The Electric Field Gradient in Device Simulations

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Abstract

Self-consistent Monte Carlo (MC) simulations of a n+/n/n+ Si diode will be compared to drift-diffusion (D-D) modelling for a range of field and fieldgradient values. The conditions under which MC and D-D results begin to differ because of velocity overshoot are pointed out as well as the magnitude of the differences expected. Finally, it is shown that by adding a term proportional to the electric field gradient to the D-D velocity, overshoot can be accounted for and the D-D simulation results are in better agreement with the MC results.

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The standard D-D modelling, with the carrier velocity a function of the local electric field only, cannot account for the appearance of velocity overshhot characteristis of large electric field gradients. In order to assess the range of fields and field gradients where the D-D results are unsatisfactory and the errors expected when using such a model, self-consistent MC simulations are compared to D-D calculations.

The device studied is the generic n+/n/n+ Si diode with a 0.4 μ m lightly doped region. The D-D results are obtained using the well known Scharfetter-Gummel discretization scheme. Field dependent values for the mobility (obtained from homogeneous MC simulations) are used and the results compared to selfconsistent ensemble MC simulations. As expected, the deviations increase as the voltage applied across the diode (and the field gradient) increases. A typical example is shown in Fig. 1 for a bias of 2.5 V at 300 K. Because of overshoot, the MC velocity and the current density are 20% and 10% higher, respectively than the D-D result.

A rather simple (and computationally inexpensive) way to account for such non-local effects in D-D models is to write the velocity as:

$$u = \mu(F)F + \mu(F)L(F)\frac{dF}{dx} - \frac{D(F)}{n}\frac{dn}{dx}$$

where L(F) is a phenomenological length constant, calculated from MC simulations [1]. The same discretization scheme is kept, while amending the current by the term:

$$n\mu(F)L(F) \frac{dF}{dx}$$

The resulting velocity, shown in Fig. 1, is in quite good agreement with the MC result, as is the calculated current density. It should be noted that the values of L(F) used in the simulations were taken directly from [1] without any adjustment or fitting. In [1], L(F) was calculated neglecting the effect of the space charge on the field. Also, the lower field values had larger uncertainties associated with them. This helps to explain the poorer agreement with the MC results in the lower field region. The velocity peak at around 0.25 μ m is due to the rather sudden appearance of overshoot as a function of electric field, as calculated in [1].

1. M. Artaki, to be published in Appl. Phys. Lett. (Jan. 11, 1988)



Position (Angstroms)

Figure 1. Drift velocity in a n+/n/n+ Si diode with a 0.4 μ m intrinsic region for an applied bias of 2.5 V.