A Robust Algorithm for Predicting Freezeout and Exhaustion Under Equilibrium Conditions

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Abstract

A numerically robust method for evaluating the temperature-dependent carrier concentrations and related Fermi levels is proposed. The method is applicable to simple cases for which analytic solutions are available as well as more complex cases in which numerical methods are required due to nonstandard effects including bandgap widening, compensation and degeneracy induced by high levels of doping.

1 Background for Analysis

The physical basis for analysis assumes that that there is sufficient spatial uniformity in the doping profiles in order to apply the condition of charge neutrality,

$$P(T) = p_0 - n_0 - \sum N_a^- + \sum N_d^+ = 0 \qquad (1)$$

where T is the Kelvin temperature, po and no are the equilibrium hole and electron carrier concentrations respectively, while N_a^- and ${}_N d^+$ are the ionized acceptors and donors atom concentrations respectively. The summations run over the numbers of impurities. The approach presented is facilitated by defining the parameter Z where:

$$Z = exp[(E_{F_i} - E_F)/kT] \qquad (2)$$

where k is Boltzman's constant, E_F is the Fermi level and E_{F_i} is the intrinsic Fermi level. In nondegenerate cases, i.e. where the Boltzman approximation can be applied to simplify the exact expression for the carrier concentrations, the Z parameter is directly proportional to the equilibrium hole concentration. The constant of proportionality is the temperature dependent intrinsic concentration. It turns out that Eq. (1) can be expressed as $P(Z)$. Numerical methods based on successive substitution in solving for the zeros in expression (1) were found to be unreliable in producing a convergent solution. However the method proposed here is derived from the numerical scheme known as interval bisection [1] and it was found work well with variety of combinations of profiles and other nonstandard conditions. Figure 1 provides a flowchart describing the salient numerical features of the calculation. The basic scheme had to be modified due to the extremely large dynamic range in the $P(Z)$. See for example, Fig. 2a, which shows that the range of values in $P(Z)$ can cover 50 decades of variation. In order to efficiently apply the method of interval bisection a rough estimate for the zero in $P(Z)$ is needed for each temperature of interest. This is obtained in a simple way through use of the 'sign' and 'diff' vector operations as illustrated on Figs. 2b and 2c, respectively. This initial rough estimate for where the zero in $P(Z)$ occurs will serve as a seed for the interval bisection method. This 2nd step produces a smooth convergent solution using only 1 decade of dynamic range centered on the seed.

2 Analysis

The normalized energy level differences between the conduction and valence bands measured relative to the Fermi level are, respectively:

$$\xi_n = \frac{E_F - E_c}{kT} \qquad (3a)$$

$$\xi_p = \frac{E_v - E_F}{kT} \qquad (3b)$$

where $E_g = E_c - E_v$. The equilibrium electron and hole concentrations can now be defined as:

$$n_0 = N_c e^{(E_F - E_c)/kT} \chi_n \qquad (4a)$$

$$p_0 = N_v e^{(E_v - E_F)/kT} \chi_p \qquad (4b)$$

where the normalized correction factors, $\chi_n \chi_p$, for degenerate statistics can be defined

$$\chi_n = \frac{F_{1/2}(\xi_n)}{e^{\xi_n}} \qquad (5a)$$

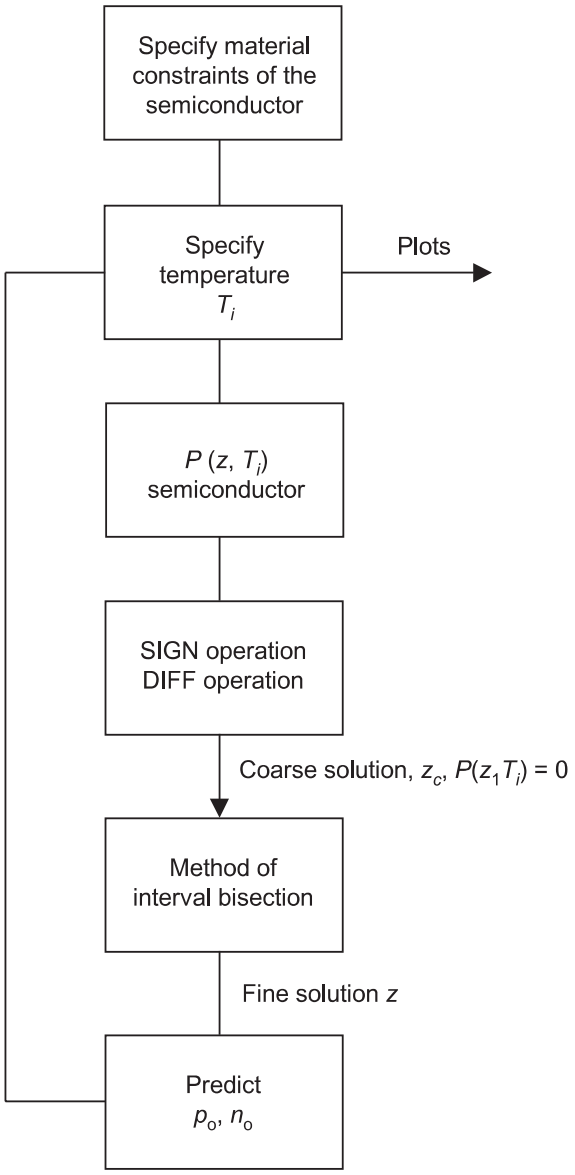

Figure 1: Flowchart

$$\chi_p = \frac{F_{1/2}(\xi_p)}{e^{\xi_n}} \tag{5b}$$

The Fermi level integral $F_{1/2}(\xi)$ with useful approximations are respectively defined [2]

$$F_{1/2}(\xi) = \frac{2}{\sqrt{\pi}} \int_0^\infty \frac{X^{1/2}}{1+\exp(x-\xi)} dx \tag{6a}$$

$$F_{1/2}(\xi) \simeq e^\xi \quad \text{for} \quad \xi < -3 \tag{6b}$$

$$\ln[F_{1/2}(\xi)] = c_0 + c_1\xi + c_2\xi^2 + c_3\xi^3 + c_4\xi^5 \quad 10 < \xi < -10 \tag{6c}$$

where $c_0 = -0.32881$, $c_1 = 0.74071$, $c_2 = -0.045427$, $c_3 = 8.797$, $c_4 = 1.5117$.

$$N_c = 2\frac{(2\pi m_n^* kT)^{3/2}}{h^2} \tag{7a}$$

$$N_v = N_c \left(\frac{m_p^*}{m_n^*}\right)^{3/2} \tag{7b}$$

where m^* is the effective mass for the respective bands [2]. For non-degenerate conditions $\chi_n \cong \chi_p \simeq 1$. In order to facilitate casting Eq. (1) into a form dependent on the Z-parameter the well known [2] relations for intrinsic concentration and Fermi level are used.

$$n_i = \sqrt{N_c N_v}\, e^{-E_g/2kT} \tag{8}$$

and

$$E_{F_i} = \frac{E_c + E_v}{2} + \frac{kT}{2} \ln\left[\frac{N_v}{N_c}\right] \tag{9}$$

Following the standard methods of transforming Eqs. (6) making use of Eqs. (8–9), it follows that

$$n_0 = n_i \frac{\chi_n}{Z} \tag{10a}$$

$$p_0 = n_i \chi_p Z \tag{10b}$$

Making use of the Fermi probability distributions to predict ionization levels of the donors and acceptors, i.e., N_a^- and N_d^+, substitution of Eqs. (10) into Eq. (1) and dividing by the intrinsic concentration leads to:

$$P'(Z,T) = \left(\chi_p Z - \sum_j^{M_a} \frac{\overline{N}_{d_j}}{1 + (g_{d_j} Z)^{-1} e^{(E_{F_1} - E_d)/kT}}\right) - \left(\chi_n Z^{-1} + \sum_j^{M_d} \frac{\overline{N}_{a_j}}{1 + g_{a_j} Z e^{(E_a - E_{F_i})/kT}}\right) = 0 \tag{11}$$

where $M_a(g_n)$ and $M_d(g_d)$ are the number of impurity components (degeneracy factors) for acceptors and donors, respectively. The donor and acceptor concentrations with the overbars are normalized by the intrinsic concentration. The energy levels for the impurities are defined relative to the valence band, i.e.,

$$E_d = E_c - E_d' \tag{12a}$$

whee E_d' is the standard cited value for donors measured with respect to the conduction band.

$$E_a = E_a' \tag{12b}$$

where E_a' is the standard cited value for acceptors measured with respect to the valence band. For degenerate conditions due to high doping it would be necessary to include χ_n and χ_p nontrivially in Eq. (11)

$$\ln \chi_n = \ln\left(F_{1/2}(\xi_n)\right) - \xi_n \tag{13a}$$

$$\ln \chi_p = \ln\left(F_{1/2}(\xi_p)\right) - \xi_p \tag{13b}$$

which would be identical in form to the RHS of Eq. (5b) after letting $c_1 \rightarrow c_1' = 0.74071 - 1$. Lastly, the explicit dependence of ξ_n and ξ_p on Z is given by:

$$\xi_n = \ln Z - \frac{1}{2} \ln \left[\frac{N_v}{N_c} \right] - \frac{E_g}{2kT} \qquad (14a)$$

$$\xi_p = -\ln Z + \frac{1}{2} \left[\frac{N_v}{N_c} \right] - \frac{E_g}{2kT} \qquad (14b)$$

which is required in evaluating the corrections, Eq. (13), for degenerate computations.

3 Example

As an example, please find in Fig. 3 the two curves $\log_{10}(p_0)$ plotted versus normalized $(1/T)$ obtained for a nondegenerate case with two acceptor impurities which are partially compensated with two donor impurities.

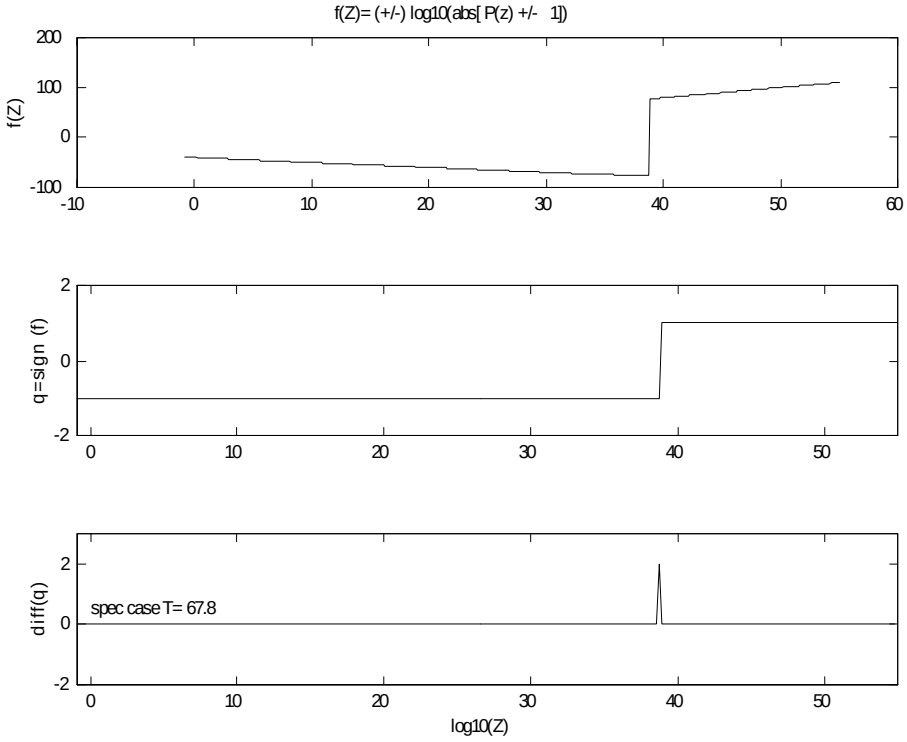

Figure 2: Finding approximate zeros of $P(Z)$, a,b,c is top, middle, and bottom respectively.

Conslusions

The method described here was found to be generally robust in producing a convergent solution under a wide range of conditions for which other numerical methods such as successive substitution would fail. The method was tested against some cases for which analytic solutions are available and there was excellent agreement. A report providing a full disclosure of details is in preparation.

References

[1] Hamming, R.W., *Numerical Methods for Scientists and Engineers*, Dover Publications, 1975.

[2] Shur, M., *Physics of Semiconductor Devices*, Prentice-Hall, Englewood Cliffs, NJ, 1990.

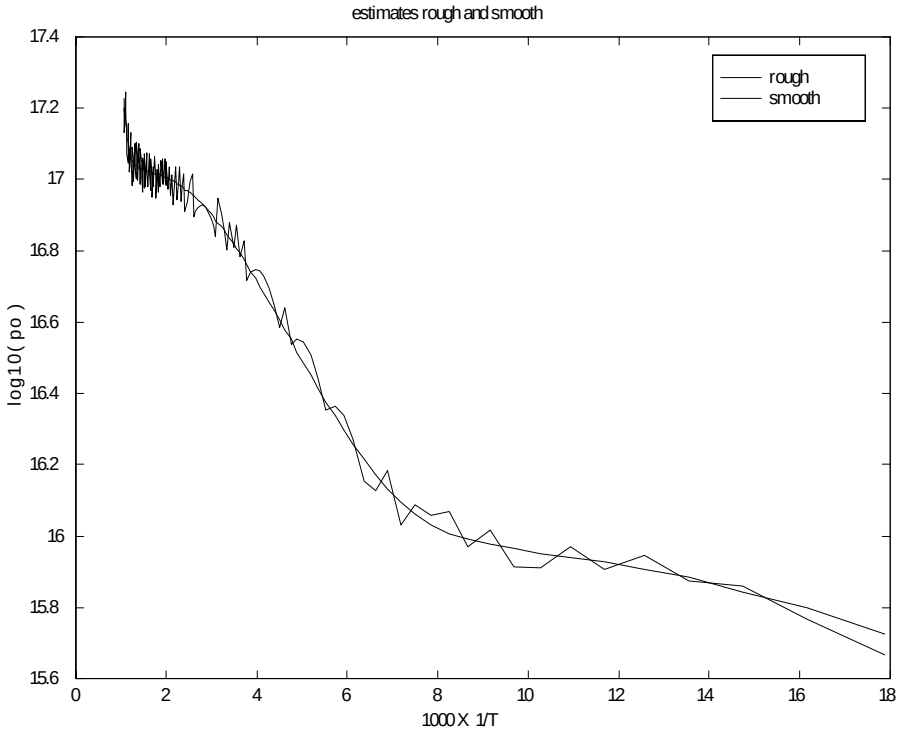

Figure 3: Results of method showing approximate solution and smooth solution obtained using interval bisection method.