Determination of Diffusion Coefficients and Mobilities Using The Effective Field Concept

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Abstract

In recent years, the effective field approach has been developed in terms of hydrodynamic variables [1, 2, 3]. In this paper, the effective field is formulated for the calculation of transport coefficients in a drift-diffusion model. With these transport parameters, it was found that calculations of the energy distribution function tail, and average velocity match suprisingly well with Monte Carlo results, for a variety of cases. Therefore, results so far encourage further investigations into the effectiveness of characterizing device performance along with device reliability in terms of the effective field concept.

I. Introduction

Recently, it has been shown that in some cases the effective field determined from the average energy is sufficient for characterizing the shape of space dependent energy distribution function tails [4]. In this work, the effective field is defined as the table of electric field values that are generated by finding, at each space point, the best match between a homogeneous field and inhomogeneous field calculation of the energy distribution function tail. Then, the effective field concept is extended to include computations of mobilities and diffusion coefficients, with justification based upon the Bogoliubov ansatz [5] .

II. Modeling

In 1-D, the following analytical formula for the effective field has been obtained from Boltzmann's equation,

$$E_{eff}(x) = \int_{xo}^{x} dx' \frac{dE}{dx'} \left(1 - e^{-\frac{x-x'}{\lambda}}\right) . \tag{1}$$

Here, it is seen that the derivative of the electric field is being attenuated by an exponential term, thus demonstrating that the faster the field varies, the more the effective field will lag behind the locally applied field. This behavior is in qualitative agreement with the observations of Ref. [6]. The quantity λ is referred to as the relaxation length, and is shown to be well characterized by the ratio of the diffusion coefficient to the average velocity $\vec{u}$,

$$\lambda = \left| \frac{D}{|\vec{u}|} \right| . \tag{2}$$

This is a transcendental equation, however approximations can be introduced by considering Fig. 1, which is a plot of the ratio of diffusion coefficient to drift velocity for a homogeneous applied field. This plot characterizes the variation of λ, and it is seen that at high fields, where velocity saturation is present, λ varies slowly.

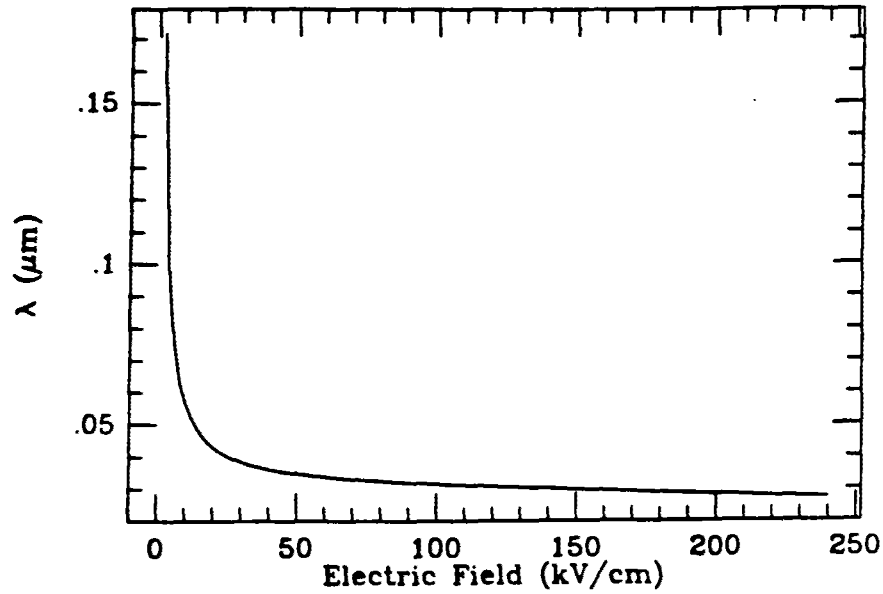

Fig. 1. This graph demonstrates the general dependence of λ upon the size of the electric field. For high fields, λ becomes the length scale over which the average envergy relaxes.

Once the effective field is known, the drift velocity is found to have the following simple form,

$$\vec{v}_d = \frac{\vec{E}}{E_{eff}} v_h(E_{eff}) \tag{3}$$

which is a formula that is not restricted to 1-D considerations. Here, $v_h(E_{eff})$ represents the average velocity of carriers in a homogeneous field E_{eff}. For low fields, where the slope of $v_h(E_{eff})$ is fairly constant, this expression reduces to the conventional, local expression for carrier mobility. In the limit that the applied field no longer varies, this expression yields the correct steady state velocity.

Though the drift velocity demonstrates the presence of velocity overshoot, and its relationship to a varying field, there are diffusive and convective contributions to the average velocity as well. In 1-D, the following drift-diffusion-convection (DDC) equation first introduced by Sanchez [6] was used to resolve these components,

$$\frac{d}{dx}(Dn) + nv_d + n < v_{\|}^2 \frac{\partial \tau}{\partial x} >= \frac{J_o}{q}. \tag{4}$$

The presence of the $\frac{\partial \tau}{\partial x}$ term is due to the effect of a spatial variation in the collision rate caused by variations in the donor impurities. Using the effective field concept, the following expressions for the transport parameters were obtained:

$$D(x) = -\int d\vec{p} v_{\|}^2 \tau(x,\varepsilon) f_s^h(x,\vec{p})$$

$$< v_{\|}^2 \frac{\partial \tau}{\partial x} > = \int d\vec{p} v_{\|}^2 \frac{\partial \tau(x,\varepsilon)}{\partial x} f_s^h(x,\vec{p})$$

where f_s^h is the distribution function obtained from the effective field. Although equation (4) represents an initial value problem, it did not pose any major problems for self-consistent device simulations where two boundaries are present. A second order version of this equation was also implemented.

III. Results

Shown in Fig. 2 is the effective field profile generated from a Monte Carlo analysis of the channel region of a MOSFET [3]. Also plotted is the effective field generated from formula (1), exhibiting a remarkable agreement. Shown in Fig. 3 is the effective field profile determined from a case studied in Ref. [7]. Also plotted is the expression of $v_h(E)$ and v_d to demonstrate that there is a significant difference between using the effective field drift term, and assuming that the drift velocity depends only upon the locally applied field.

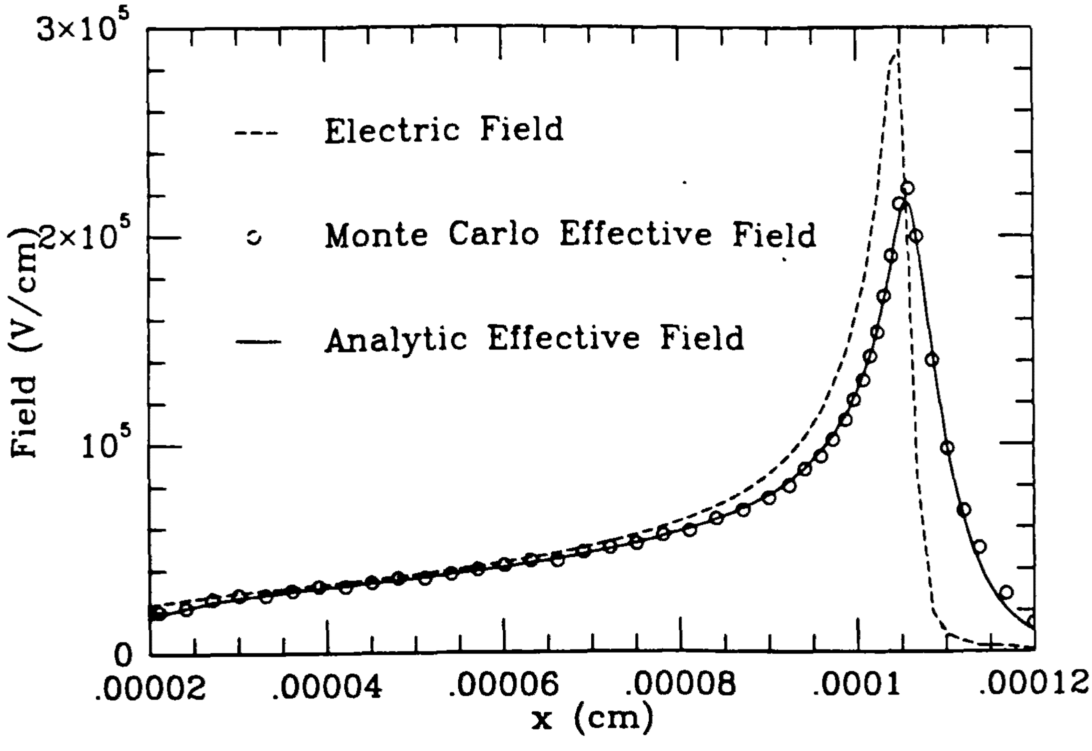

Fig. 2. A comparison of effective fields from ref. [1] and formula (1). A Monte Carlo simulation was used to verify the value of the effective field for most of the points in ref. [1].

In Fig. 4, a comparison of the average velocity obtained from equation (4) and a Monte Carlo calculation is performed. For additional comparison, the first order (P_1) Legendre polynomial calculation performed in Ref. [7] is also included. As can be seen, good agreement between the Monte Carlo calculation and the effective field calculation of the average velocity is obtained. The agreement is better than the P_1 calculation probably due to an implicit avoidance of truncation error in the effective field approach.

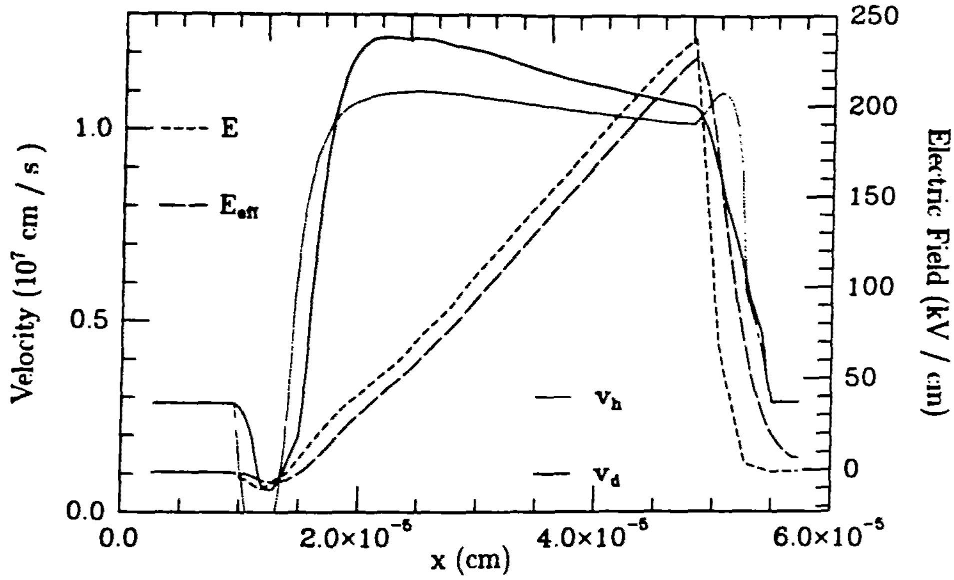

Fig. 3. The drift velocity (v_d), homogeneous field velocity(v_h), self-consistent electric field (E), and effective field(E_{eff})are plotted for a n^+nn^+diode simulation, Bias = 5.0 Volts. The discrepancy between v_h and v_d demonstrate the importance of the non-local dependence of the mobility.

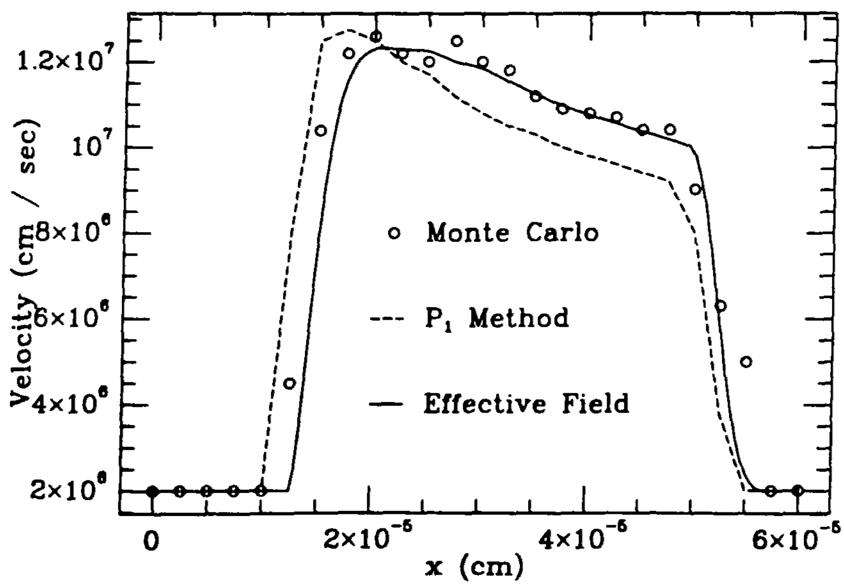

Fig. 4. The average velocity from a drift-diffusion (DD) equation, a Monte Carlo (MC) simulation, and a 1st order Legendre polynomial (P1) calculation found in ref. [4] are plotted for comparison. Better agreement than the P1 approach is attributed to an implicit avoidance of truncation error.

The discrepancy in the barrier region of the device is due to the fact that the diffusion coefficient has been overestimated by the effective field formulation presented so far. To account for temperature reduction due to the barrier, the effective field is reformulated using a different approximation scheme. This approximation scheme insures that the correct equilibrium behavior is obtained, and predicts temperature lowering. However, a detailed comparison and study in this region of the device is left for future work.

III. Summary

An approach for device modeling using the drift-diffusion model has been developed which does not use any empirically determined parameters except for those that are associated with deformation potentials and band structures. Considerations so far have been restricted to a single-valley model of silicon. However, the generality of the approach encourages an investigation into considerations of multiple bands and anisotropic effects.

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