Simulation of THz Emission by Plasma Waves in GaAs Devices Based on the Boltzmann Transport Equation

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***Abstract*—Plasma oscillation in a submicron gate length field effect transistor is a promising candidate for terahertz emissions. The transport model plays a significant role for the simulation of the instability leading to the self excitation of plasma oscillations. For this purpose, the growth rate and frequency of the plasma instability are compared using a simple transport model based on the Euler equation and the complete Boltzmann transport equation. The comparison shows that the simple transport model fails to capture important aspects included in the Boltzmann equation concerning the generation of plasma waves at high electric fields and low temperatures.**

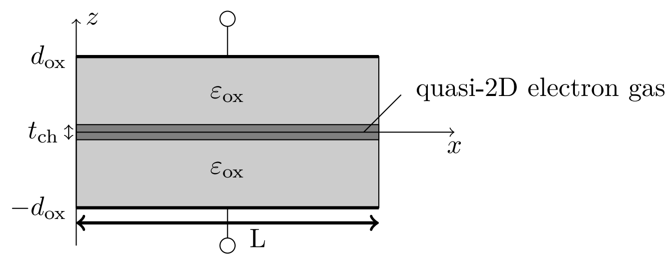

Figure 1: A symmetric double gate structure with a quasi-2D electron gas at $z = 0$ in a GaAs layer and the channel length L.

I. Introduction

Generation and detection of THz waves based on plasma waves − electron density oscillations in time and space − in two dimensional electron channels is a possible way to fill the so called *terahertz gap* [1]. The excitation of electron plasma waves in a field effect transistor can lead to the emission of terahertz radiations which relies on the instability of the propagating steady-state current [2]. A large body of theoretical work based on transport equations derived from the first two moments of the semi-classical Boltzmann Transport Equation (BTE) exists with many simplifications like the assumption of equilibrium transport conditions [3]. We call these kinds of approximations of the BTE the Semiconductor Equations (SE) [4]. With the ongoing miniaturization of semiconductor devices where distances become smaller than the mean free path of carriers, it is essential to consider non-equilibrium transport. Rather than a moments-based approach, solving the BTE directly is much more accurate [5].

Reference [4] shows how to calculate plasma waves at arbitrary frequencies and wave numbers by the BTE. This paper is based on the methods developed in Ref. [6] where the BTE is solved together with the Poisson Equation (PE) to obtain the plasma dispersion of the two Vlasov modes for equilibrium and non-equilibrium states. In addition the plasma instability is calculated according to the Dyakonov-Shur approach [2]. In this work the accuracy of using the SE as a transport model to get the Vlasov modes' dispersion relation and the plasma instability is assessed by comparison with numerical solutions of the BTE at different temperatures for a device with a GaAs channel.

II. Approach

We consider a homogeneous electron gas in the quasi-2D **k**-space of a system confined in one dimension, as shown in Fig. 1. To be consistent with the approach of Dyakonov-Shur, the electron gas is located in the plane $z = 0$ and the channel thickness (t_{ch}) is assumed to be negligible compared to the oxide thickness (d_{ox}).

Furthermore, we assume that the linear response of the electronic system is sufficient to model plasma wave propagation. Therefore all variables are split into a stationary part and a small signal part at a complex angular frequency and wave number [4], [6].

The two equations for the SE are the first moment of the BTE which is the continuity equation for the electron density, and the second moment which gives the balance equation for the electron current density and includes the convective derivative [7], [8]. The small signal SE is obtained by expanding the electron density and current density around the stationary states up to the first order in harmonic functions [4].

The stationary BTE is solved deterministically based on an expansion in Fourier harmonics which is described in detail in Refs. [9], [10]. Similarly to the SE the small signal BTE can be evaluated by a linearization around the stationary state [6], [10].

The analytic solution of the linearized PE yields a small signal electric field in the x-direction which is assumed to be independent of the z-coordinate within the channel [4].

In order to obtain the plasma dispersion relation, i.e. the wave number behavior as a function of frequency, the linearized transport model – either the BTE or the SE – and the result of the PE are solved together as a generalized eigenvalue problem.

Using the SE as a transport model gives a dispersion relation with two branches $\underline{q}^{+}(\underline{\omega})$ and $\underline{q}^{-}(\underline{\omega})$ which are often referred to as Vlasov modes. The $\underline{q}^{\pm}(\underline{\omega})$ are the results of the following generalized eigenvalue problem:

$$\begin{pmatrix} 1+\mathrm{j}\underline{\omega}\tau & -e\mu_0 E_0 \\ 0 & -\mathrm{j}e\underline{\omega} \end{pmatrix} \begin{pmatrix} \underline{J} \\ \underline{n} \end{pmatrix}$$
$$= \mathrm{j}\underline{q} \begin{pmatrix} -\tau\frac{2J_0}{en_0} & -e^2 n_0 \mu_0 \frac{d_{\mathrm{ox}}}{2\varepsilon_{\mathrm{ox}}} - e\mu_0 V_{\mathrm{T}} + \tau \frac{J_0^2}{en_0^2} \\ 1 & 0 \end{pmatrix} \begin{pmatrix} \underline{J} \\ \underline{n} \end{pmatrix} \quad (1)$$

where τ is the macroscopic relaxation time of the velocity, $\underline{\omega}$ the angular frequency, $\underline{q}$ the wave number, V_{T} the thermal voltage, μ_0 the low-field mobility, E_0 the electric field in the transport direction, e the positive electron charge, n_0 and J_0 are the stationary electron density and current density at the electric field E_0, respectively [4].

On the other hand, solving the generalized eigenvalue problem with the BTE gives us a multitude of modes in addition to the two Vlasov modes. At equilibrium and low frequencies two Vlasov modes are distinguishable. By ramping up the electric field and frequency in small steps to the desired values and comparing the eigenvectors, the two Vlasov modes can be tracked and identified even for strong non-equilibrium states [6].

To simulate the plasma excitation we use the Dyakonov-Shur approach [2]. A device with asymmetric boundary conditions with a short circuited source and open drain and length L in x-direction is considered [11]. The result of applying these conditions is a complex angular frequency of the form of $\underline{\omega} = \omega' - \mathrm{j}\omega''$, in which the sign of the imaginary part ω'' determines the stability of the waves. The real part with $\omega' = 2\pi f$ defines the plasma wave's oscillation frequency f [6].

In this paper we will investigate the possibility of THz wave generation by self-excitation of plasma oscillations; we will also show that to simulate the correct behavior a more sophisticated transport model like the BTE is needed.

III. Results

We simulate a homogeneous 2D double gate nMOSFET with a 5nm thick GaAs channel and 20nm thick oxide depicted in Fig. 1. The non-parabolic conduction band structure of GaAs comprises the Γ-valley, four equivalent L-valleys, and three equivalent X-valleys.

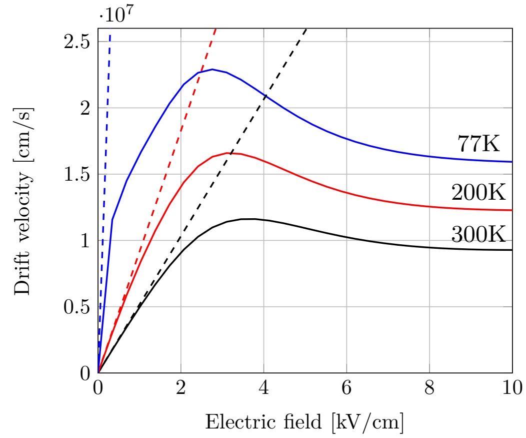

Figure 2: Drift velocity versus stationary electric field at different temperatures for a GaAs quantum well using the BTE (solid lines) and SE (dashed lines).

T (K)	300	200	77
μ_0 (cm^2/Vs)	5.1×10^3	9.1×10^3	8.7×10^4

Table I: Low-field mobility μ_0 for GaAs at different temperatures

The scattering term includes the Pauli principle and consists of elastic acoustic intra-valley, and inelastic inter-valley phonon as well as non-isotropic polar optical phonon scattering [12], [13].

The quasi-2D electron sheet density is $n_0 = 1 \times 10^{12}$ cm^{-2}. Oxide permittivity is set to $\varepsilon_{\mathrm{ox}} = 3.9\epsilon_0$. The FEAST eigenvalue solver [14] and LAPACK library [15] are used to compute the eigenvalues.

The electron drift velocity versus the electric field is shown for the GaAs quantum well at different temperatures in Fig. 2. The magnitude of the velocity overshoot as well as the saturation velocity rise when the temperature is reduced. In the SE the velocity overshoot and saturation is neglected and the relation between the drift velocity and the stationary electric field ($v_d = \mu_0 E_0$) is linear as shown in Fig. 2 with dashed lines. Therefore the drift velocity can be larger than the maximum velocity predicted by the BTE. Table I shows the low-field mobility for GaAs at different temperatures. By reducing the temperature the low-field mobility increases.

Figure 3 illustrates the Vlasov modes calculated by the BTE and SE for $E_0 = 0$kV/cm at different temperatures for real-valued frequencies. In equilibrium we do have inversion symmetry and therefore the modes occur in pairs with $\underline{q}^{+} = -\underline{q}^{-}$. The real part of the plasma dispersion shows a square root behavior at lower frequencies and a linear behavior at higher ones. By raising the temperature, the transition between the two regions shifts to higher frequencies. At low frequencies, the results of the BTE and SE are very similar for $E_0 = 0$kV/cm. The combination of higher frequencies and lower temperatures however leads to a growing

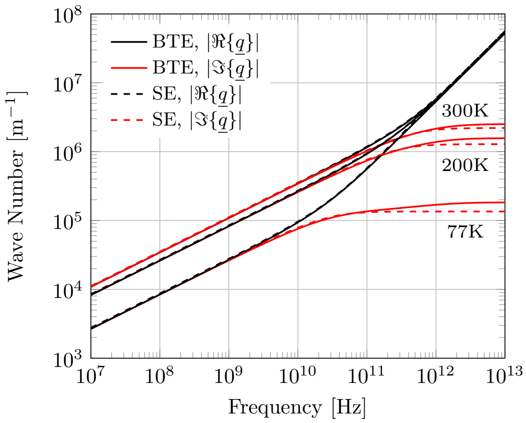

Figure 3: Vlasov modes for $E_0 = 0$kV/cm at different temperature; BTE (solid line), SE(dashed line)

difference between the two. This difference is more obvious in the imaginary part.

Figure 4 shows the plasma dispersion of the two Vlasov modes for a drift velocity of $v_d = 1 \times 10^7$ cm/s at different temperatures. According to Fig. 2 to get the same velocity for the SE and BTE we need to apply different electric fields, where the BTE requires a larger electric field. With increasing temperatures the electric field also needs to be increased. Comparison of the plasma dispersion shows that at lower temperatures the SE results differ significantly from the BTE results.

As mentioned before the self-excited plasma oscillation is a promising candidate to generate terahertz waves. To investigate the plasma wave instability, we use the Dyakonov-Shur approach [2], where the plasma dispersion is calculated based on either the BTE or the SE.

The imaginary part (ω'') and real part (ω') of the complex angular frequency versus the drift velocity are depicted in Fig. 5 for a device with a 60nm channel in the transport direction. The unstable oscillations occur when ω'' becomes positive, and this instability can lead to an active device and THz wave generation.

By reducing the temperature, ω'' increases in both cases but we can see a clear difference between the results. ω'' has a higher value when using the SE in comparison to the results of the BTE. In the case of the SE the saturation velocity is neglected and velocities much larger than the saturation velocity can be obtained.

The drift velocity depends on the applied drain/source bias and for large voltages velocity saturation occurs and scattering of electrons in the channel increases which leads to strong dissipation and damping of the plasma waves, and consequently to a reduction of the growth rate. There is no instability at 300 and 200K when using the BTE, but by reducing the temperature further for instance to 77K, ω'' becomes positive and the instability occurs. At low

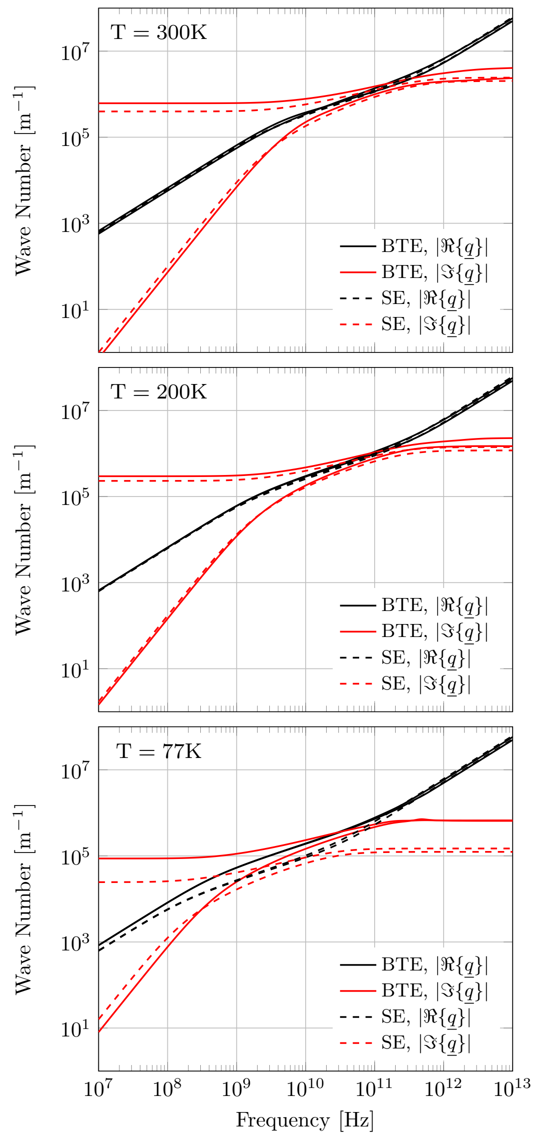

Figure 4: Vlasov modes for the drift velocity of -10^7cm/s at different temperatures using the BTE (solid line) and SE (dashed line)

drift velocity, in both cases ω'' is proportional to the drift velocity and the device is passive. The lower graph in Fig. 5 shows the effect of the drift velocity and temperature on the oscillation frequency. The BTE has more pronounced effects on the angular frequency than the SE.

IV. Conclusion

In this work we compared the results of the SE and BTE for the plasma dispersion at equilibrium and non-equilibrium and for the plasma instability based on the Dyakonov-Shur approach. The comparison shows that at high temperatures and low frequencies the SE results are in good agreement with the numerical solutions of the BTE. To simulate the plasma instability at higher frequencies, higher wave numbers and low temperatures

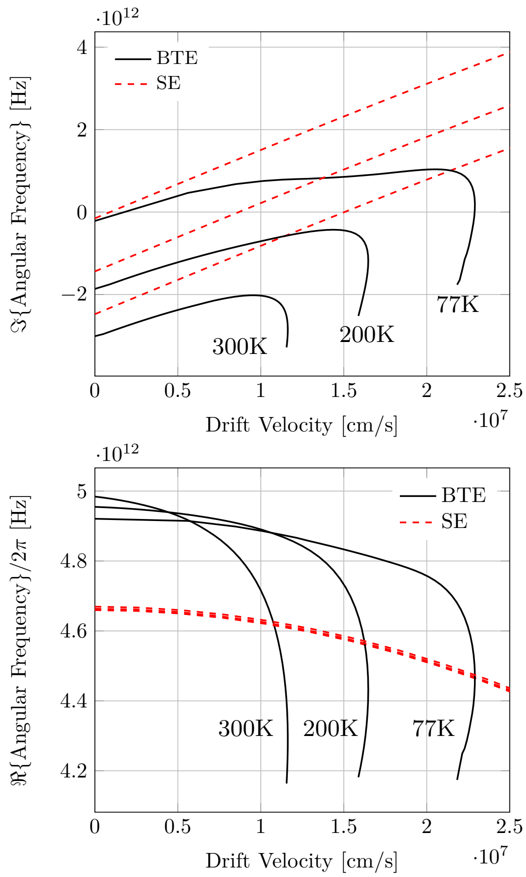

Figure 5: Imaginary part (upper graph) and real part (lower graph) of the angular frequency for a GaAs FET with a 60nm channel at different temperatures using the BTE (solid line) and SE (dashed line).

are required for which the SE fails to capture the correct behavior of the plasma waves.

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