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Monte Carlo simulation of plasma oscillations in ultra-thin layers

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We investigate the dispersion of the plasma frequency associated with the free carriers in a InGaAs layer of length L in the range 0.1-1 µm as a function of the thickness W and carrier concentration at thermal equilibrium $T = 300$ K. To this purpose we use a Monte Carlo simulator coupled with a two dimensional Poisson solver. To take into account the fringing effects of the electric field, the layer is embedded in a dielectric medium (vacuum) along the transverse direction. The fluctuations of the voltage at the center of the sample are extracted and their spectral density calculated by Fourier transform of their autocorrelation function. For $W = 100$ nm and carrier concentrations of $10^{16} \div 10^{18}\text{cm}^{-3}$ the spectral density shows peaks which are in good agreement with the 3D expression of the plasma frequency. For $W \leq 10$ nm the spectral density of voltage fluctuations exhibits a peak that depends on L, thus implying that the oscillation mode exhibits a dispersion. The corresponding frequency values are in good agreement with the 2D expression of the plasma frequency obtained for a ballistic regime within the in-plane approximation for the electric field. Simulations evidence a region of cross-over between the 2D and 3D plasma frequencies for width W around 20 nm.

1 Introduction Due to its specifical physical properties, TeraHertz (THz) radiation, usually defined in the frequency window 0.3 to 30 THz, offers an important range of potential applications within different domains, such as broadband communications, high-resolution spectroscopy, radars, environment monitoring, biomedical testing, materials and device inspection, close wireless networks, security, etc. [1,2]. As a consequence, this region of the electromagnetic spectrum is the object of a relevant research effort. As a matter of fact, the realization of a room-temperature operating, compact and affordable, solid-state THz radiation source with coherent, powerful, and tunable characteristics is still an open issue. If THz radiation generation and detection can be envisaged by using optical or electronic systems, then one of the most promising strategies lies in the plasmonic approach. In this framework, Dyakonov and Shur have considered, through an analytical approach, the case of two dimensional electron layers constituted by the ungated channel of a nanometric transistor [3, 4]. The electron gas has been assumed as highly concentrated but non degenerate, and supposed to undergo only long-range electron-electron interaction. As concerns the active region of the device, the in-plane field approximation has been employed. In these conditions, the electron gas behaves as the support of plasma waves whose propagation velocity can be greater than the electron drift velocity. Through the oscillations of the plasma, nanometric HEMT have been considered as possible emitters and detectors of electromagnetic radiation in the THz range. The purpose of this work is to investigate the dispersion of the plasma frequency, associated with the free carriers, in a InGaAs layer of submicron length L from 0.1 to 1 µm as function of the thickness W and carrier concentration. To this purposes, within a microscopic model based on the

Monte Carlo method, the frequency spectrum of voltage fluctuations has been investigated.

2 Analytical model The analytical model for the dispersive 2D plasma frequency is [5]

$$\omega_p^{2D} = \sqrt{\frac{e^2 n_0^{2D} k}{2 m_0 m \varepsilon_0 \varepsilon_{diel}}} \qquad (1)$$

where ω_p^{2D} is the 2D plasma frequency, $k = \frac{2\pi}{L}$ with L the channel length, m_0 and m the free and effective electron mass, respectivcely, ε_{diel} the relative dielectric constant of the dielectric and ε_0 the vacuum permittivity, respectively $n_0^{2D} = n_0^{3D} * W$ with W the channel thickness, and n_0^{3D} the corresponding 3D carrier concentration. We notice that the 2D plasma frequency depends on the relative dielectric constant of the external dielectric. Plasma waves also exist in bulk and their 3D dispersionless frequency is [5]

$$\omega_p^{3D} = \sqrt{\frac{e^2 n_0^{3D}}{m_0 m \varepsilon_0 \varepsilon_{mat}}} \qquad (2)$$

3 Monte Carlo simulations In order to be able to attribute accurately the different experimental observations to the corresponding physical phenomena, a microscopic investigation has to be performed. In particular the physical model must describe correctly the different microscopic phenomena influencing the charge transport and take into account different conditions such as device geometry, temperature, bias, etc.

Since it offers a great sensitivity to the microscopic features of the carrier dynamics, a special attention is given to the calculation of noise spectra at $T = 300$ K under thermodynamic equilibrium conditions. In particular, the fluctuations of the voltage in the center of the considered device are calculated, and the spectral density of this quantity is extracted. To this purpose, we use the microscopic Monte Carlo approach coupled with a two dimensional Poisson solver which has already shown its capabilities and detailed in recent works [6, 7]. In brief, the band model accounts for a three valley conduction band, scattering mechanisms consider acoustic, polar optical and intervalley deformation potential phonons, ionized impurities, and degeneracy effects.

To study the plasma oscillations in the 3D and 2D cases, we simulate a bar of $In_{0.53}Ga_{0.47}As$ of length L in the range $0.1 \div 1$ µm for different thicknesses W and carrier concentrations. One of the terminal is kept at a voltage V = 0 and is connected to an ideal thermal reservoir of electrons which are injected at a constant rate into the bar. Carriers are reflected at the boundaries between the bar and the dielectric as well as when reaching the open terminal of the opposite side. The bar is surrounded by a perfect dielectric (Fig. 1) (taken as the vacuum) 10 µm wide in the upper and lower region of the bar, where the 2D Poisson equation in the xz-plane is solved to account for the fringing of the

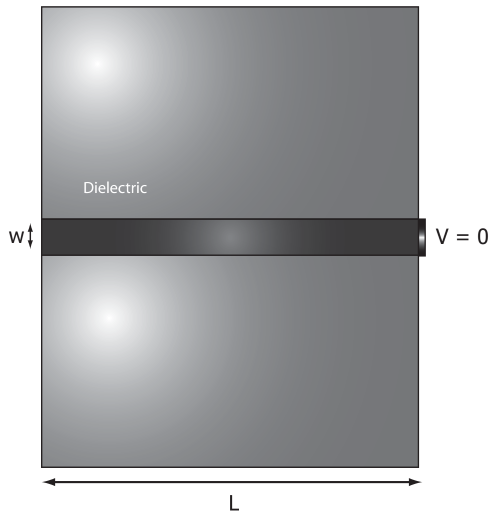

Figure 1 Schematic of the device (not in scale) studied within the Monte Carlo simulation. The free charge is present only in the bar of length L along the x direction and thickness W along the z direction.

external electric field. To this purpose, as boundary conditions a zero value of the perpendicular component of the electric field is taken all-over the outside region of the simulated structure. The structure, which is depicted in Fig. 1, represents a simplified version of the transistor channel for the ungated case. The time and space discretizations take typical values of $0.2 \div 10$ fs for the time steps, $0.1 \div 2$ nm for the spatial scale of the bar, 500 nm for the spatial scale of the dielectric. Typically there are 80 carriers inside a mesh of the bar, which is found to provide a correct solution of the Poisson equation. After a transient of a few picoseconds, the electron gas is found to achieve steady state conditions, with an energy distribution which well reproduces an equilibrium Fermi-Dirac shape. Accordingly, short range carrier-carrier interaction are implicitely accounted for.

4 Results In a first step, we consider the case of a channel of thickness $W = 100$ nm. Figure 2 reports the spectral density of voltage fluctuations, for a length of the device $L = 0.1$ µm and for a free electron density n_0^{3D} = 10^{18} cm^{-3}, which corresponds to the autocorrelation function of voltage fluctuations whose temporal evolution is given in the figure insert. We can observe that the amplitude of the autocorrelation function decreases exponentially as a function of time by oscillating around the zero value. Accordingly, the spectral density shows that the oscillation spectrum is centered around a unique frequency $f = 10$ THz, in good agreement with the expected 3D plasma value of Eq. (4). From this result it is evident that voltage fluctuations exhibit a strongly deterministic behavior characterized by a periodic process whose associated frequency lies in the THz range.

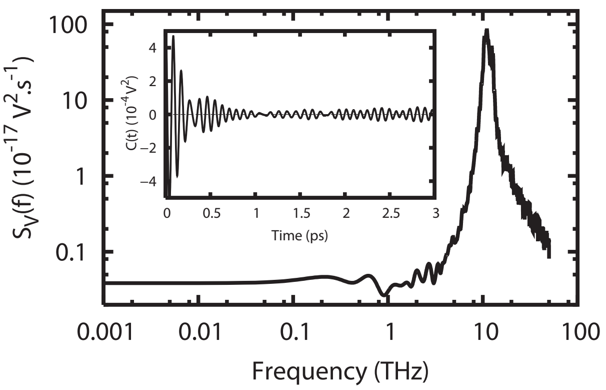

Figure 2 Spectral density of voltage fluctuations as a function of frequency for a InGaAs channel of thickness $W = 100$ nm with $n_0^{3D} = 10^{18}$ cm^{-3} and L = 0.1 µm at room temperature. The insert reports the corresponding autocorrelation function of voltage fluctuations.

Figure 3 reports the peak frequency $f_p = \omega/(2\pi)$ as a function of the device length for different values of the carrier concentration. We remark that, for a given value of the channel length, the oscillation frequency is greater for higher values of the electron density. On the other hand, we observe that for a given value of the electron density, the oscillation frequency is nearly constant with the channel length, which implies that the oscillation mode is independent of geometry. This situation corresponds to the 3D electron gas case where the plasma oscillations of the voltage have an angular frequency ω_p^{3D} following Eq. (2).

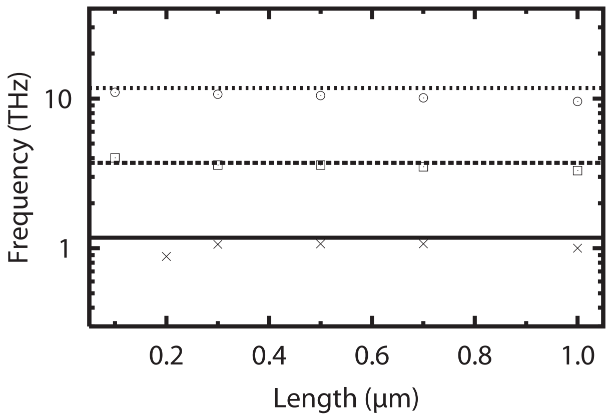

Figure 3 Plasma frequency as a function of the channel length for a thickness $W = 100$ nm and for free electron densities n_0^{3D} = 10^{16} cm^{-3} (crosses and continuous lines), n_0^{3D} = 10^{17} cm^{-3} (squares and dashed lines), n_0^{3D} = 10^{18} cm^{-3} (circles and dotted lines). Lines correspond to Eq. (2) and symbols refer to Monte Carlo simulations

Let us now consider the case of a channel of thickness $W = 1$ nm and perform the same calculations as previously. The obtained Monte Carlo results for the frequency peak are reported in Fig. 4 as symbols. We remark that, for a given value of the length, the oscillation frequency is still greater for the higher concentrations. However, for a given value of the sheet electron density, the oscillation frequency increases with the decrease of the sample length, which shows that the electron flow behaves as the 2D fluid described by the analytical theory.

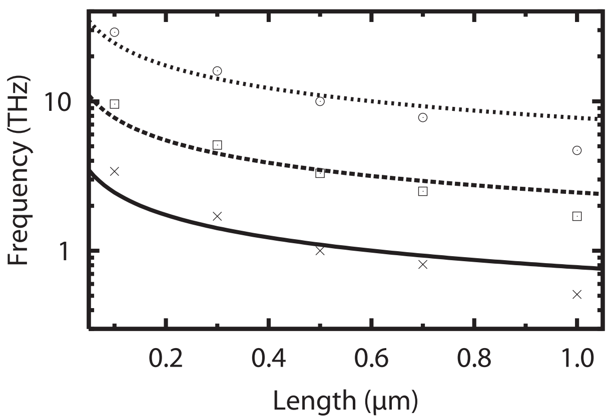

Figure 4 Plasma frequency as a function of the channel length for a thickness $W = 1$ nm and for free electron densities n_0^{2D} = 10^{10} cm^{-3} (crosses and continuous lines), n_0^{2D} = 10^{11} cm^{-3} (squares and dashed lines), n_0^{2D} = 10^{12} cm^{-3} (circles and dotted lines). Lines correspond to Eq. (1) and symbols refer to Monte Carlo simulations.

For the purpose of checking the validity of the 2D model, we studied the voltage fluctuation dependence on the dielectric constant of the insulator which surrounds the channel. Figure 5 represents the spectral density for three different values of ε_r: 1 the constant of the vacuum, 13.88 the case of a dielectric with the same permittivity of the channel, and 100 an extremely high value seen in some ceramics.

We can see that the frequency of plasma oscillations decreases proportionally to the inverse of the square root of dielectric constant as predicted by Eq. (1). The microscopic model thus validates the analytical predictions of the 2D charge carriers even in the presence of scattering mechanisms.

The results for the 1 nm and 100 nm thicknesses represent asymptotic behaviours of a 2D and 3D plasma. The natural question of looking for the cross-over region between these two behaviors has been investigated by simulating diffent intermediate thicknesses in the region $10 \div 50$ nm. The results are summarized in Fig. 6, which reports the plasma frequency obtained by simulations as function of the width. Together with the data, calculated for two 3D carrier concentrations of 10^{17} and 10^{18} cm^{-3} we reported in the figure the interpolating curve obtained from

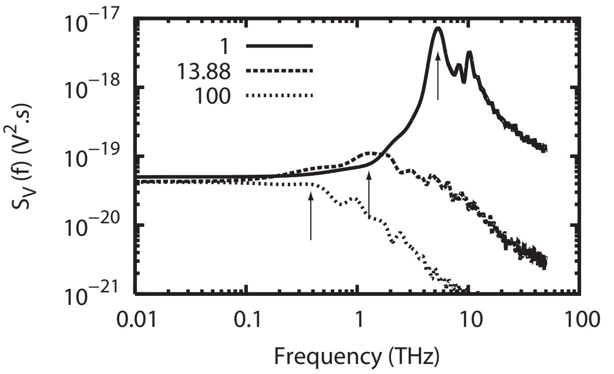

Figure 5 Spectral density of voltage fluctuations as a function of frequency for three different external dielectrics in a InGaAs channel of thickness $W = 1$ nm with n_0^{2D} = 10^{11} cm^{-2} and $L =$ 0.3 µm at room temperature. The arrows signal the frequency peak corresponding to the value of the relative dielectric constant

the asymptotic behaviours

$$\frac{\omega_p}{\omega_p^{3D}} = \frac{\omega_p^{2D}}{\omega_p^{3D} + \omega_p^{2D}} = \frac{\sqrt{\frac{W}{W_0}}}{1 + \sqrt{\frac{W}{W_0}}} \tag{3}$$

with $W_0 = L\varepsilon_{diel}/(\pi\varepsilon_{mat})$. The agreement between the results of the simulation and the interpolating curves is reasonably good. We notice that the cross-over length $W_0 =$ 23 nm is comparable with the 3D Debye length, L_D, which for the above concentrations is in the range $4.4 \div 14$ nm.

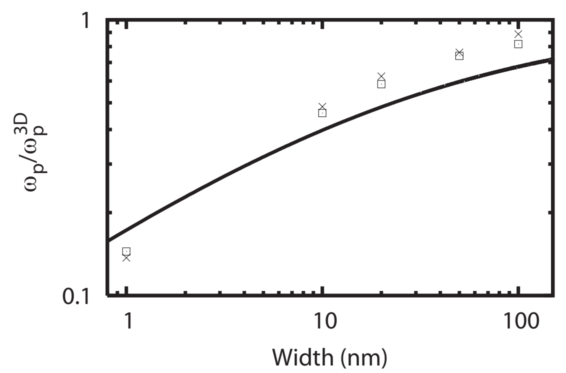

Figure 6 Normalized plasma frequency as a function of the channel width for a length L = 1 µm and for free electron densities n_0^{3D} = 10^{17} cm^{-3} (crosses) and n_0^{3D} = 10^{18} cm^{-3} (squares). The line correspond to Eq. (3) and symbols refer to Monte Carlo simulations

5 Conclusion Through the calculation of the spectral density of voltage fluctuations we have investigated plasma oscillations in InGaAs channels of different lengths, thicknesses and carrier concentrations. The results of Monte Carlo simulations show that for thick channels 3D plasma oscillations appear which depend only on carrier concentration. In contrast, for thin channels, we have observed the transition from 3D to 2D plasma modes where the oscillation frequency exhibits a dispersion decreasing with the length of the channel in close agreement with the analytical model [4]. The microscopic model provided by the simulations evidences that: (i) the presence of scattering does not influence the results predicted by the ballistic theory, and (ii) the existence of a cross-over between the 2D and 3D behaviour of the plasma frequency controlled by the charatecristic length $W_0 = L\varepsilon_{diel}/(\pi\varepsilon_{mat})$.

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