Analytic Tests for a Robust Numerical Algorithm for Predicting Semiconductor Freeze-out and Exhaustion

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Abstract- In this report a complete analytic description for the temperature dependence of the majority carrier in a single impurity doped equilibrium semiconductor is proposed. This model should provide an attractive alternative to commonly used rules predicting the temperature boundaries for the exhaustion regime. This model is used to provide a confidence test for a less restrictive robust numerical model recently proposed in the literature. Both the analytic description and results for the numerical algorithm are compared under a variety of assumed conditions including band-gap narrowing. Limitations of the analytic model are also clarified.

Key-Words Semiconductor, simulation, exhaustion, freeze-out

1. Introduction

Integrated Circuits are specified to operate between designated temperature limits. The circuit designer selects the doping level or levels and typically assumes that the dopants are approximately 100% ionized, i.e. exhaustion and the temperature is not too high. There can be a significant impact on the value of a plethora of device parameters such as depletions widths and/or FET threshold voltages if the assumption is violated. In the domain that the temperature is too low the percentage ionization of dopant or dopants will be significantly less than 100%. The value for the majority carrier concentration is depressed significantly below the design value. On the other hand if the temperature is too high the thermal generation effect causes the majority carrier concentration to become excessively higher than the design value in what is called the intrinsic temperature regime. The exhaustion regime lies between this two extremes, intrinsic and freeze-out. It is well known that for a multiple impurity dopant process this "simple" three regime description can be inadequate. What is important to the designer is the plot of the majority carrier versus the temperature, or what is more commonly done, a plot of majority carrier concentration versus reciprocal of the temperature.

To-date most "analytic" methods for determining dominant features in such plots make use of multiple ad-hoc arguments, which taken one at a time, applies in only two of the three regimes mentioned above. Numerical methods based on one-dimensional analysis are applicable and provide significant flexibility in terms of making predictions when there are multiple dopants and when taking into account 2^{nd} order effects. It can be argued that numerical methods are generally going to be applicable over a wider range of problems than what can be solved with exact analysis. On the other hand analytic solutions are extremely useful for at least two reasons. First, they provide limited but essential checking of more flexible numerical algorithms. Second, they are more amenable to sensitivity analysis. The analytic model developed here will be applied to test just such a recently proposed numerical algorithm [1], [2].

2. Basic Analysis

The physical basis [1] for analysis assumes that there is sufficient spatial uniformity in the

doping profiles in order to apply the condition of local charge neutrality,

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

where T is the Kelvin temperature, p_o and n_o 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:

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

where k is Boltzman's constant, E_F is the Fermi level and E_{Fi} 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 [3] 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 one decade of dynamic range centered on the seed. Although this numerical algorithm can in principle be applied in conditions for which the Boltzman approximation is invalid[2,4], those details are not essential to the main point and will be excluded here to conserve space.

The effective density of states, which is derived in most introductory semiconductor texts, is given by:

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

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

where m^* is the effective mass for the respective bands [4]. In order to facilitate casting Eq. (1) into a form dependent on the Z-parameter the well known [4] relations for intrinsic concentration and Fermi level are used.

$$n_i = \sqrt{N_c N_v}\; e^{-\frac{E_g}{2kT}} \qquad (4)$$

$$E_{Fi} = \frac{E_c + E_v}{2} + kT\;\ln\left(\frac{N_v}{N_c}\right) \qquad (5)$$

Following the standard methods [1,4]of expressing carrier concentrations in terms of intrinsic parameters Eqs(4-5), it follows that:

$$n_o = \frac{n_i}{Z} \qquad (6a)$$

$$p_o = n_i Z \qquad (6b)$$

Making use of the Fermi probability distributions[4] to predict ionization levels of the donors and acceptors, i.e., N_a^- and N_d^+, and substitution of Eqs(6) Eq. (1) and then dividing by the intrinsic concentration [1] leads to a condition on P(Z,T):

$$Z + \sum_{l=1}^{M_d}\frac{\overline{N}_{d_l}}{1+K_{d_l}Z^{-1}} - Z^{-1} - \sum_{l=1}^{M_a}\frac{\overline{N}_{a_l}}{1+K_{a_l}Z} = 0 \qquad (7)$$

in which the temperature dependent constants,

$$K_{d_l} \equiv g_d e^{\left(E_{Fi}-E_{d_l}\right)/kT} \quad (8a)$$

$$K_{a_l} \equiv g_a e^{\left(E_{a_l}-E_{Fi}\right)/kT} \quad (8b)$$

are needed to characterize partial ionization. Also M_a and M_d are the numbers of impurity components, and g_a (4 typical for Silicon) and g_d (2 typical for Silicon) are the occupation degeneracies, for acceptors and donors, respectively. The donor and acceptor concentrations with the over-bars are normalized by the intrinsic concentration. The energy levels for the impurities E_a, E_d are defined relative to the valence band, i.e.,

$$E_d = E_c - E_d^{'} \quad (9)$$

where $E_d^{'}$ is the standard cited value for donors measured with respect to the conduction band. The polynomial $P^{'}(Z,T)$ as defined by Eq(7) is used in the numerical algorithm Fig 1. This analysis will also be the basis for an analytic description provided in the next section.

3. Analytic Solution, single impurity

Situation is described by the special case that M_a=1 and M_d=0 the summation subscript in Eq(7) can be dropped to lighten the notation. Straight-forward algebra leads to a cubic equation in Z.

$$Z^3 + \frac{1}{K_a}Z^2 - \left(\frac{\overline{N}_a}{1+K_a}\right)Z - \frac{1}{K_a} = 0 \quad (10)$$

The corresponding result for a single impurity N-type is exactly the same form, producing a cubic in Y=1/Z revised coefficients obtained by letting the 'a' subscript (for acceptor) be replaced with the 'd' subscript (for donor). The solution can be defined in terms of coefficients for the reference cubic equation:

$$x^3 + a_1x^2 + a_2x + a_3 = 0 \quad (11)$$

To facilitate representation of the solution the following intermediate parameterization of the problem is commonly taken[5].

$$Q = (3a_2 - a_1^2)/9 \quad (12a)$$

$$R = (9a_1a_2 - 27a_3 - 2a_1^3)/54 \quad (12b)$$

$$D \equiv Q^3 + R^2 \quad (12c)$$

where, D, which is referred to as the "discriminant" for the cubic problem will dictate the type of solutions possible. As per the fundamental theorem of algebra there will be three roots. For D negative all roots are real while for D positive only one root is real while the other two are complex conjugate. If D is zero there will be repeated root. For the problem being evaluated it can be shown using symbolic mathematical methods that Q and D will always be negative. Furthermore it can then be shown that of the three roots only one is positive and therefore physically acceptable. That root will be predicted by the following recipe [5] ,

$$Z = x = 2\sqrt{-Q}\cos(\theta/3) - \frac{1}{3}a_1 \quad (13)$$

where $\theta = \cos^{-1}\left(R/\sqrt{-Q^3}\right)$. Once Z is determined the majority carrier concentration, p_o, can be predicted from Eq(6b).

4. Examples

The first example should illustrate the agreement in both the numerical method (as per algorithm described in Fig 1) and the analytic solution the following tests were performed. Specifically it should prove interesting to apply solution approaches to the situation in which there is band-gap narrowing [6].

$$E_g(T) = E_{go} - \frac{\alpha T^2}{(T+\beta)} \quad (14)$$

where for Silicon recommended values for α and β are provided on the Figure(3). Figure (3) also shows both the comparison of solution approaches for a test with bandgap narrowing (BGN) and a test without. The first observation is that the numerical and analytic solutions are in perfect agreement. Furthermore, as expected

the impact of BGN is apparent in the curves at the higher temperatures.

As a second example the analytic solution is tested on a number of cases in which the doping level is changed. Details for the examples are provided on Fig 4. The break point lines were generated with typical "rules of thumb" [7], which depend on the temperature dependent intrinsic concentration and effective density of states. Reliable results are obtained with an iterative process. The disadvantage of this method is clarified by noting that it was not unusual for the number of iterative cycles to ran over twenty for the break points shown on Figure (4).

The third example tests a situation in which there are multiple donors. This situation does now fall in the umbrella of problems the cubic analytic solution can handle. The details of the problem are specified on Fig 5 and the results shown demonstrate a number of points. First, the numerical method is a two step method with the first "rough " solution serving as a seed for producing a more accurate smooth solution. Second, this example illustrates the fact that with multiple dopants the standard 3 regime description for majority carrier concentration temperature dependence no longer applies. One can identify 2 exhaustion regimes associated with $10^{17}/cm^3$ and $10^{16}/cm^3$.

5. Conclusions

An analytic formulation of the freezeout, exhaustion problem has been proposed. It can describe all three regimes for a single impurity dopant. The advantage of the analytic approach is that it provides a reliable but limited test for the more robust and flexible numerical algorithm also described here. Both approaches also agreed for the situation that temperature dependent band-gap narrowing is included

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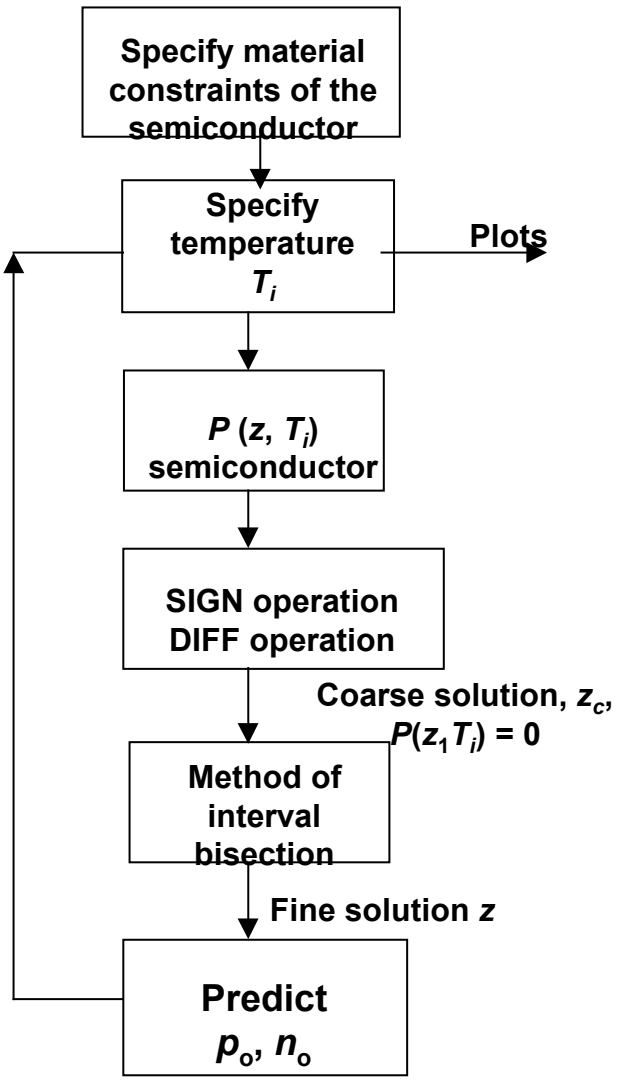

Figure 1 Flow Chart for Numerical Algorithm

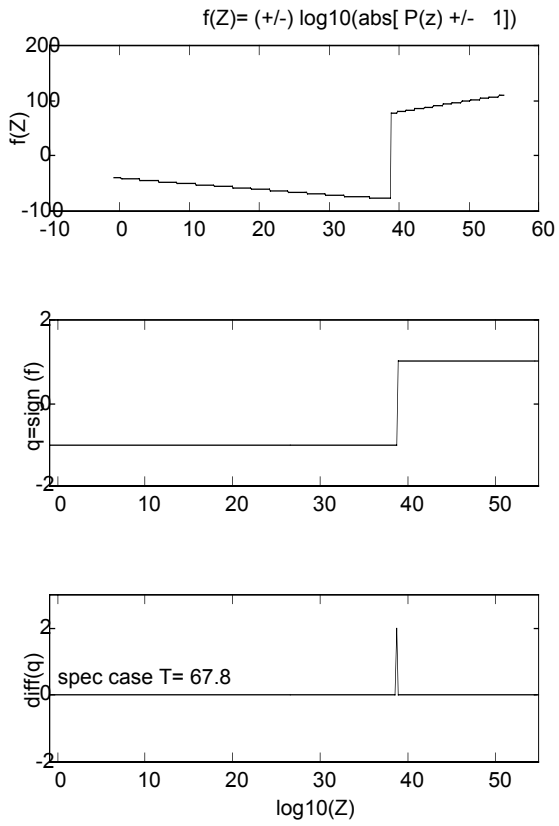

Figure 2, Finding Approximate zeros for P(Z)

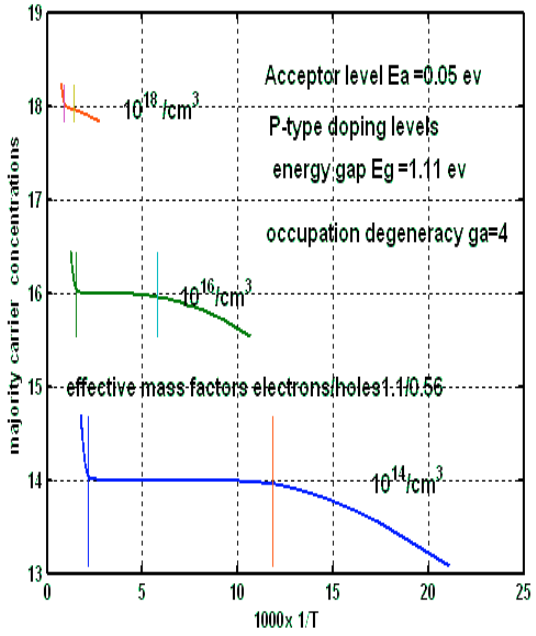

Figure 4, Examples for Analytic Model

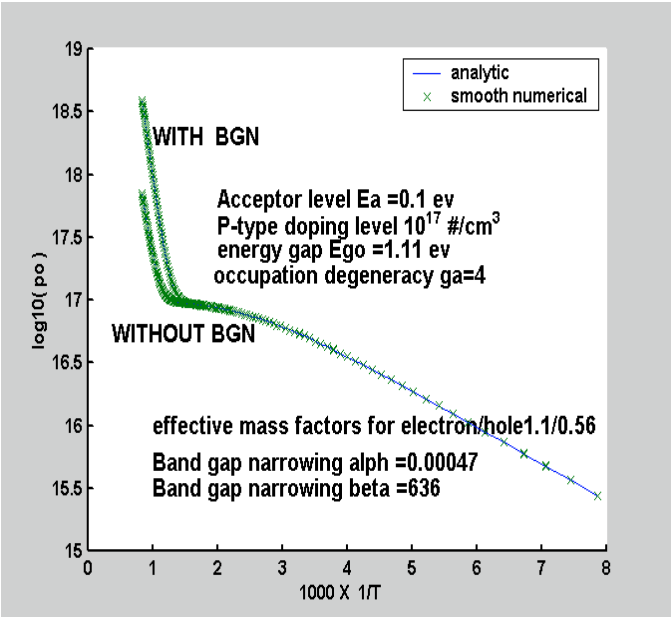

Figure 3, Comparison of analytic equation with numerical algorithm with and without band-gap narrowing (BGN).

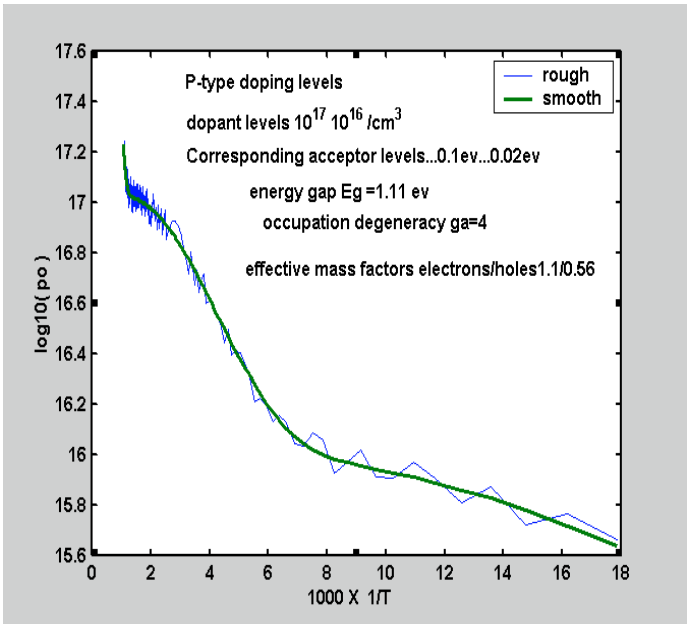

Figure 5 Multiple dopant test of numerical algorithm for which analytic model does not apply.