MONTE CARLO ANALYSIS OF REPEATED OVERSHOOT STRUCTURES

Tim Crandle and Jack East
Department of Electrical Engineering and Computer Science
The University of Michigan
Ann Arbor, Michigan 48109

Peter Blakey
Department of Electrical and Computer Engineering
Arizona State University
Tempe, Arizona 85287

(Received 13 August 1984 by John D. Dow)

The effectiveness of two recently proposed repeated overshoot structures is investigated using Monte Carlo simulation. Results are presented showing electron velocity, energy and valley occupancy as a function of bias conditions. High local peak velocities sometimes are observed, but for a given mean field across a unit cell the average velocities are always relatively low; less than or at best equal to the steady state velocity in bulk GaAs with the same average fields. The reasons for this are explained in terms of the diffusion process.

1. Introduction

A repeated overshoot structure is a multilayer device with a doping profile arranged to provide a spatially modulated field profile. Typical doping, electric field and potential profiles are shown in Figure 1. The principle of operation relies on periodic acceleration in short high field regions to produce periodic velocity overshoot, resulting in a high mean velocity. The basic concept was proposed by Cooper et al. [1], who suggested the structure 1 of Table 1. Golio et al. recently proposed structure 2 of Table 1 as a possible improvement. Structure 2 is designed to increase mean velocity by reversing electrons with negative velocities, rather than simply accelerating electrons with positive velocities [2].

The purpose of the present paper is to calculate the characteristics of these two structures, using a detailed model of electron transport, for GaAs devices operating at 300°K. The primary quantity of interest is the mean electron velocity in each structure as a function of mean electric field. The mean field is determined by the external bias voltage.

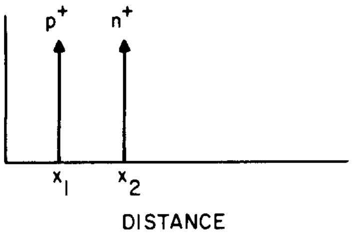
2. The Model

The underlying treatment of electron transport is the Monte Carlo simulation model developed by Fawcett [3]. Features of the specific implementation have been described elsewhere [4]. This electron transport kernel is used in conjunction with a prescribed electric field as a function of distance. The field is calculated within a single cell for a given structure and bias condition, assuming negligible perturbation due to space charge. A single electron is simulated in this field. Periodic boundary conditions are adopted, i.e., on crossing either boundary the electron is reinjected at the other boundary with the same velocity. This 'periodic' boundary condition corresponds to the limit that the number of cells tends to infinity, and neglects injecting and collecting contacts. Information from several thousand cell transits is averaged to yield estimates of electron velocity, valley occupancy and energy as a function of position within the cell.

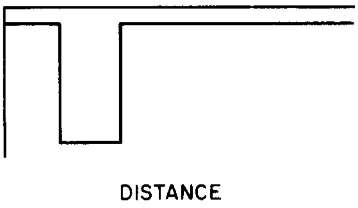
3. Overall Results

The overall results of the comparison between the two structures is shown in Figure 2. This shows the mean electron velocity in each structure as a function of the mean electric field. The 'static' velocity-field curve for undoped GaAs is also shown. Structure 1 has low field velocities much lower than the 'static' results. Structure 2 represents an improvement over Structure 1. However its velocity-field characteristic is at best equal to the static case. The obvious conclusion to be drawn from these results is that the repeated velocity overshoot concept does not appear promising as a means of obtaining high mean velocities in semiconductor devices.

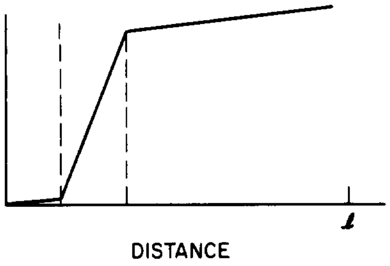
0749-6036/85/010091+06 $02.00/0



(a) DOPING



(b) ELECTRIC FIELD



(c) VOLTAGE

Figure 1 Typical doping electric field and potential profile.

Detailed results for the two structures must be examined to establish why the concept is less successful than predicted by idealized theories. Information available for each structure and bias point is (as a function of position) field, potential, mean energy of central valley electrons, central valley electron population fraction, fraction of central valley electrons with positive velocity and, mean electron velocity. Space limitations preclude a comprehensive presentation of the detailed results, but some key features will be presented for each structure.

4. Detailed Results

A complete set of results for structure 2 at a mean bias field of 2300 V/cm is shown in Figure 3. It is clear that the increase in central valley energy across the field step (Figure 3(c)) is much less than the 0.048 V potential across the high field region (Figure 3(a)). This failure of the high field region to produce a corresponding increase in central valley energy helps explain why there is hardly any velocity overshoot. The failure is not associated with intervalley transfer since, as shown in Figure 3(d), there is almost no transfer under these conditions. The answer therefore must lie with what happens to the central valley electrons crossing the high field region.

Some electrons will enter the high field region with positive velocity, be accelerated across the region without scattering, and gain the entire 0.048 volt energy step. Other electrons will enter with positive velocity but will scatter within the high field region. These electrons may lose energy directly (e.g. as a result of inelastic polar optical phonon scattering) or indirectly, due to deceleration by the field following a momentum randomizing

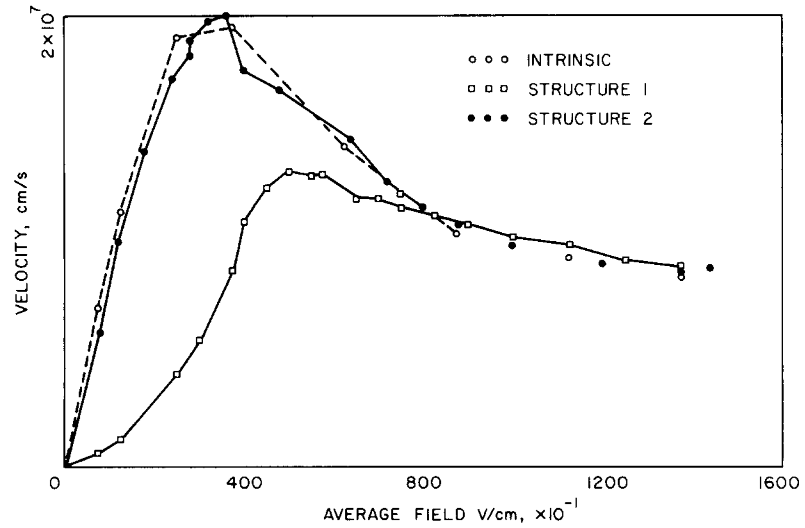


Figure 2 Comparison of structure 1, structure 2 and uniform material.

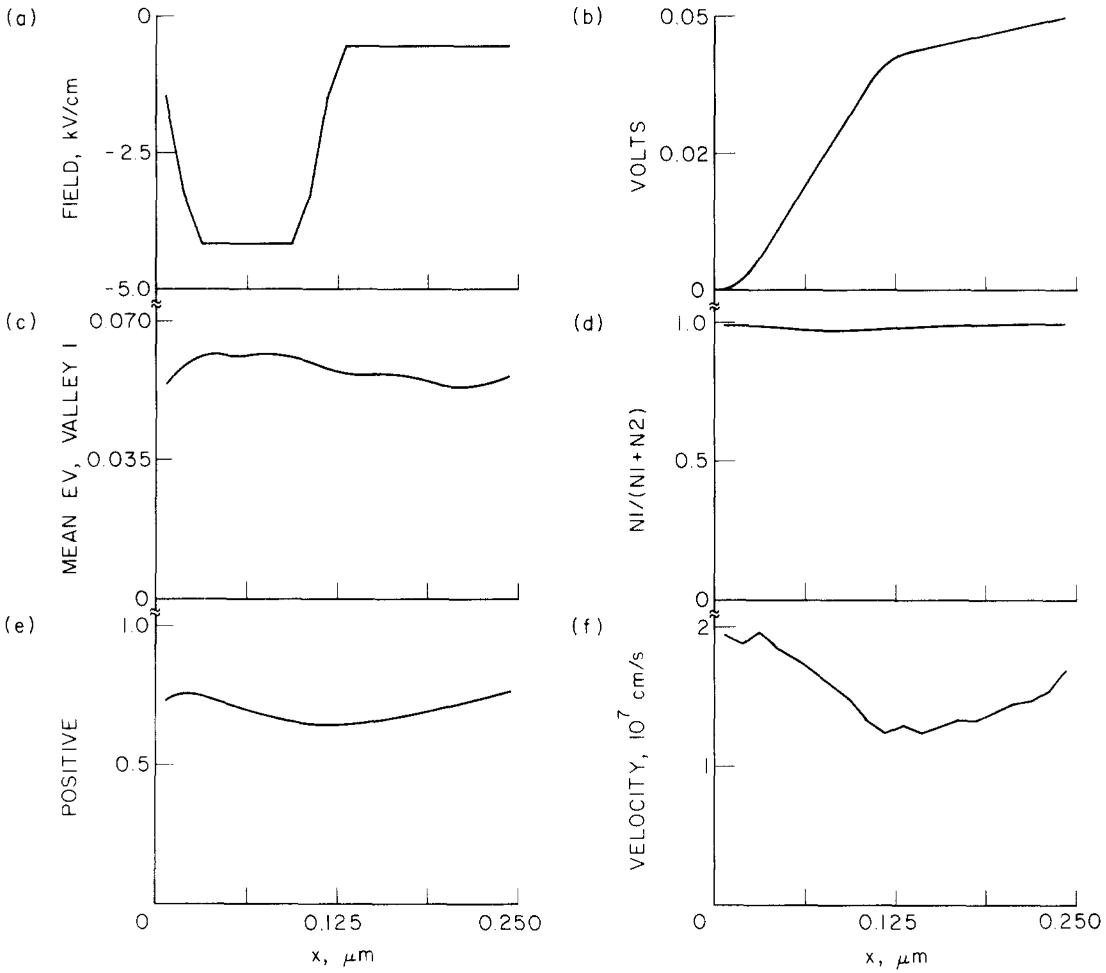


Figure 3a Electric field profile for structure 2 (2300 volt/cm average field)

3b Voltage profile

3c Energy Profile

3d Central valley electron fraction profile

3e Positive velocity fraction profile

3f Velocity profile

collision to a negative velocity. A third type of electron will enter the high field region with negative velocity. Figure 3(e) shows that at all points in the cell between 20 percent and 40 percent of the electrons have negative velocities, so this third class of electrons is significant. Such electrons will lose energy until their velocity becomes positive, as a result of being turned around by the field, as a result of a scattering event, or until they transit the entire layer. Simple repeated overshoot theory considers only the first class of electrons. 'Near-ballistic' theory makes some attempt to include the second class, but generally fails to account for energy loss following elastic collisions to negative velocities. The results of this study indicate that departures from average behavior (resulting in, among other things, significant numbers of electrons with negative velocity) are of first order importance and must be included in device models. In the context of the scattering process transport models used in this work, these effects will be referred to as 'diffusion-like'.

Similar results are obtained at higher bias fields, with the exception that intervalley transfer effects have become important. Figure 4 shows the central valley population fraction for a mean bias field of 4000 V/cm, very close to the maximum velocity for the structure. Significant intervalley transfer is occurring,

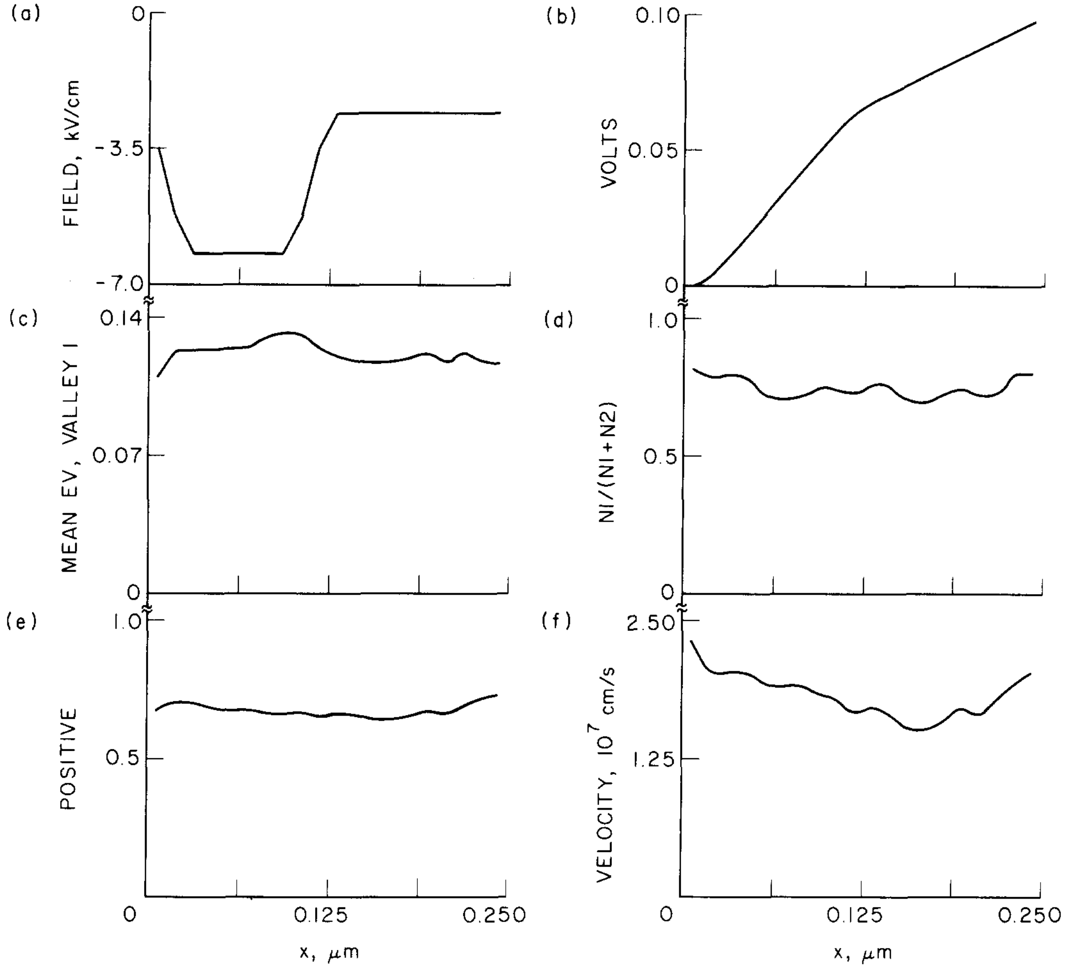


Figure 4a Electric field profile for structure 2 (4000 volt/cm average field)

4b Voltage profile

4c Energy profile

4d Central valley electron fraction profile

4e Positive velocity fraction profile

4f Velocity

but the population fraction is almost constant, indicating that the cell length is short with respect to distances travelled between intervalley scattering events. Idealized models should not assume that most satellite valley electrons return to the central valley before encountering the next high field region.

Structure 1 provides a larger accelerating potential across the high field at mean fields below 4000 V/cm, however the low field region must be positive to compensate this voltage, resulting in a retarding field. A complete set of detailed results for a mean field of 2500 V/cm is shown in Figure 5. The accelerating potential does result in an increase in electron energy (Figure 5(c)), and causes a local velocity overshoot (Figure 5(f)), but the mean velocity is low because of the extensive region of low local electron velocity. At higher mean fields the same type of behavior is observed except that intervalley transfer effects become more significant, the peak velocities reduce and the minimum velocities increase. For mean fields up to about 4000 V/cm this increases the mean velocity, but at higher fields increasing transfer to the satellite valley causes the velocity to degrade.

5. Discussion

The computed results are only surprising when viewed from a ballistic or near-ballistic

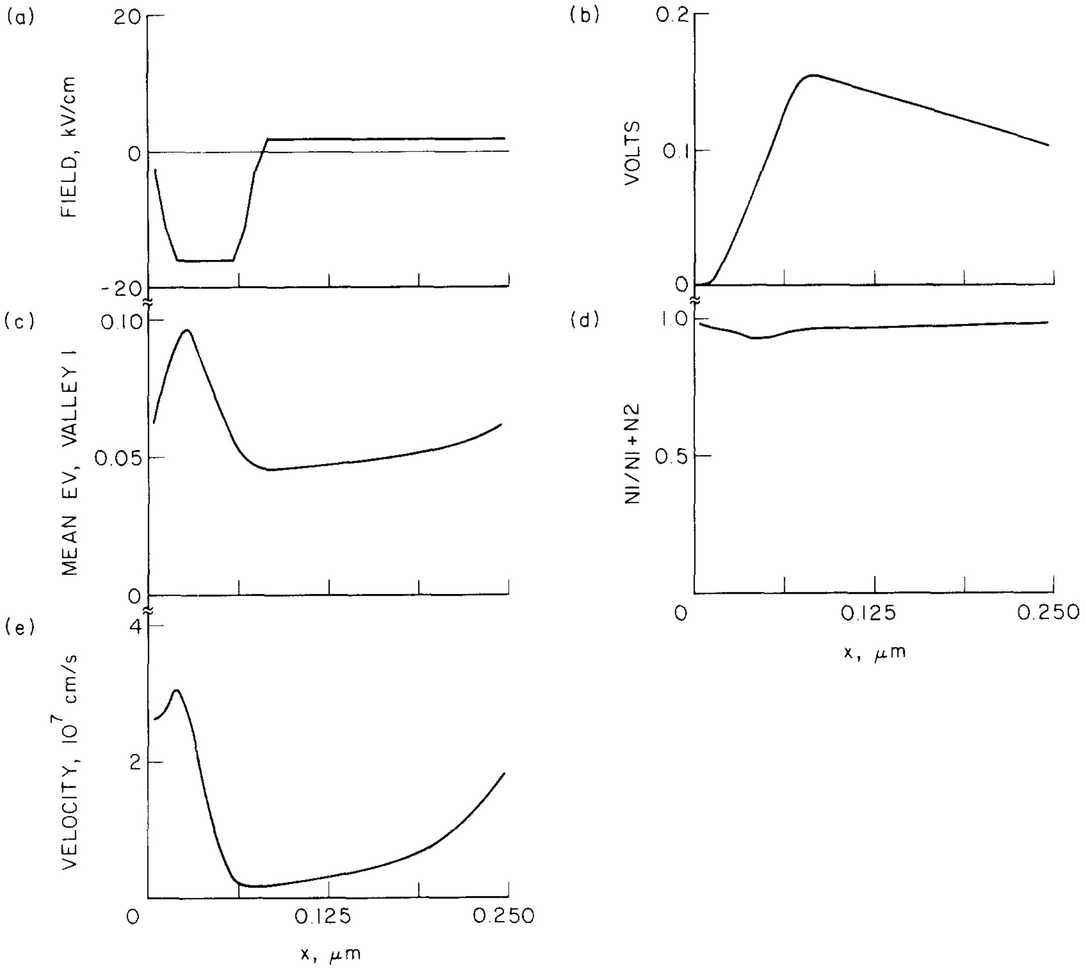


Figure 5a Electric field profile for sturcture 1 (2500 volt/cm average field)

5b Voltage profile

5c Energy profile

5d Central valley electron fraction profile

5e Velocity profile

perspective. They are quite consistent with the requirements of current continuity and a drift-diffusion perspective. Current continuity requires that the product of the electron concentration and the mean net electron velocity be constant in a one dimensional structure under dc conditions. The net carrier velocity may be thought of as the algebraic sum of a 'drift' velocity representing 'mean' behavior and a 'diffusion' velocity representing the effect of the distribution of behaviors around the mean. Simple ballistic models predict regions of locally higher velocity and electron energy due to local steps in the electric field. The present results show that these local peaks are reduced and spread out by the diffusion-like nature of the electron transport. The drift-diffusion model shows that steep gradients are difficult to obtain in materials with high diffusion coefficients. Sharp peaks in energy or velocity are difficult to obtain for the same reason.

Although the results presented strongly suggest that the repeated overshoot concept is unpromising, they are not wholly conclusive. Other structures may be superior to the two investigated; in particular structures with a few cells may have properties superior to the infinite cell limit. Investigation of such structures would require detailed consideration of Debye tailing at the injecting and collecting contacts in homojunction devices, and the series resistance of heterojunction launchers and collectors in heterojunction devices. Additional problems which have not been considered in this paper are charge instabilities, these can be investigated using a self-consistent particle-field simulation, and the limited bias conditions for which devices incorporating repeated overshoot cells would operate correctly.

6. Conclusions

Two repeated overshoot structures have been investigated theoretically using Monte Carlo simulation. Neither structure represents an improvement over bulk GaAs, and the prospects for the underlying concept are judged unpromising. The main problem appears to be that departures from mean behavior (diffusion-like effects) counteract efforts to explicit assumed mean behavior. Similar diffusion-like effects may impair the performance capabilities of other ballistic and overshoot devices.

Acknowledgements

It is a pleasure to acknowledge useful discussions with M. Golio, M. Tischler and R. Trew.

References

(1) J. A. Cooper, F. Capasso, K. K. Thorbar, "Semiconductor Structures for Repeated Velocity Overshoot," Electron Device Letters, Vol. EDL 3, No. 12, p. 407, 1982.

(2) M. Golio, M. Tischler, R. Trew, personal communication.

(3) W. Fawcett, "Non-Ohmic Transport in Semiconductors," in Electrons in Crystalline Solids, International Atomic Energy Agency, Vienna, 1973.

(4) R. O. Grondin, P. A. Blakey, J. R. East and E. D. Rothman, "Monte Carlo Estimation of Hot Carrier Noise at Millimeter and Submillimeter-Wave Frequencies", IEEE Trans. on Electron Devices, Vol. ED-28, No. 8, pp. 914-923, August 1981.