Temperature and Surface Traps Influence on the THz Emission from InGaAs Diodes

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Abstract. Monte Carlo simulations forecast Gunn-like oscillations at ~0.75-1.25 THz in InGaAs planar recessed diodes (slot diodes); however, up to date no experimental evidence of this effect has been observed. The effects of temperature and surface charges on the emission parameters from InGaAs diodes are analyzed by means of an ensemble Monte Carlo simulator. Cooling the device down to 77 K strongly improves the amplitude of the oscillations and can increase their frequency. On the other hand, the ratio between cap and recess charges plays an important role for the onset of oscillations. A high level of traps in the recess region may completely attenuate the emission.

1. Introduction
The millimeter and sub-millimeter frequency range has found an increasing number of applications in several fields as defence, pharmacy, engineering or medicine among others [1]. However, compact sources of signals in this region of the electromagnetic spectrum are scarce and this fact is limiting the progress of terahertz (THz) technologies and applications [2,3]. Previous studies [4] of electronic transport in InGaAs slot diodes, based on Monte Carlo (MC) simulations, have shown the possibility to generate ultrafast Gunn-like oscillations. Nevertheless, up to date no experimental evidence of this effect has been observed in the performed experiments neither with a Schottky nor with a bolometer detectors [5]. The main objective of this work is trying to identify possible mechanisms that prevent the onset of oscillations in real devices. By means of MC simulations we analyse the influence of temperature and surface charges, located on the cap and recess region of the devices, on the THz emission.

2. Device structure and Monte Carlo simulation
The layer structure of the simulated slot diodes, similar to that used for the fabrication on InGaAs HEMTs [6], is shown in Figure 1. For the calculations we have used an ensemble MC tool, which is self-consistently coupled with a two dimensional Poisson solver. The material parameters based on a three valley system are reported in [6]. The devices are divided into 5 nm long and 1-10 nm wide
meshes depending on the doping and the required resolution of the potential along the structure. Ohmic boundary conditions are applied in the source and drain contacts, which are vertically placed adjacent to the different materials. Accordingly, no uniform potential and concentration profiles are considered along these contacts, but those that would be obtained if real top electrodes were simulated.

The effect of degeneracy has been introduced by using locally the classical rejection technique, with electron heating and non-equilibrium screening effects introduced by means of the local electron temperature. No other quantum effects are considered in the simulation in order to have reasonable computer simulation times. The validity of this approach (mainly under high field conditions) and that of the whole MC model has been confirmed in previous work [6]. In order to detect the presence of ultrafast Gunn oscillations, special attention is devoted to the calculation of the Fast Fourier Transform of the current.

3. Results and discussion

As shown in previous works [4,7], a planar InAlAs/InGaAs slot diode exhibits self-generated Gunn-like terahertz current oscillations operating under DC bias due to the modulation of the injection of electrons into the recess-to-drain region, which alternatively takes place in the $\Gamma$ or L valley. The influence of bias, recess-to-drain length and $\delta$-doping has been also reported in previous studies [8]. But unfortunately up to date no experimental evidence of this effect is obtained. In order to satisfactorily achieve emission in future attempts, the influence of lowering the operating temperature of the device and the impact of the surface charges density on the cap layer, $\sigma_C$, and recess region, $\sigma_R$, are analyzed.

3.1. Influence of the operating temperature

Figure 2(a) shows MC simulated time sequences of the current of a slot diode at different temperatures. In the inset the IV characteristics are plotted. We have used the following values for the surface charge density: $\sigma_C=4\times10^{12}$ cm$^{-2}$ for the cap layer and $\sigma_R$ for the surface charges density on the cap layer and recess region respectively.

![Figure 1. Geometry of the simulated InAlAs/InGaAs slot diode. n.i.d. stands for non-intentionally doped, and $\sigma_C$, $\sigma_R$ for the surface charges density on the cap layer and recess region respectively.]

![Figure 2. (a) Simulated time sequences of the current for a bias range from 0 to 1.5 V (steps of 0.1 V of 10 ps each), at different temperatures (500, 300, 150 and 77 K). Inset: I-V characteristics. For comparison, the experimental DC current measured in a fabricated device with the same geometry is also plotted (triangles). (b) Oscillation frequencies (left y-axis) and amplitudes (right y-axis) in a slot-diode obtained by means of Monte Carlo simulations at different temperatures. ($V_{DC}>0.8$ V).]
σ_r = 5 \times 10^{12} \text{ cm}^{-2} for the recess. These values have been carefully chosen in order to reproduce the 300 K experimental DC I-V characteristic of the devices fabricated in Chalmers[5]. Lowering the temperature in the MC simulations clearly benefits the onset of the oscillation for V_Dc \sim 1 \text{ V}. Conversely, excessive temperatures around 500 K inhibit the oscillatory behavior. Figure 2(b) shows, for stable oscillation conditions (V_Dc \sim 0.8 \text{ V}), a \times 3 factor of increase in the oscillation amplitude at 77 K besides a slight decrease in the operation frequency. The decrease in the amplitude around 1.1 V is attributed to the beginning of the population of the X-valley. However, the predicted MC oscillations around 1 \text{ THz} at 300 K were not observed in several experimental attempts neither with a Schottky detector up to 900 GHz with a noise floor < 50 \text{ nW} nor with a bolometer detector up to 1 \text{ THz} with a noise floor < 10 \text{ nW}.

3.2. Dependence on the surface charges of the cap and recess regions

Other possible origin of the absence of oscillations in the real device can be the existence of an excessive amount of carrier traps on the surface of the device. These surface charges are very sensitive, and not easily controllable in the fabrication process. Therefore, here we analyze with our MC tool the effect on the oscillating phenomena of several values of trap densities on the cap and recess regions. In particular, the presence of detectable oscillations is strongly determined by the value of the surface charge in the recess region, which can almost attenuate the emission as can be seen below. Simulated time sequences of the current are shown in Figure 3. Comparing the results shown in Figure 4(a) and Figure 4(b), it is observed that the increase of σ_R degrades the

![Figure 3](image-url) Simulated time sequences of the current for a bias range from 0 to 1.5 V (steps of 0.1 V of 10 ps each) at values of σ_R: (a) σ_R = 4 \times 10^{12} \text{ cm}^{-2} and (b) σ_R = 5 \times 10^{12} \text{ cm}^{-2}. Values of σ_C = (5, 4 and 3) \times 10^{12} \text{ cm}^{-2} are considered. Insets: IV characteristics.

![Figure 4](image-url) Oscillation frequencies (symbols and left y-axis) and amplitudes (right y-axis) in a slot-diode obtained with Monte Carlo simulations at values of σ_R: (a) σ_R = 4 \times 10^{12} \text{ cm}^{-2} and (b) σ_R = 5 \times 10^{12} \text{ cm}^{-2}. Values of σ_C = (5, 4 and 3) \times 10^{12} \text{ cm}^{-2} are considered.
performance of the emitter by reducing very significantly the amplitude of the oscillations, although the fundamental oscillation frequency slightly increases for higher $\sigma_R$. Note that the scale for the amplitude in the y-axis in (b) is 2 times smaller than in (a). With regard to the surface charge on the cap, Figure 4 shows that an increase of $\sigma_C$ causes a reduction of the fundamental frequency. The amplitude of the oscillation increases with the cap surface charge density in the case of Figure 4(b), whereas it remains similar in the case of Figure 4(a). In addition, the lower the value of $\sigma_C$, the higher the DC threshold voltage for the onset of oscillation. Thus the presence of detectable oscillations is strongly determined by $\sigma_R$ and $\sigma_C$. Note that an increase of $\sigma_R$ from 4 to $5 \times 10^{12}$ cm$^{-2}$ strongly attenuates the emission and for $\sigma_R=6 \times 10^{12}$ cm$^{-2}$, the emission disappears (result not shown here). Consequently the surface charges can be considered as a key parameter in order to obtain the onset of oscillations.

4. Conclusions
We have shown by means of MC simulations, how the operation of the slot diodes as THz emitters benefits from cooling the devices down to 77 K with a $\times 3$ factor in the oscillation amplitude. This result opens the possibility that the fabricated slot diodes could show some evidence of THz emission at low temperature. In addition, we have studied the amplitude and frequency of the oscillations for different values of the surface charges densities in cap and recess finding that they are key parameters for the onset of the oscillating phenomena.

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