Simulation of the frequency comb induced by a periodically excited tunnel junction in silicon

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***Abstract*—In this article we use the ensemble Monte-Carlo method to study the frequency comb induced by a periodically excited tunnel junction on a semiconductor. The electron transport is modeled by solving the Boltzmann transport in p-type silicon doped with a concentration of 10^{17} cm^{-3}. For a laser-pulse frequency of 100 MHz, we observe that, if the distance between the STM probe and the second electrode is under 1 μm and we apply a negative bias on the STM tip, the harmonics of the frequency spectrum are not reduced significantly by the electron diffusion and resistance spreading effects in the semiconductor. In this case we obtain a wide frequency comb spectrum, relatively similar to the ones measured experimentally in metals and other materials with high electron conductivity.**

Keywords—scanning tunneling microscopy, microwave frequency comb, spreading resistance

I. Introduction

It is well known that a mode-locked ultrafast laser can induce pulse currents with a wide frequency comb in metals and other materials with high electric conductivity [1]. The frequency comb can extend in the terahertz spectrum and the analysis of its spectral characteristics could provide a new, non-destructive way to probe these materials. One such application that our group has recently proposed is to use a mode-locked ultrafast laser to induce small currents inside a semiconductor material and to determine the local conductivity, compute the doping profile, and localize the impurities in the semiconductor by analyzing the waveforms of the signal collected by a second electrode [2-4].

When a mode-locked ultrafast laser is focused on a tunneling junction, such as in a scanning tunneling microscope (STM), optical rectification occurs because of the nonlinear current-voltage response to cause a current having a waveform equal to that of the envelope of the laser radiation. This current, which is superimposed on the DC tunneling current, consists of short pulses, typically 15 fs in length, with a pulse repetition frequency equal to that of the mode-locked laser. The spectrum of this current, found by taking the Fourier transform, is a microwave frequency comb containing hundreds of harmonics with frequencies equal to integer multiples of the laser pulse repetition frequency. With a metal sample electrode in the STM hundreds of harmonics are measured in the tip or sample circuit of the STM because the tunneling electrons are rapidly transferred from the tunneling junction by the tip and sample electrodes [1]. However, with a semiconductor as the sample electrode in the STM, the microwave harmonics are attenuated, primarily by the spreading resistance at the surface of the semiconductor [5]. This measurable attenuation is proportional to the spreading resistance [5]. Thus, the spreading resistance, which is also measured for carrier profiling in Scanning Spreading Resistance Microscopy (SSRM), may be determined nondestructively, with greater speed, and without requiring calibration, by measuring the microwave attenuation [5].

The modeling of the charge transport induced by mode-locked ultrafast lasers in semiconductor materials is relatively difficult because of two reasons. First, the semiconductor material is under strong non-equilibrium conditions after each laser pulse which injects a large number of electrons in a very small region in the material. Second, the time scales at which the transport takes place are very short, of the order of a few femtoseconds to a few picoseconds. For these reasons, as well as because we currently do not have reliable mobility models to investigate the charge transport at these time scale and high non-equilibrium conditions, the classical drift-diffusion model is expected to fail, at least shortly after the electrons are injected in the semiconductor. Therefore, in this article we analyze for the first time the current transport by solving the Boltzmann transport equation in the semiconductor and investigate the spectrum of the collected signal.

In the next section we present the geometry of the simulated structure and give details about the simulation technique. Then, we present the simulation results for a 100 MHz laser train pulse and discuss the spectrum of the collected signals. Finally, conclusions are drawn in the last section.

II. Simulation Results

The simulated structure is represented schematically in Fig. 1. An STM tip, situated at 0.5 nm above the surface of a p-type semiconductor, is used in conjunction with a mode-locked ultrafast laser to inject a small a.c. current in the semiconductor. The laser introduces 400 electrons at a frequency of 100 MHz. The width of the pulse is 15 fs, which is much shorter than the period of the laser that is 10 ps. When the electrons arrive on the surface of the semiconductor they are localized within a very small volume below the STM tip. In our numerical simulations we consider that, after the 15 fs pulse, all the electrons are uniformly distributed within a small 3 nm × 3 nm × 3 nm region below the STM tip, which was

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estimated approximately by considering that the electrons have an initial electron thermal velocity of 2×10^5 m/s. However, as our simulations will reveal, the size of the region where the electrons are initially distributed does change the results of the numerical simulations significantly because of the relatively long time interval between two laser pulses.

After the electrons are introduced in the semiconductor, the electric current is collected by a fixed contact situated at a distance of 0.4 µm away from a STM tip and its spectrum is computed numerically using the FFT method. In order to increase the electron current collected by the fixed contact, the STM tip is slightly negatively biased with an electrostatic potential of -1.2 V.

In the simulations presented in this article, we consider that the semiconductor material is silicon with a p-type doping concentration of 10^{17} cm^{-3}. The concentration of electrons in the conduction band at room temperature is very small at equilibrium and can be neglected in the simulations. The electron transport is computed by solving the Boltzmann transport equation coupled with the nonlinear Poisson equation using the ensemble Monte-Carlo technique [6]. All the six non-parabolic equivalent valleys along the <100> directions as well as the second minima in the energy bad structure of silicon are considered during simulations [7].

Modeling electron scattering accurately is also essential describing the charge transport correctly. In our simulations we consider non-polar acoustic phonons, non-polar optical phonons, and polar optical phonons to model the electron scattering after the laser pulse. At this stage, quantum mechanical effects are not yet taken into consideration but they will be included in our future work. Quantum confinement effects are expected to play an important role during the first hundreds of picoseconds and particularly when the distance between the STM tip and the fixed electrode becomes smaller than a few hundred meters.

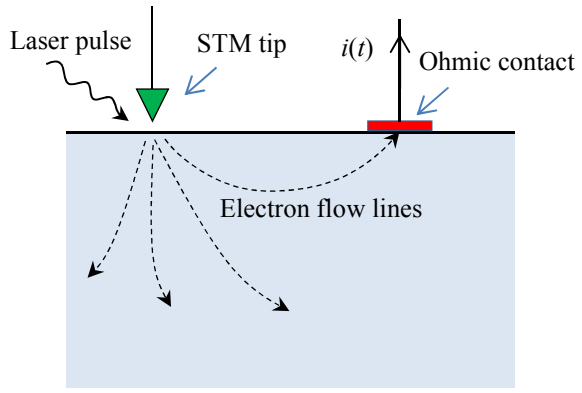

Fig. 1 Electron trajectories generated by STM tip driven by a mode-locked ultrafact laser.

Immediately after the electrons are injected in the semiconductor, due to the high charge density of the electron cloud under the STM tip, the electrons suffer a sudden Coulomb explosion. After the Coulomb explosion, which significantly increases the average velocity of the electrons during the hundreds of femtoseconds, the electrons will diffuse slowly towards the fixed electrode [5]. To estimate the time scales during which the Coulomb explosion and diffusion process take place, we represent the position and energy of the electrons at different times after the laser pulse in Figs. 2 and 3. Fig. 2(a) and (b) presents the position and energy of the electrons 50 fs and 1 ps after the laser pulse. The average electron concentration under the STM tip is of the order of 10^{24} cm^{-3} and 10^{21} cm^{-3} in Figs. 2(a) and 2(b), respectively. During the first picosecond, the electrons can be considered to move under the strong electrostatic forces of the Coulomb explosion.

After a few picoseconds, the electron-electron interaction has decrease significantly and the electrons are moving slowly, in the presence of the electrostatic field created by the STM tip and the fixed electrode. Fig. 3 presents the position and energy of the electrons during this slow drift-diffusion process. The drift-diffusion process lasts approximately from a few picoseconds to 100 ps. After 100 ps an important fraction of the electrons from the laser pulse have been collected by the fixed electrode, while the other electrons have diffused towards the middle of the semiconductor where they are slowly recombining with holes.

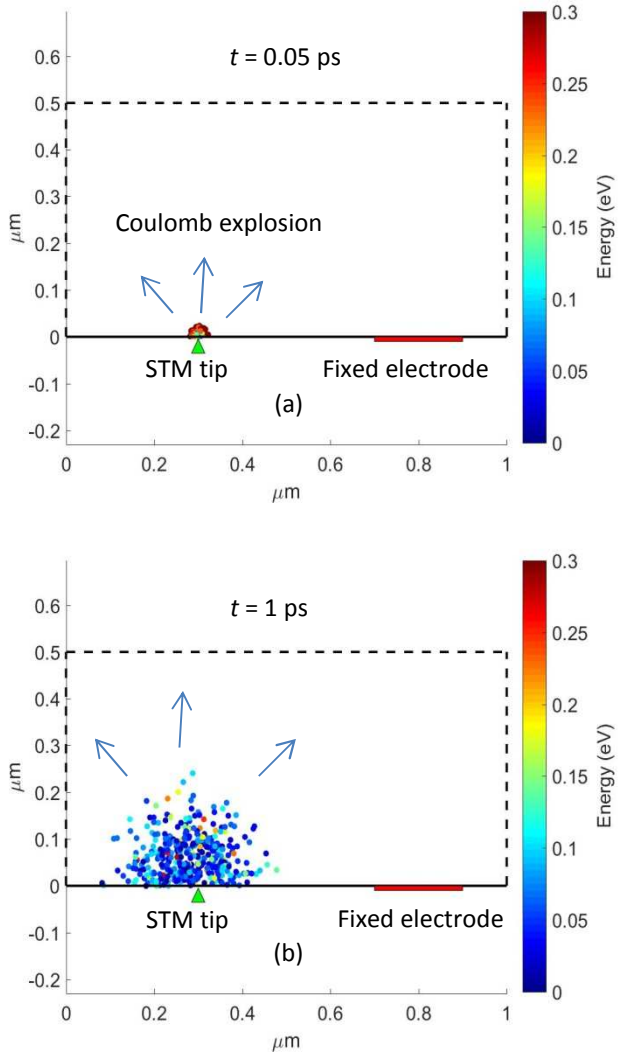

Fig. 2 Electron energy during the Coulomb explosion.

The number of electrons collected by the fixed electrode during each laser pulse is represented in Fig. 4 with vertical bars. Notice that approximately 60-70 electrons of the total of 400 electrons are collected by the fixed electrode during each laser pulse, while, as mentioned before, the remaining electrons diffuse inside the semiconductor and recombine with holes. This recombination process results in an additional hole current that appears as noise at the fixed electrode. Since the electron's life-time in silicon is of the order of 1 μs, which is much larger than the period of the laser pulses, the electron-hole recombination current is distributed randomly and approximately uniformly during the measurement. Experimentally, this current appears as generation-recombination noise current, 1/f noise, or other types of noise in the collected signal.

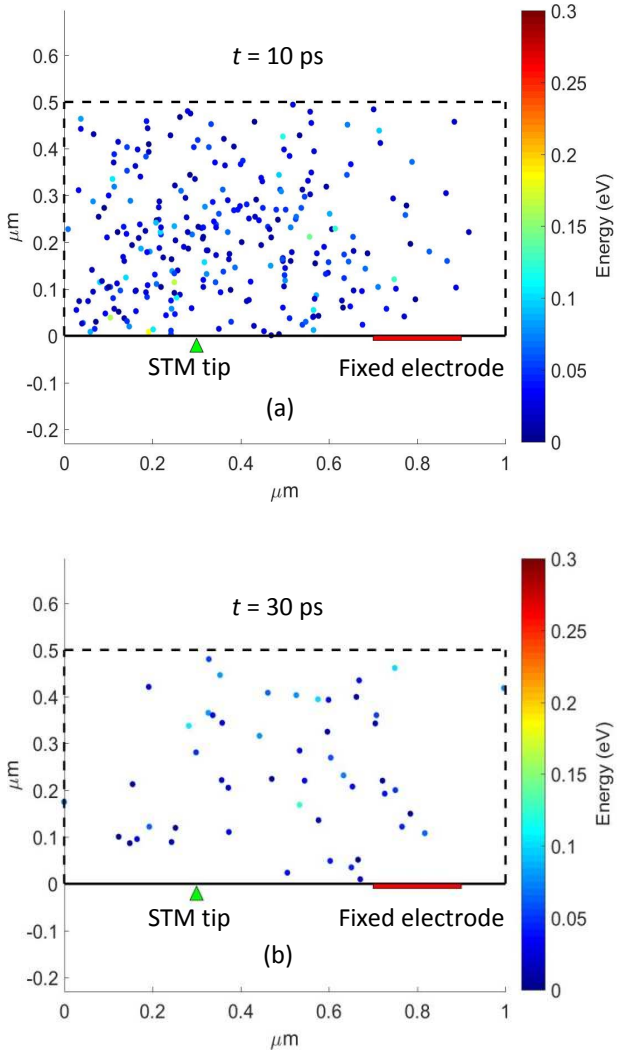

Fig. 3 Electron energy during the drift-diffusion process.

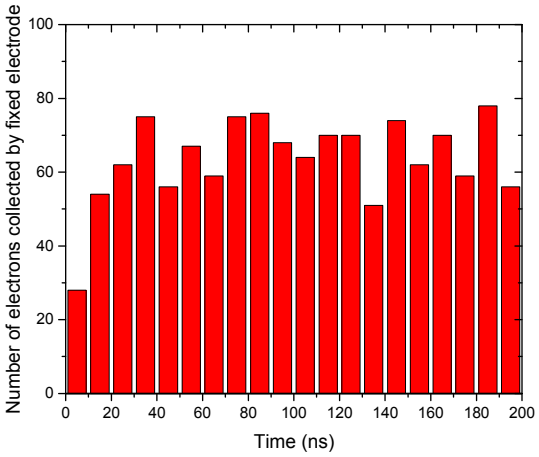

Fig. 4 Number of electrons collected by the fixed electrode during each laser pulse..

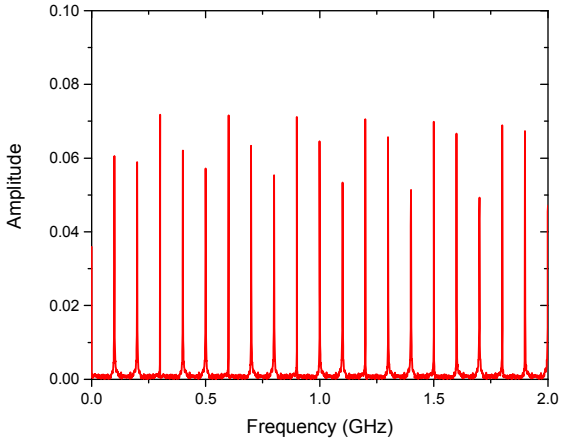

Fig. 5 First 20 harmonics of the frequency spectrum measured at the fixed electrode. The main harmonic is at 100 MHz.

To compute the spectrum of the signal collected by the fixed electrode, we accumulate statistics for 100 laser pulses and take the FFT of the collected signal. Fig. 5 presents the frequency spectrum obtained by using the FFT analysis. The main harmonic at 100 MHz corresponds to the frequency of the laser pulses. Similar to previous experimental results performed on metals [1], we obtain that the frequency spectrum is not attenuated much by the diffusion of the electrons in the substrate and there is a wide frequency comb that extends for more than a few hundred harmonics. This result is due to the fact that electrons arrive at the fixed electrode in a much shorter time than the period of the laser. If the pulse repletion frequency (PRF) of the laser is increased, the higher harmonics of the frequency spectrum are significantly reduced because the fixed electrode does not have enough time to collect the electrons generated by the laser between two laser pulses. This fact can be observed in the simulations presented in Figs. 6(a) and 6(b), which present the frequency spectrum of the current measured at the fixed

electrode when the PRF is equal to 1 GHz and 10 GHz, respectively. As shown by these simulations, in the case of a laser with a PRF of 1 GHz the harmonics are slowly decreasing with frequency; a decrease of 6 dB below the fundamental is obtain after approximately 20 harmonics. In the case of a laser with a PRF of 10 GHz, the harmonics of the spectrum are decreasing much faster with frequency and, in fact, the second harmonic is 7 dB below the fundamental.

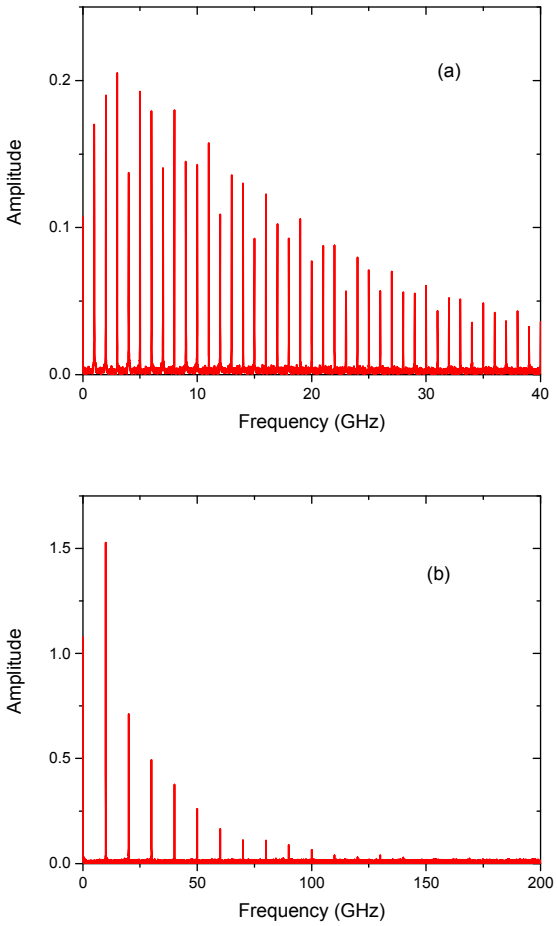

Fig. 6 Frequency spectrum of the signal measured at the fixed electrode for a pulse repetition frequency of 1 GHz (a) and 10 GHz (b). The fixed electrode is located at 400 nm away from the STM tip.

III. Conclusion

Frequency comb microscopy is a promising technique for analyzing the spreading resistance effects in semiconductor materials. If the distance between the STM tip and the fixed electrode is of the order of a few micrometers a significantly proportion of the electrons induced by the laser pulse have enough time to diffuse towards and be collected by the fixed electrode. By analyzing the spectrum of the collected current one can determine information about the scattering rates in the semiconductor. Such information includes the density and locations of doping impurities and carrier mobilities.

Our Monte-Carlo simulations reveal that the current collected by the fixed electrode is a superposition of the electron current coming from the STM probe and a random hole current generated by the electron-hole recombination processes in the semiconductor. In order to increase the SNR we need to increase the magnitude of the electron current collected by the fixed electrode with respect to the random hole current. This can be achieved by increasing the bias between the STM tip and the fixed electrode so that more electrons will drift towards the electrode.

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