

Harmonic Balance Boltzmann Equation Solver for Gunn Domains

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Abstract—In Gunn diodes a negative differential mobility leads to the formation of dipole domains. At high frequencies the underlying electron transport becomes strongly nonlocal in time and space, and the full Boltzmann equation is required to accurately describe Gunn domains. A versatile deterministic approach based on the harmonic balance method is presented by which the Boltzmann equation can be solved for the homogeneous bulk case in space and time, and the ultimate performance limits of semiconductor materials can be explored before a specific device design is investigated. As an example, Gunn domains in bulk GaAs are investigated, but the approach can be easily extended to other materials.

Index Terms—Gunn effect, GaAs, Boltzmann equation

I. INTRODUCTION

Gunn diodes are versatile microwave power sources [1], in which a negative differential mobility leads to soft plasma modes [2] and dipole domains [3], [4]. The occurrence of new materials (e.g. GaN, 2D materials) has led to a renewed interest in the Gunn effect (e.g. [5], [6]), and we simulate homogeneous bulk systems to investigate whether Gunn oscillations are, in principle, possible and what the peak performance of the material might be. The semiconductors are modeled on a microscopic level by the Boltzmann equation (BE) [7]. We use a deterministic solver instead of the usual Monte Carlo method because analysis in the complex Fourier domain is much more efficient and capable than in the spatiotemporal domain.

II. THEORY

As an example, an infinitely large homogeneous GaAs bulk system with a constant doping N_D and constant external electric field E_0 in x -direction is investigated.¹ We assume that all vectorial quantities have only x -components, and all solution variables depend only on x w.r.t. space.

In the semi-classical framework the BE is the fundamental equation of electron transport [8], [9]

$$\frac{\partial f}{\partial t} - \frac{e}{\hbar} E \frac{\partial f}{\partial k_x} + v_x \frac{\partial f}{\partial x} = \mathcal{S}\{f\} . \quad (1)$$

$f_\gamma(\mathbf{k}, x, t)$ is the electron distribution function, γ the index of the conduction band valley, $\mathbf{k}$ the wave vector, x the position in space, t the time, $\hbar$ Planck's reduced constant,

¹In a Gunn diode with a drift zone of length L the field $E_0 = -V_{\text{appl}}/L$ would be due to the applied bias V_{appl} .

$E(x, t)$ the x -component of the electric field, $v_{x,\gamma}(\mathbf{k})$ the x -component of the group velocity, and $\mathcal{S}\{f\}$ the scattering integral. For the sake of legibility of the equations we will drop wherever possible all arguments and indices of the distribution function, etc. We use a conduction band structure with spherical non-parabolic Γ , L and X valleys and the most relevant scattering processes (acoustic, optical, polar optical phonons and impurity scattering) [10], [11]. The Pauli principle is neglected due to the low densities and/or high electric fields. The BE is solved by a deterministic approach based on a spherical harmonics expansion (SHE) up to third order, which is sufficiently accurate for the cases investigated in this work [12]. This approach has the advantage of being versatile because transport models (band structure, scattering processes) exist for many types of materials (e.g. [9]), and the stringent approximations of simpler models (e.g. hydrodynamic models) are avoided.

The electric field is obtained by Gauss's law² (GL) [13]

$$\frac{\partial E}{\partial x} = e \frac{N_D - n}{\varepsilon_{\text{sc}}} \quad (2)$$

with the electron density

$$n(x, t) = \frac{2}{(2\pi)^3} \sum_{\gamma} \int f_{\gamma}(\mathbf{k}, x, t) d^3k , \quad (3)$$

and ε_{sc} is the permittivity of the semiconductor. The total current density (electron plus displacement current density) must be solenoidal (charge conservation) [13]

$$\frac{\partial}{\partial x} \left(-ej + \varepsilon_{\text{sc}} \frac{\partial E}{\partial t} \right) = 0 \quad (4)$$

with the particle current density

$$j(x, t) = \frac{2}{(2\pi)^3} \sum_{\gamma} \int v_{x,\gamma}(\mathbf{k}) f_{\gamma}(\mathbf{k}, x, t) d^3k . \quad (5)$$

²If instead of a bulk system a lateral structure with translation invariance in x -direction (e.g. a 2D material) is investigated, Gauss's law has to be replaced by the corresponding solution of the Poisson equation resulting in minor modifications of the approach.

The distribution function is expanded in a Fourier series of order N_H with coefficients $\underline{f}_l = \underline{f}_{-l}^*$ to ensure a real distribution function (harmonic balance approach)

$$f_\gamma(\mathbf{k}, x, t) = \sum_{l=-N_H}^{N_H} \underline{f}_{\gamma,l}(\mathbf{k}) \exp(iql\eta) \exp(\sigma|l|t) \quad (6)$$

with $\eta = v_{pl}t - x$, the fundamental wave number $q = 2\pi/L$, fundamental angular frequency $\omega = v_{pl}q$ and the growth constant σ which is in this case a continuation parameter used to ease the numerical solution of the equation system and which must vanish [14]. For $\sigma = 0$ the domains are periodic in space with wave length $\lambda = L$ and in time with period $T = 2\pi/\omega$. They are plane waves with the speed v_{pl} . The domains are by construction charge neutral, and only dipole domains can be simulated. A similar expression is used for the electric field

$$E(x, t) = \sum_{l=-N_H}^{N_H} \underline{E}_l \exp(iql\eta) \exp(\sigma|l|t) . \quad (7)$$

The BE is given for $t = 0$ by

$$[\sigma|l| + iql(v_{pl} - v_x)] \underline{f}_l - \frac{e}{\hbar} \sum_{l'=\max(-N_H, l-N_H)}^{\min(N_H, l+N_H)} \underline{E}_{l'} \frac{\partial \underline{f}_{l-l'}}{\partial k_x} = \mathcal{S}\{\underline{f}_l\} . \quad (8)$$

In the case of $\sigma = 0$ the solution is valid for all times t . The nonlinear drift term of the BE results in a discrete convolution [15]. GL yields for $l \neq 0$

$$iql\varepsilon_{sc}\underline{E}_l = e\underline{n}_l . \quad (9)$$

We have the constraints that $E_0 = -V_{appl}/L$ and that the bulk is charge neutral with $n_0 = N_D$. Since the phase of the domain is arbitrary, we fix it by requiring that $\underline{E}_1$ must be real and should have the opposite sign of E_0 to center the domain at about $x \approx L/2$. This constraint is implemented by $\Re\{\underline{n}_1\} = 0$, which results in a real E_1 (cf. (9)). For a nonzero E_1 charge conservation (4) yields $\Re\{\underline{j}_1\} = 0$, which results in $\sigma = 0$. We solve these equations with the Newton-Raphson method starting with a suitable initial solution including a nonzero σ . The harmonic balance approach is implemented in such a way that it can handle various forms of the discrete BE and GL.

In the linear response regime (small-signal case) we linearize the BE and GL and retain only the equations for $l = 1$. In this case the growth constant is in general nonzero and we get soft-mode plasma waves [2]. The small-signal electric field, for example, is given by a plane wave

$$\delta E(x, t) = \Re\{\underline{E}_1 \exp[i(\omega t - qx)]\} \exp(\sigma t) , \quad (10)$$

where σ and $\omega = 2\pi\nu$ are functions of q . A positive σ leads to exponential growth and indicates the possibility of domain formation [4].

III. RESULTS

As an example we solve the BE for a well-established GaAs model with a band structure including three valleys [10], [11] by the spherical harmonics expansion method [12] at room temperature. In Fig. 1 the electron drift velocity is shown for various donor concentrations, and a negative differential mobility occurs, indicating the possibility of Gunn oscillations.

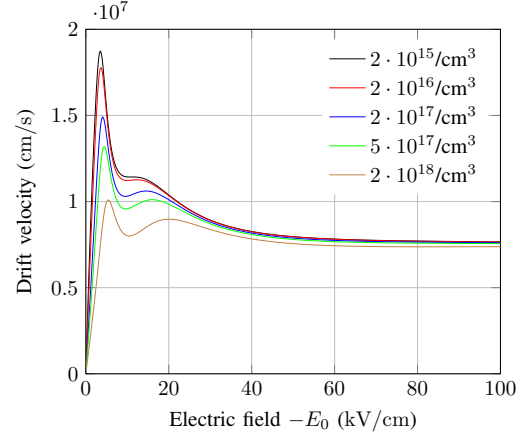


Fig. 1. Electron drift velocity for different donor concentrations N_D at room temperature.

First, we investigate the small-signal case of soft-mode plasma waves. In Fig. 2 σ is shown as a function of E_0 and two distinct peaks occur at fields for which the differential mobility is negative (cf. Fig. 1). At low E_0 electron transfer occurs between the Γ and L valleys of GaAs [3] resulting in the first peak, whereas at higher E_0 all three valleys (Γ , L , X) are involved. Although the differential mobility is lower for the second peak, the growth factor is higher (at least for the higher doping concentrations), demonstrating the importance of solving the full BE.

In Fig. 3 the dependence of σ and ν on q is shown. The frequency ν increases with q , whereas the growth constant

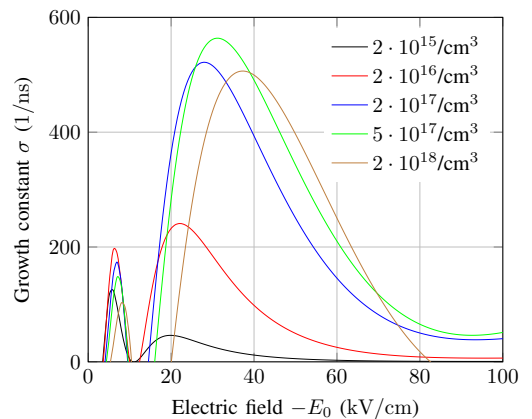


Fig. 2. Growth constant of plasma waves at $q = 0$ for different donor concentrations N_D and room temperature.

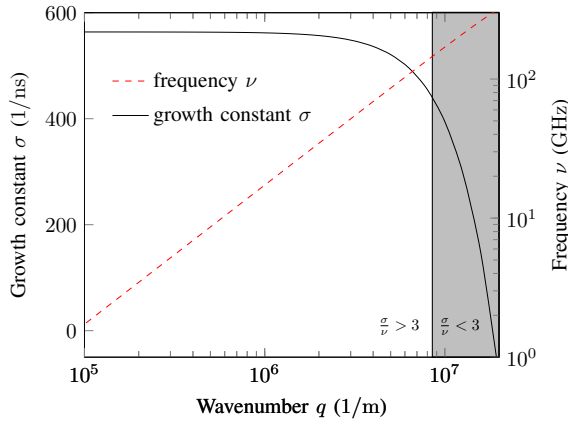


Fig. 3. Growth constant and frequency of a plasma wave at $N_D = 5 \cdot 10^{17}/\text{cm}^3$, $E_0 = -31 \text{ kV/cm}$. To the left of the gray area Kroemer's criterion is satisfied.

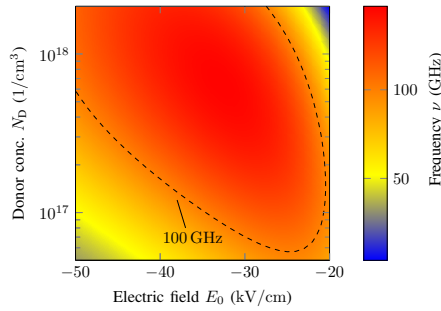


Fig. 4. Frequency for $\sigma = 3\nu$. Peak frequency at $N_D = 5 \cdot 10^{17}/\text{cm}^3$, $E_0 = -31 \text{ kV/cm}$.

drops. For domain forming the growth constant should be at least three times larger than the frequency $\sigma > 3\nu$ [4]. For $q > 8.6 \cdot 10^6/\text{m}$ the criterion for domain forming is no longer satisfied limiting the maximum frequency to 147 GHz. The velocity of the plasma wave $v_{pl} = 1.07 \cdot 10^7 \text{ cm/s}$ is higher than the drift velocity of the electron gas ($0.863 \cdot 10^7 \text{ cm/s}$).

In Fig. 4 the maximum oscillation frequency (q such that $\sigma = 3\nu$) is shown for various electric fields E_0 and donor concentrations N_D . The peak frequency of 147 GHz is found for $N_D = 5 \cdot 10^{17}/\text{cm}^3$ and $E_0 = -31 \text{ kV/cm}$. Thus, it is possible to CPU-efficiently scan the configuration space of a material (15 CPU seconds per configuration) to find an upper limit for the peak performance. Together with, for example, a DC power constrain it is possible to search for an optimal operating point.

The plasma wave grows exponentially in time for $\sigma > 0$, and nonlinear effects lead to the formation of a stable dipole domain [4]. The electric field and electron density of the Gunn domain for the condition of peak frequency are shown in Fig. 5 together with the relative valley occupancy evaluated by the harmonic balance method. The electron transfer clearly involves all three valleys. The domain travels with $v_{pl} = 8.98 \cdot 10^6 \text{ cm/s}$ which is slower than the corresponding plasma wave, and the frequency is reduced from 147 GHz to

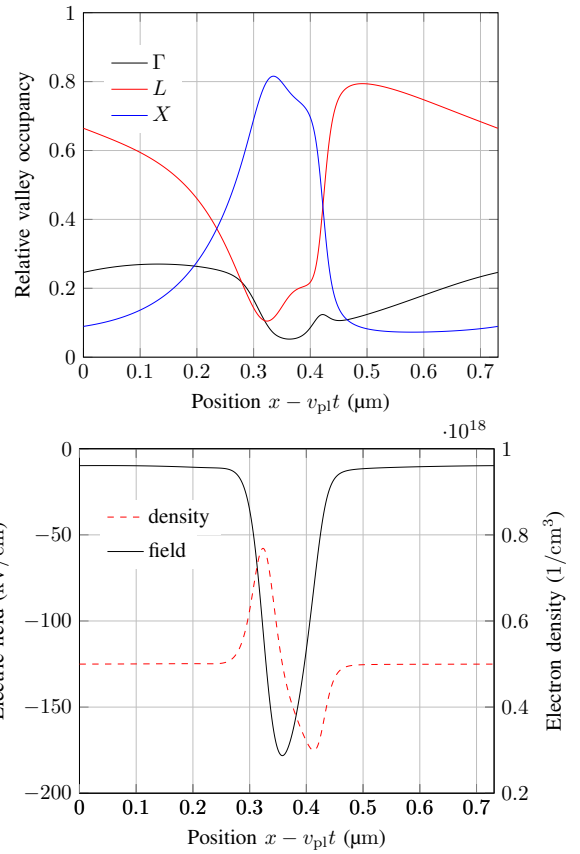


Fig. 5. Occupancy of the valleys (left), the electric field and electron density (both right) for the Gunn domain at $N_D = 5 \cdot 10^{17}/\text{cm}^3$, $E_0 = -31 \text{ kV/cm}$, $q = 8.6 \cdot 10^6/\text{m}$. The domain moves to the right.

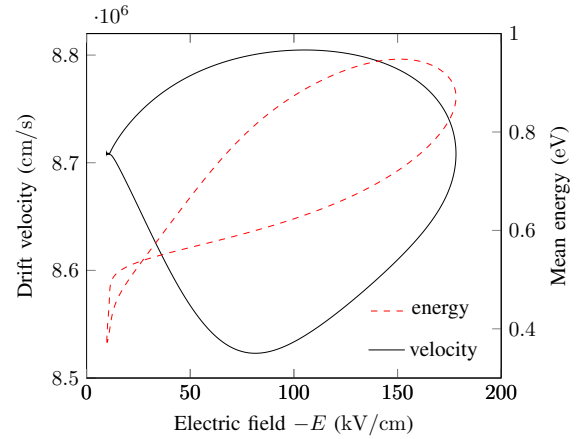


Fig. 6. Drift velocity and mean energy vs. electric field for the Gunn domain at $N_D = 5 \cdot 10^{17}/\text{cm}^3$, $E_0 = -31 \text{ kV/cm}$, $q = 8.6 \cdot 10^6/\text{m}$.

122 GHz. The drift velocity varies only by about 3% over the domain (Fig. 6) despite the huge change in the electric field clearly demonstrating that even a weak negative differential mobility does not preclude a strong Gunn effect. The variation of the mean energy, on the other hand, is large.

The DC power should be as low as possible to conserve

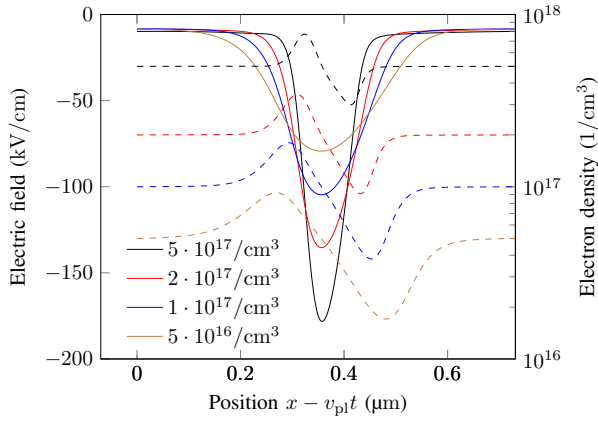


Fig. 7. Electric field (solid lines) and electron density (dashed lines) for Gunn domains at $E_0 = -31$ kV/cm, $q = 8.6 \cdot 10^6$ /m and different donor concentrations N_D .

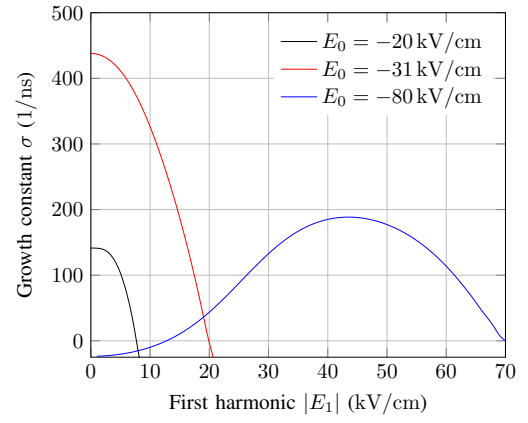


Fig. 8. Growth constant of the domain vs. the field of the first harmonic for different external fields E_0 at $N_D = 5 \cdot 10^{17}$ /cm³, and $q = 8.6 \cdot 10^6$ /m.

energy and to reduce self-heating. It is proportional to the DC electric field and donor concentration, which both should be as small as possible. On the other hand, if the donor concentration and thus electron density is reduced, the electric field spreads in space (Fig. 7), and since it cannot spread beyond the given wave length $\lambda = L = 2\pi/q$, a lower limit of the donor concentration occurs. Thus, a minimum DC power is required, which increases with q and thus frequency.

We can solve the harmonic balance BE with σ as a variable and fix the magnitude of the first harmonic of the electric field $\underline{E}_1$. For small values of $|\underline{E}_1|$ we obtain again the small-signal solution. This is shown in Fig. 8 for three values of E_0 , where the third value is so large that for the given q the growth constant σ is negative at low $|\underline{E}_1|$. With growing $|\underline{E}_1|$ nonlinear effects occur and σ changes. In the first two cases it decreases and when it becomes zero a stable solution is found with $d\sigma/d|\underline{E}_1| < 0$. In contrast, for the largest E_0 the growth constant is negative for $|\underline{E}_1| = 0$ and grows with $|\underline{E}_1|$. Thus, two stable states exist: $|\underline{E}_1| = 0$ without a domain and $|\underline{E}_1| = 70$ kV/cm with a strong stable domain, but this domain does not form spontaneously. Only if the initial $|\underline{E}_1|$ is larger than 13 kV/cm (e.g. due to a launcher in a Gunn diode) a domain can form.

IV. CONCLUSIONS

We have presented a versatile simulation approach for Gunn domains in bulk GaAs by solving the full BE with the harmonic balance method. With this approach the configuration space (E_0 , N_D) can be CPU-efficiently scanned for peak frequency and the properties of the corresponding Gunn domains can be determined. The approach can be easily adapted to the case of other materials, geometries (e.g. 2D materials), etc.

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