm^{-3} < N_D < 3.16*10^{20}cm^{-3}$)

$$a1(T) = -1.99765*10^{+1} + 2.01814*10^{-1}*T - 1.97040*10^{-4}*T^2$$
$$a2(T) = +7.95811*10^{-1} - 3.20439*10^{-3}*T + 3.54153*10^{-6}*T^2$$
$$a3(T) = +2.97104*10^{-1} + 6.75707*10^{-4}*T - 4.90892*10^{-7}*T^2$$

and for Mock's model ($10^{12}cm^{-3} < N_D < 10^{20}cm^{-3}$)

$$a1(T) = -2.00536*10^{+1} + 2.02186*10^{-1}*T - 1.97509*10^{-4}*T^2$$
$$a2(T) = +9.60563*10^{-1} - 3.94127*10^{-3}*T + 4.41488*10^{-6}*T^2$$
$$a3(T) = +1.29363*10^{-1} + 1.10709*10^{-3}*T - 9.56981*10^{-7}*T^2.$$

6. Validity range of Boltzmann statistics

We try to find out how far Boltzmann statistics can describe the relations between n and F_n or p and F_p. For the exact models we calculated for thermodynamic equilibrium n, p and F and set $n_{ie}^2 = n*p$. Then we calculated F'_n and F'_p using the classical formulae

$$n' = 0.5*(N_D - N_A) + (0.25*(N_D - N_A)^2 + n_{ie}^2)^{1/2} \qquad F'_n = k*T*\log(n'/n_{ie})$$

$$p' = 0.5*(N_A - N_D) + (0.25*(N_D - N_A)^2 + n_{ie}^2)^{1/2} \qquad F'_p = k*T*\log(p'/n_{ie})$$

Then we calculate F''_n and F''_p in the same way, using a well established formula for the doping dependent intrinsic number /6/.

$$n''_i(T) = 6.43*10^{15}*T^{1.5}*\exp((4.07*T^2/(T+1108) - 6370)/T)$$

$$n''_{ie}(N,T) = n_i(T)*\exp((52.2/T)*(C + (C^2+0.5))^{0.5}) \text{ with } C = \log(N_D/10^{17}cm^{-3}).$$

The results of the calculations are plotted in Fig.11 to Fig.16.

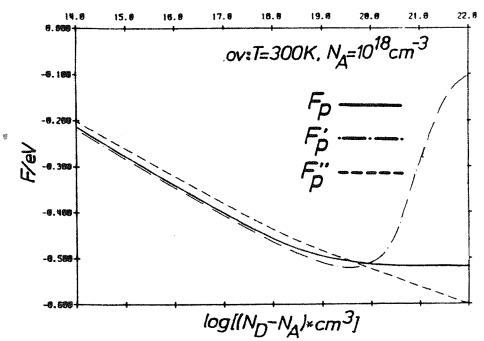

Fig.11: F_p for model "ov"

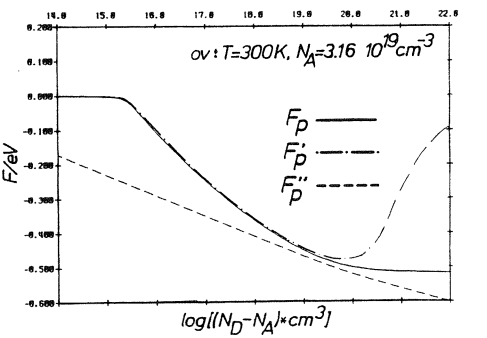

Fig.12: F_p for model "ov"

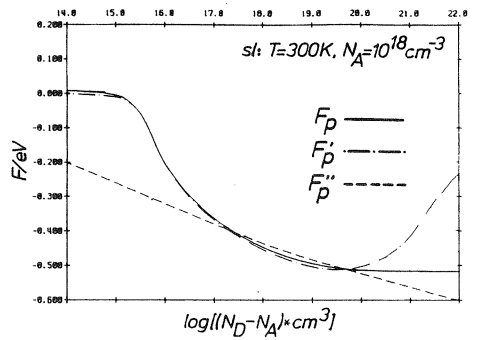

Fig.13: F_p for model "sl"

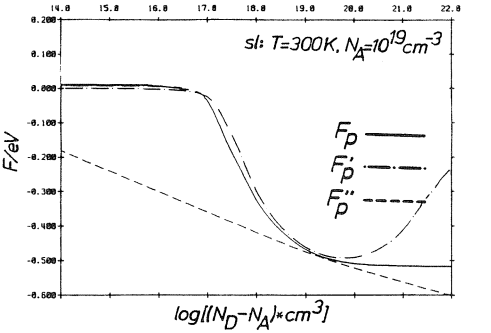

Fig.14: F_p for model "sl"

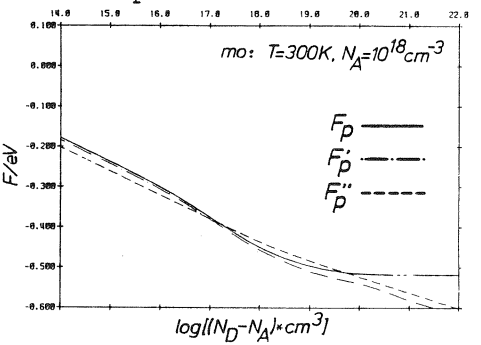

Fig.15: F_p for model "mo"

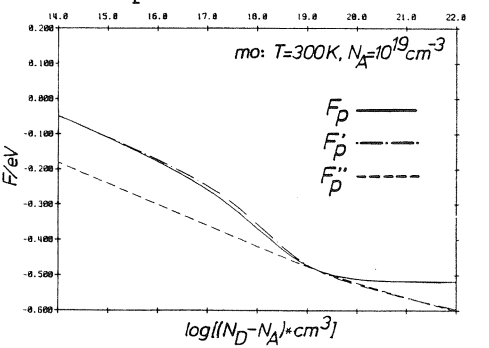

Fig.16: F_p for model "mo"

Fig.11 to 16 show that Boltzmann statistics can only be used up to total doping ranges of $3...10*10^{19}cm^{-3}$. F_p' follows F_p even for the case of higly compenated silicon below this doping level. F_p'' differs strongly if $(N_D-N_A)/N_D \ll 1$, but does not decrease extremely for uncompensated material.

Acknowledgements: Many helpful discussions with Prof. Pötzl are very acknowledged. This work was sponsored by the Fonds zur Förderung der wiss. Forschung, project No.22/11.

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