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Cathode Modeling and Diode Performance in a Planar Geometry using Space-charge-limited Emission

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***Abstract*—Space-charge-limited (SCL) emission parameters are varied to study the performance effects in a planar diode using an electromagnetic particle-in-cell simulation software suite, EMPIRE. Oscillations in the simulations are found and linked to the emission parameters, namely the breakdown threshold, the emission delay time, and the current density ramp time. The oscillations are suggested to be a transverse oscillator due to the perfect magnetic conductor boundary condition in steady-state operation and the formation of a virtual cathode in the diode driven by the SCL boundary condition.**

I. Introduction

EXPLOSIVE electron emission due to high electric field stresses on vacuum cathodes is a common occurrence in pulsed power machines. As the electric field in a pulsed diode surpasses the electrostatic field breakdown threshold, electrons explosively emit from the cathode and are accelerated across the anode-cathode (AK) gap. The numerical modeling of this process is crucial to understanding the performance of pulsed diodes. Breakdown happens at various field strengths depending on the cathode material used. These field strengths are generally on the order of 10^7 V/m.

Several computational algorithms have been developed to model this process, one of which is a simple space-charge-limited (SCL) model. Once the prescribed breakdown threshold is surpassed, electron computational macroparticles (i.e. a lumped computational particle with some weight that represents many electrons to save memory) are injected into the simulation domain with a current density that inductively drives the electric field at the cathode surface to near zero. The current density that achieves this is the Child-Langmuir current density for a 1D planar model [1]

$$J_{SCL} = \frac{4\epsilon_0}{9}\sqrt{\frac{2e}{m}}\frac{V^{3/2}}{d^2} \tag{1}$$

If the emission model is allowed to inject particles immediately without extra regulation, the simulation can become noisy and unstable in a couple ways, often yielding unphysical and misleading results. The first of these problems to typically occur is ”patchy” emission. EMPIRE, an electromagnetic finite element particle-in-cell code suite, uses unstructured tetrahedral meshes for simulating 3-dimensional models. Suppose the bottom boundary of Figure 1 is the cathode and the top boundary is the anode such that there is a pulsed electric field across them in the -z-direction that is near the breakdown field strength prescribed to the cathode surface. Since the breakdown and particle injection conditions are calculated on a cell-by-cell basis, any numerical noise could allow one cell or a small set of cells to exceed the breakdown threshold while neighboring cells are not quite past the threshold. Then in the next timestep, the surfaces that have exceeded the breakdown threshold will have particles injected into the cells directly above them, forcing the electric field in those cells to to nearly zero. This has the consequence of also lowering the electric fields of neighboring cells in that timestep. Then the neighboring cell will no longer be near to the breakdown field strength, and neither will it emit current. Thus the current can become localized and appear “patchy”.

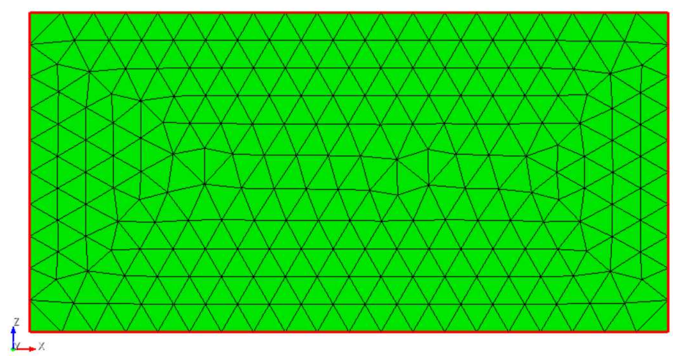

Fig. 1. Side view of a 3-dimensional tetrahedral mesh. For simplicity, this can be thought of as a 2-dimensional triangular mesh.

Another problem that can arise while using the SCL emission model is the driving of numerical instabilities and modes. One example of this is the transit-time-oscillator (TTO). Real TTOs are of interest for high-power microwave (HPM) applications [2], and are induced by the transfer of energy between electrons accelerating across the gap to fundamental structure modes. The inverse of the transit time, $t_{transit}$, of the electrons from cathode to anode will give the TTO frequency, f_{TTO}. For example, in a planar waveguide the most probable mode set for a TTO is the TM$_n$ mode. Using the TM$_n$ cutoff frequency [3], the condition for a TTO at this frequency set is

$$\frac{1}{t_{transit}} = \frac{2d}{nc} \tag{2}$$

where d is the AK gap distance and c is the speed of light. Physical TTOs will have some quality factor and oscillation growth rate depending on the ratio of the diode impedance to the load resistance [2]. In simulation, TTO growth rates are not

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only dependent on the impedance ratio, but also to numerical noise in that frequency regime.

One more simple type of oscillation that can occur is due to the formation of a virtual cathode. Essentially the system will over-emit, causing a build up of space charge that reverses the local electric field. These oscillations are generally at the plasma frequency, ω_P, given by [4]

$$\omega_P = \sqrt{\frac{n_e e^2}{\gamma_0 m_e \epsilon_0}} \tag{3}$$

Two simple measures can be implemented to smooth out these instabilities in the hopes of capturing more accurate replication of experimental diode performances. The first and simplest is adding a delay time to the emission. This is implemented in the following manner. Once a cell exceeds the breakdown field threshold, emission for the entire cathode surface is delayed by a user-specified delay time. This allows neighboring cells time to also exceed the breakdown threshold. Then once the delay time has passed, every cell above breakdown will emit at once. This is a simple way to ensure uniform beam emission with the drawback of adding more shock to the initial emission, which may be unphysical.

The second method to smooth out instabilities is to add a current fraction and ramp time. Essentially, EMPIRE will begin emitting current at the specified initial fraction of the current density to be injected based on the normalized electric field value, E_0, via

$$J = \frac{1}{4}(2 + (2 - 3E_0)\sqrt{1 + 3E_0}) \tag{4}$$

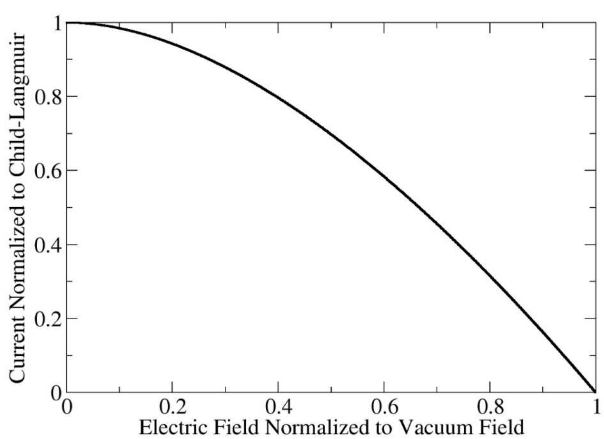

Fig. 2. Injected current per timestep injected into cells normalized to SCL current from equation (1) from the electric field at the cathode normalized to the vacuum field.

where J is normalized to the SCL current given in equation (1). Figure 2 shows the relation if the electric field were normalized to the vacuum electric field. Suppose the specified initial fraction were set to 0.1. The current emitted would then be in the bottom right corner of Figure 2. Then the emitted current would increase, following the curve of Figure 2, and ending in the top left corner after the specified ramp time. Something important to understand, however, is that under-emitting will leave a residual electric field at the cathode surface corresponding to the electric field value from Figure 2. Adding this to the applied electric field in the next timestep will increase the electric field at the cathode even more. Although the emitted current fraction will linearly ramp, depending on the time derivative of the input pulse, the electric field at the cathode surface will compound and thereby quickly ramp the current to where it quickly approaches the full SCL current. In most cases full SCL current is achieved well before the specified ramp time.

Lastly, it is desired to understand the effects of the ramp and delay time on various cathode materials and operating regimes (i.e. ratio of breakdown field to maximum electric field). Thus the breakdown threshold will also be varied to capture any effect that this might have.

II. Modeling

Keeping the geometry as simple as possible simplifies the math and expedites analysis. So a simple planar geometry was chosen for this problem. The applied electric field points in the -z-direction in Figure 3, and so the top boundary is the anode surface while the bottom boundary is the cathode. The anode and cathode boundary conditions chosen in EMPIRE are Dirichlet boundary conditions with the electric field tangential to the surface set to zero, which is essentially perfectly electrically conducting (PEC). The sides of the model at minimum and maximum x-values are set using Dirichlet once again, but setting the tangential magnetic field to zero, constituting a perfect magnetic conductor (PMC). The minimum and maximum y-valued boundaries are given a resistance equal to the geometric impedance [3] of the vacuum planar waveguide for a TEM wave, which is

$$Z_0 = \sqrt{\frac{\mu_0}{\epsilon_0}}\frac{d}{W} \tag{5}$$

This resistance is set in the input deck of the code using a transmission line boundary condition - a 1-dimensional circuit that also serves as a wavelaunch boundary condition. These transmission line boundary conditions are on either side of the model as the goal is to have the same waveform launched from either end and meet in the middle diode region. They are given a finite length of 1m, which is set so that there can be some resolution of the wave structure on the transmission line before the wave encounters the 3-dimensional model.

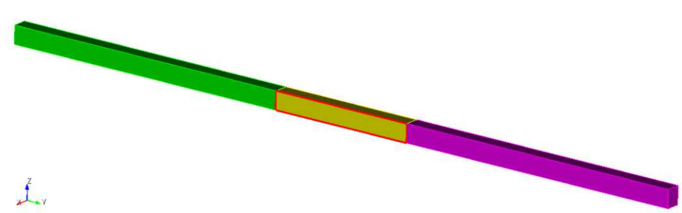

Fig. 3. Simple diode model with the left and right volumes (green and pink) being vacuum transmission lines and the middle (yellow) volume is the diode region where electron emission is allowed.

The entire length of the 3D model is 1m, exceeding the general numerical rule of thumb which is to allow a 3D wave 3 AK gaps or more of distance to "set up" before the emission region. In addition to ensuring pulse quality, this also allows for time-separated diagnostics which is useful for being able to quickly identify the source of any unwanted reflections, instabilities, etc. without adding too much to the computation time. The emission region was chosen to be 20cm in length, and the width of the entire model in the x-direction is 2cm. An AK gap of 2.5cm gives the transmission line (both 1D and 3D) a 471Ω impedance from equation (5). Field emission is only allowed from the cathode surface in the middle (yellow) block, which will change its impedance. In steady state with current flowing, the diode impedance should follow the Child-Langmuir space-charge limited flow [4]

$$Z_D = 429\frac{d^2}{A}\frac{1}{\sqrt{V_0}} \tag{6}$$

where d and A are the AK gap and the emitting cathode area in cm and V_0 is the applied voltage in MV. The applied voltage profile is shown in Figure 4. The steady state voltage of 1MV will give a diode impedance of

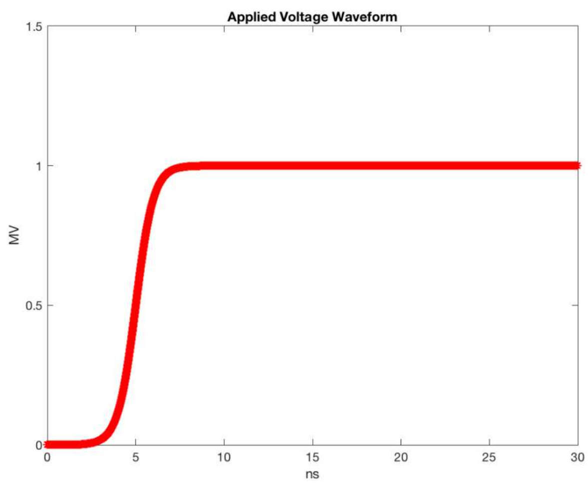

Fig. 4. Applied voltage waveform with a 4ns risetime, 1MV maximum, and a hyperbolic tangent profile.

As previously mentioned, the simulation code is EMPIRE, which accepts multiple mesh types. The mesh used here is similar to that pictured in Figure 1. An unstructured tetrahedral mesh was made using CUBIT, a code-based modeling software. For the vacuum transmission line regions of the model, only electric and magnetic fields exist. Since the wavelength of the electromagnetics (based on the risetime of the pulse) is large compared to the model, vacuum regions need not be heavily refined. However when particles and their motion are involved, the mesh must resolve parameters such as the cyclotron radius or diode plasma oscillations. Following a rule of thumb, the diode region is defined to have at least 20 cells across the gap. For this problem, particle orbits are expected to be much larger than the AK gap distance. Thus refining oscillations across the gap will be sufficient - as mentioned previously, these simulations are prone to developing early instabilities such as TTOs. Seeing as these oscillations should be in a fundamental structure mode, the mesh resolution is set to $dx = \frac{d}{20}$ so that a wavelength across the gap will have 20 points resolving it. For the vacuum regions, both limiting the use of computational memory and limiting a mesh mismatch between vacuum and diode regions are important. Meshes have a numerical impedance based on their resolution. If the mismatch between two regions is too high, this can yield unphysical numerical reflections. So the mesh size, dx, was increased by only a factor of 2 for the vacuum regions.

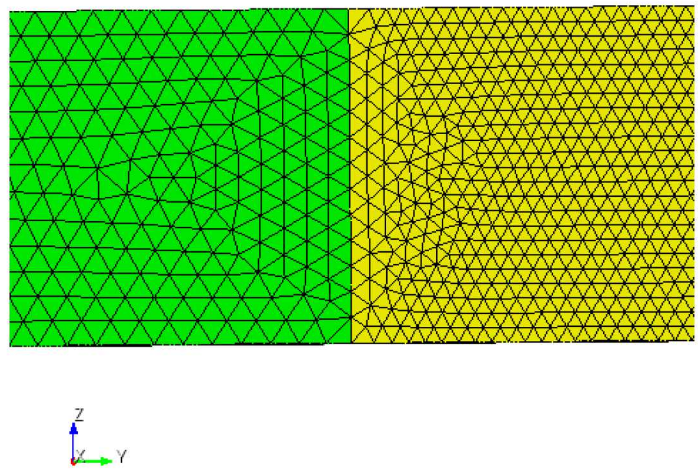

Fig. 5. A view of the mesh resolution change from vacuum (green) to diode (yellow). As a general rule of thumb, keeping mesh transitions smooth reduces numerical reflections from mesh impedance mismatching.

III. Simulation Results and Analysis

A. Varying Delay Time

The first study conducted was a sweep of the delay time parameter with the variation of the breakdown threshold. The delay time was swept as a percentage of the pulse ramp time in order to discern any dependence. Figure 6 shows one set of runs with the breakdown voltage set to 2.5% of the maximum electric field value. Clearly the delay does exactly what is advertised. After this set of runs was performed, it became clear that varying the delay time by so large of a time interval had a very similar effect to simply raising the breakdown threshold. The benefit of the delay time, as opposed to simply increasing the breakdown threshold, resides in the uniform turn on of the cathode. For such a simple geometry and long pulse risetime, the effect of the delay time is most likely seen within 100 timesteps after the breakdown threshold is surpassed. Since the timestep used in these simulations is 1ps and the time derivative of the pulse so high, delaying emission by nanoseconds is simply not going to have any additional benefit. Unfortunately, the simulations run for this setup were not refined enough to show any striping or patchy emission in the cathode.

B. Varying Ramp Time

1) Steady State Oscillations: In this study, the ramp time of the current was varied in similar fashion to the delay

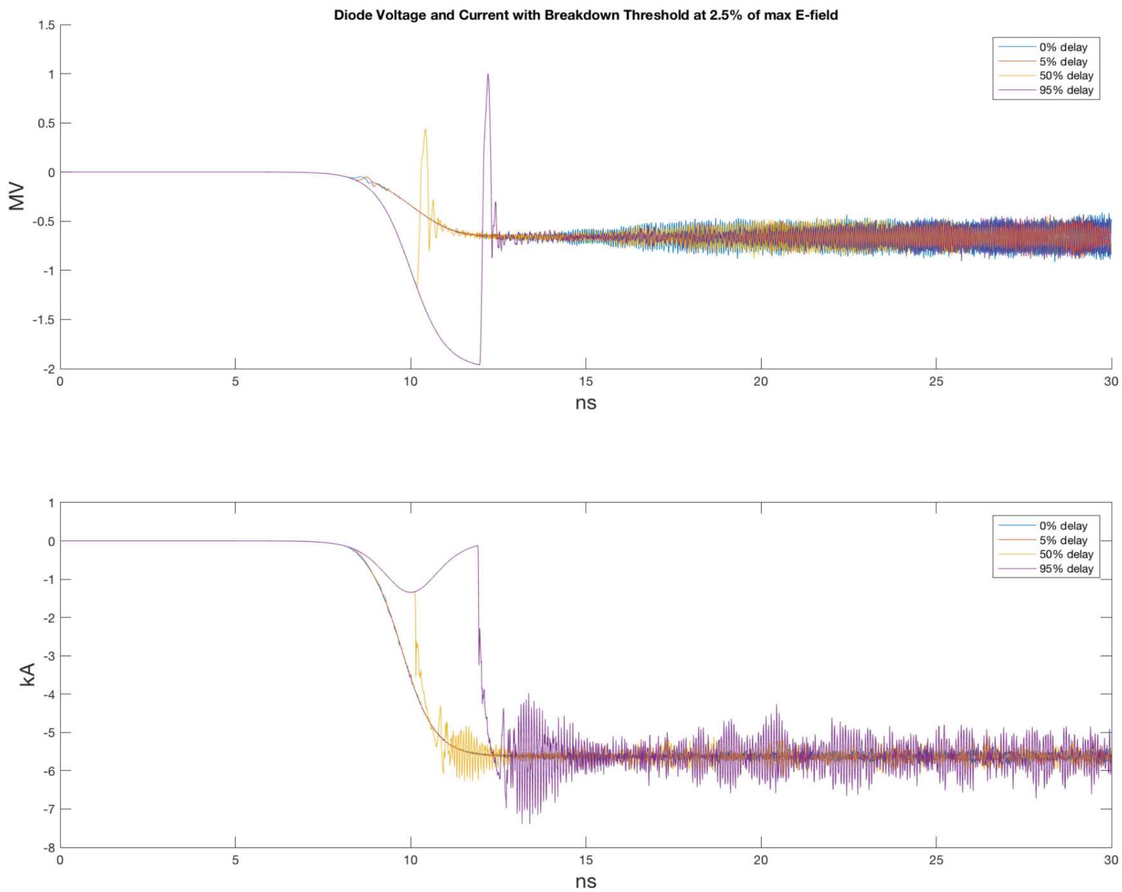

Fig. 6. Varying delay time with breakdown threshold set to 2.5% of the maximum electric field value.

time as it was varied according to a percentage of the pulse risetime. This is misleading, as is explained in the introduction. Without further analysis of the dynamics of equation (4), the ramp times will seem arbitrary. This is acceptable for the moment - the effect of increasing the ramp time is still a visible phenomenon that can be discussed. Figure 8 shows the example of increasing ramp time while holding the breakdown threshold constant at 2.5% of the max E-field while Figure 9 shows the same set of ramp times with the breakdown threshold set to 45% of the max E-field. Earlier it was mentioned that TTO behavior can be excited early via numerical noise. Indeed this seems to be the case as in steady state for either breakdown threshold case, some late time oscillation begins at an earlier time than the rest for the case ran with no delay. This was originally thought to be a TTO, however a fast Fourier transform (FFT) of these signals, Figures 10 and 11, shows something is wrong with this assumption. In each of these, the peak is shown to reside at about 15GHz for the voltage FFT (top of each figure). Using equation (2) with n = 1, this frequency corresponds to an oscillation at d = 2cm. The AK gap distance is actually 2.5cm, which should yield an oscillation at around 1.2GHz. However, the transverse gap distance (in the x-direction between the PMC boundaries) is actually 2cm.

To investigate this oscillation, another model was generated and simulated with every parameter remaining unchanged except for the transverse dimension, which was decreased to 1cm. This was simulated only for one somewhat arbitrarily chosen case: that with 45% breakdown E-field and 75% ramp time. Those results are shown in Figures 12 and 13. The oscillation in Figure 12 is smaller, however the peak frequency indeed shifts to 30GHz, which is exactly what is expected for a transverse oscillation. Clearly something is wrong at these boundaries since this mode does not actually exist in this geometry. This is where it must be introduced that EMPIRE is a developing code. The PMC boundary conditions have historically given EMPIRE developers and analysts poor answers and odd-looking flow patterns whenever used, especially when they are used so near one another. Most likely this will take much more effort to solve for the EMPIRE development team.

The fact remains, however, that the growth of this transverse instability is affected by the ramp time parameter. Just eyeballing it, the dark blue lines in Figures 8 and 9 which correspond to a 0% ramp time (i.e. no damping of emission) do grow this instability around 5ns earlier than the rest. Indeed, if the FFT sample window is cut off at 15ns (as in Figures 14 and 15), the oscillation is stronger in the 0% case for both breakdown thresholds.

Taking another look at the FFTs of these signals, it becomes apparent that the voltage and current tend to oscillate at varied frequencies. The current, whose oscillations are not nearly as pronounced compared to the voltage, does ring at about 12GHz - the expected TTO frequency. This only occurs for a larger breakdown case, which would make sense given the rather large time derivative of the current following breakdown in Figure 9. It would also seem from Figures 9 and 15 that the damping of the supposed TTO oscillation is inversely proportional to the ramp time. This would imply that the SCL ramp-time is indeed limiting the growth of the TTO, an expected outcome.

2) Near Breakdown: The effects of the ramp time parameter are easily visible in the timescale near breakdown. This can be seen in Figures 16 and 17. Unfortunately the oscillations seen near breakdown yield a flat FFT (not pictured to save space). However differentiating the current peak times by hand, one gets an oscillation that seems to be at roughly 1.1GHz. This is an order of magnitude away from the TTO oscillation. A virtual cathode oscillation at this frequency would require an electron density of roughly $5 \times 10^{16}\mathrm{m}^{-3}$. Figure 7 shows the electron density, ρ_e, shortly after breakdown. ρ_e seems to be around a value of $1 \times 10^{17} m^{-3}$ and $5 \times 10^{16} m^{-3}$ for the top and bottom Paraview plots respectively.

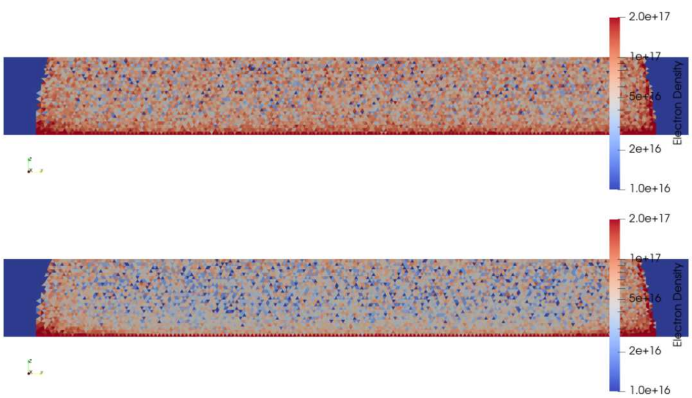

Fig. 7. **Top**: ρ_e at 10.04ns, corresponding to the trough of the first oscillation in Figure 16 for 75% ramp time. **Bottom**: ρ_e at 10.09ns, corresponding to the peak of the second oscillation in Figure 16 for 75% ramp time.

The density does not oscillate between these values - the diode density depletes as the pulse ramps. However, it is suspected that this oscillation is due to a virtual cathode-like oscillation, but it does not show up in the FFTs because it is not an actual virtual cathode oscillation as it is driven by a damped SCL emission boundary that does not match the frequency of the space-charge oscillation. Higher resolution runs and further analysis needs to be conducted to discern this as a virtual cathode oscillation and understand the mechanics of the oscillation more clearly.

IV. Conclusions and Future Work

This project set out to find the correlation between the SCL emission parameters in EMPIRE and diode performance. Even in a simple geometry such as this planar diode, there is clearly plenty of room for instabilities and oscillations to form. Understanding these in simulation is key to the replicability of diode performance in experiment.

Varying the delay time parameter was unfortunately poorly conducted. It was shown that for large delay times, the diode performance is not severely changed from that of raising the breakdown voltage. More work needs to be done to understand the effect of the delay time at short delays. As was discussed, it is expected that the delay time should be small (on the order of a few timesteps perhaps) in order to distinguish ”patchy” emission and then fixing it. For this work, the output of the simulations was unfortunately not resolved enough to capture poor cathode emission quality. This must be resolved and simulations rerun with smaller delay times.

The most unphysical of the oscillations shown in this report are those in steady-state. As was discussed, these are due to some quality of the PMC boundary conditions that excite a non-physical mode. The exact source of this is currently unknown. As has been discussed, the PMC boundary condition and its implementation could be the culprit. Another idea is that the particle boundary condition at that surface, which is separately defined from the electromagnetic boundary condition, is having some effect. This boundary condition is set to ”reflecting”, and thus could be exciting this mode with just the particles. More work needs to be done to understand this oscillation fully and fixing it. Several paths for this work can exist. One is to change the particle boundary condition and observe its effect. Another more lengthy path is to delve into the implementation of the PMC and find if this is a bug in the code. Regardless, it has also been seen that this oscillation is at least dependent on the existence of a ramp time. Without current ramping, the oscillation grew much more readily in magnitude that those runs with any ramp time.

Diode turn-on oscillations are what the ramp time parameter is geared at changing. It is unfortunate for this paper that more time was not spent on the analysis of this problem as the transverse PMC oscillation was particularly puzzling and took much of the analysis. More work will certainly be done in the future to understand this oscillation and especially its validity compared to a real diode. The oscillation itself seems to be of a physically possible source: virtual cathode formation. Fleshing this out analytically seems to be more challenging, however, as there are multiple variables that affect this oscillation. Varying the operating voltage, the ramp time, and even the breakdown threshold can change this oscillation. Apparently in these simulations the oscillation is not sinusoidal, and therefore not picked up by an FFT. It is unclear whether the oscillations must be sinusoidal. Clearly more work must be performed here to fully understand this oscillation and its effect. Plotting the electrons in phase-space may be illuminating. This would require a rerun of all simulations with a higher resolution output, adding of new diagnostics, and ultimately nearly a terabyte of data to be generated by EMPIRE for this to be done. This is possible for future work, but it is not in the timeline of this report. Ultimately, however, two diode oscillations were discovered and linked to the delay and ramp time SCL emission parameters, albeit loosely. This will shed light on future research into the comparison of simulation to experimental diodes.

V. Acknowledgements

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References

[1] Child, C. D. "Discharge from hot CaO". *Physical Review*. Series I. 32(5): 492-511. May 1911

[2] Luginsland, J. W., Arman, M. J., and Lau, Y. Y., "High-power transit-time oscillator: onset of oscillation and saturation" *Physics of Plasmas* 4, 4404. September 1997

[3] Pozar, D. M., "Microwave Engineering" *Wiley*, 1998

[4] Benford, J., Swegle, J. A., Schamiloglu, E., "High Power Microwaves" 3rd. Edition. *CRC Press*. 2016

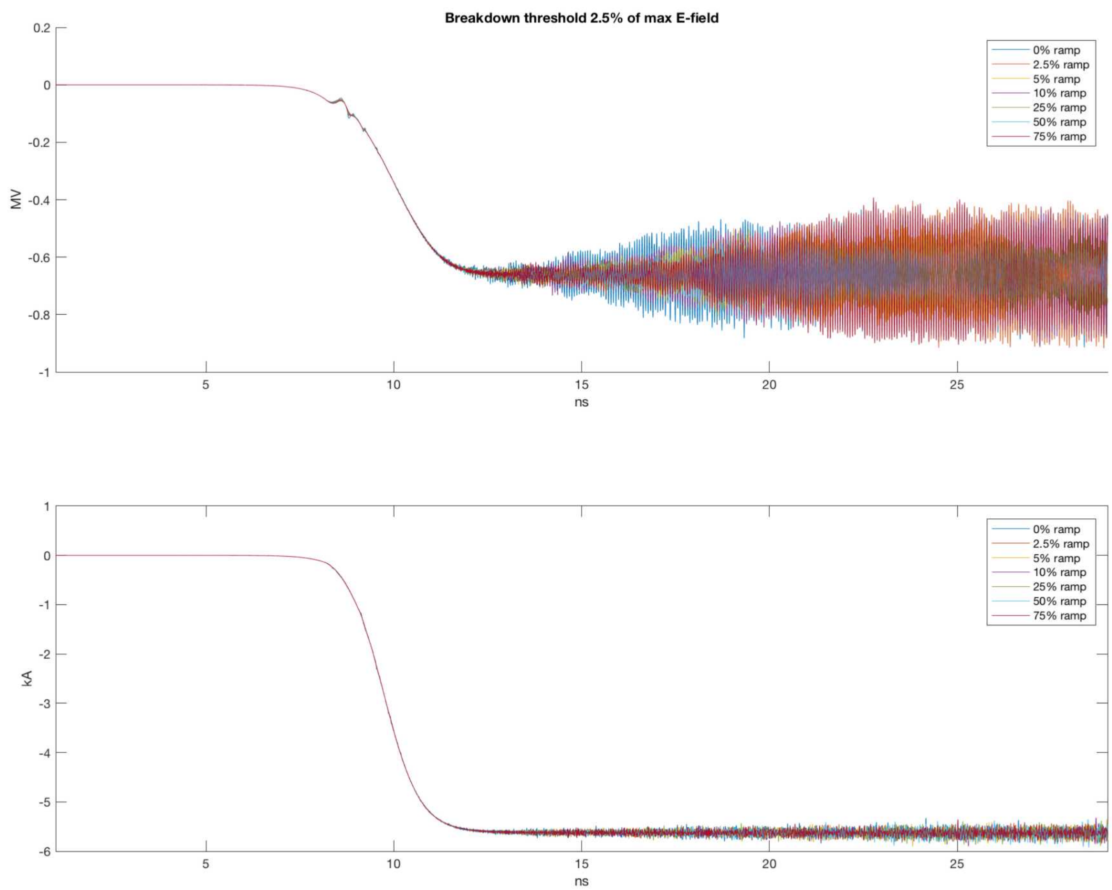


Fig. 8. Voltage and current in the simple diode, varying ramp time with breakdown threshold set to 2.5% of the maximum electric field value.

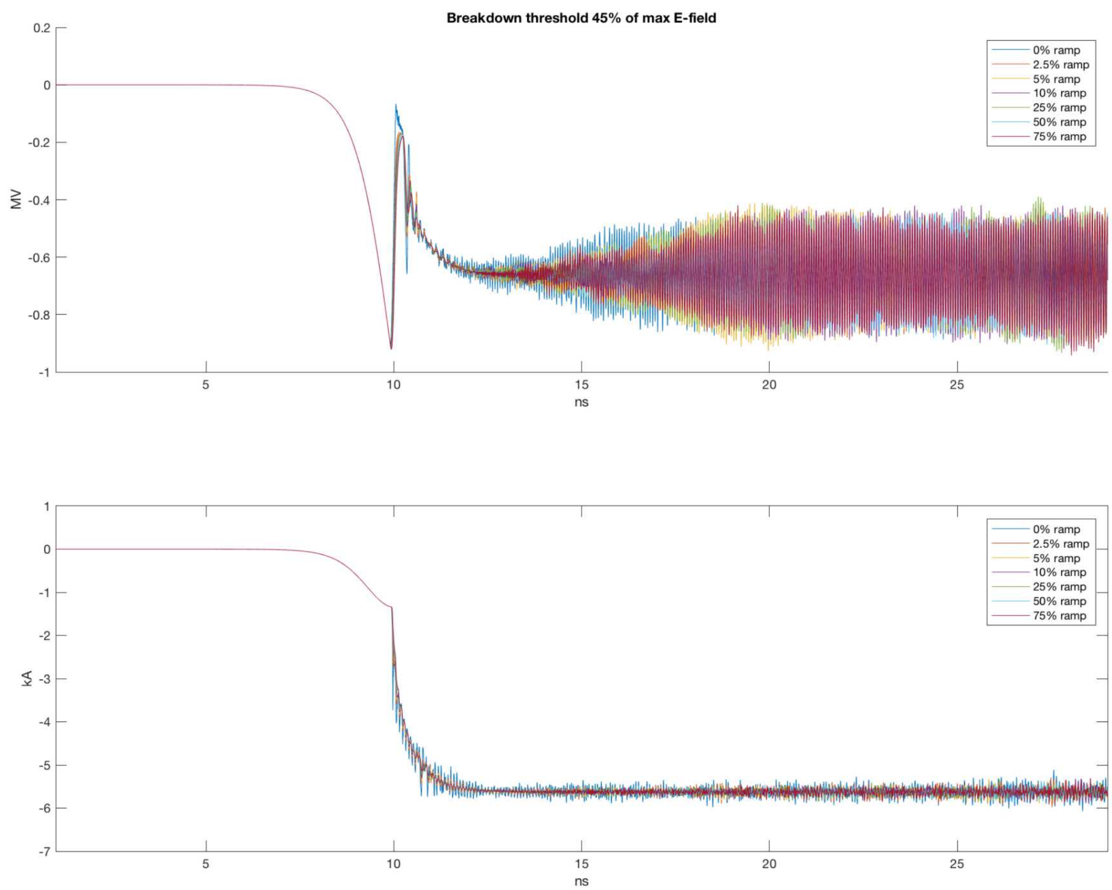
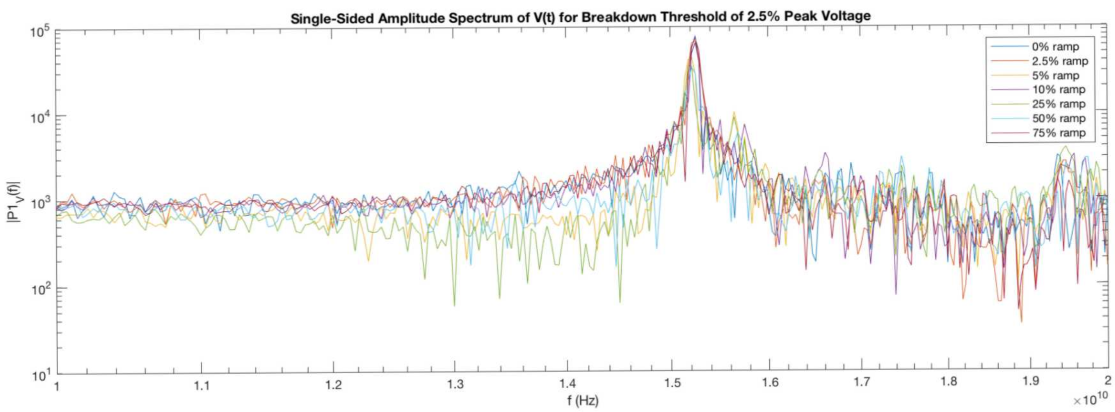


Fig. 9. Voltage and current in the simple diode, varying ramp time with breakdown threshold set to 45% of the maximum electric field value.



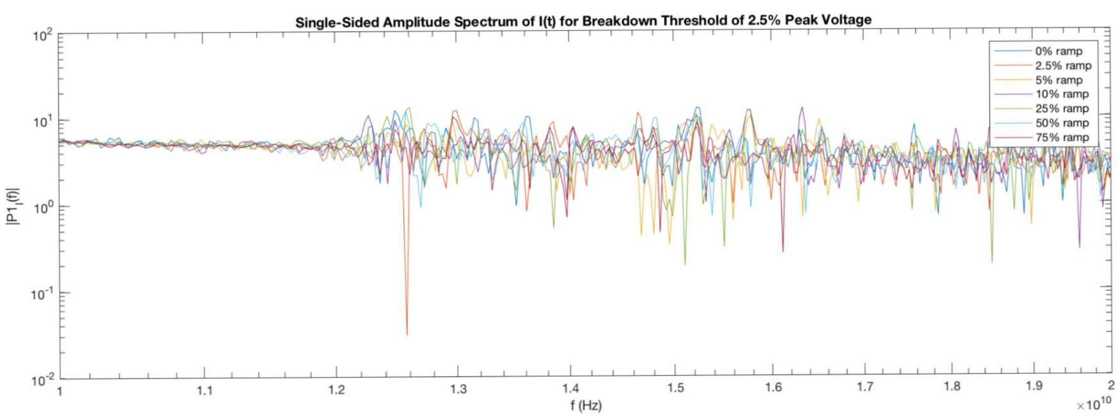


Fig. 10. **Top**: FFT of the voltage curves (top) in Figure 8 for 2.5% breakdown threshold. Clearly visible is the peak at about 15.2GHz. **Bottom**: FFT of the current curves (bottom) in Figure 8. The diode current does not oscillate with the voltage as the FFT is flat in the same frequency range.

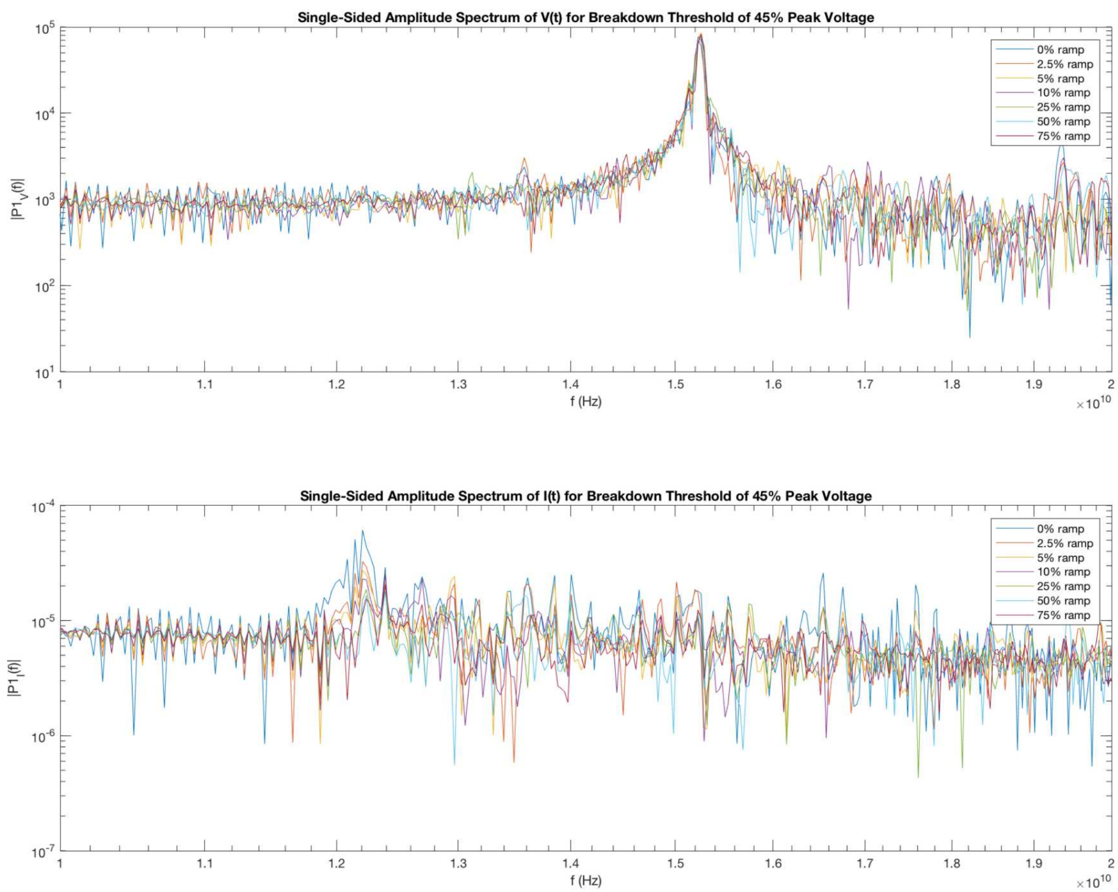


Fig. 11. **Top**: FFT of the voltage curves (top) in Figure 9 for 45% breakdown threshold. Clearly visible is the peak at about 15.2GHz. **Bottom**: FFT of the current curves (bottom) in Figure 9. The diode current oscillates here near 12GHz, the expected frequency for the TTO.

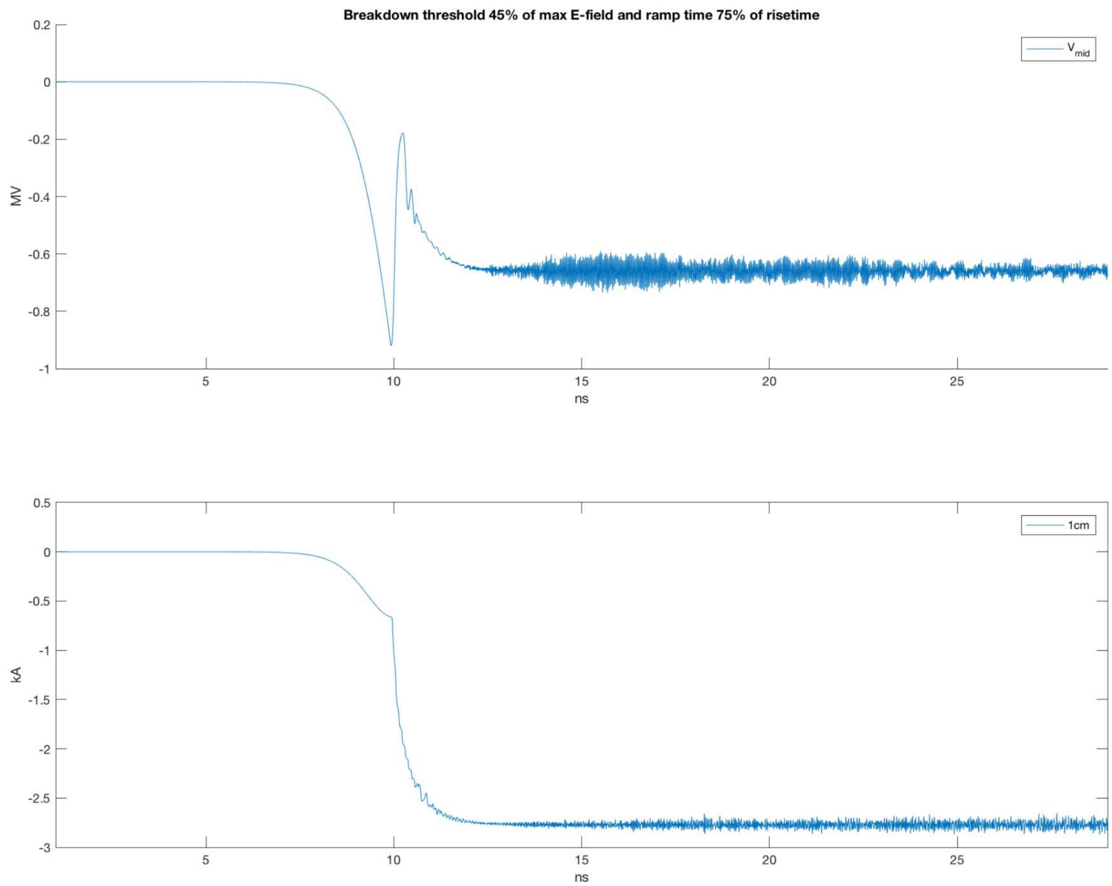


Fig. 12. Varying ramp time with breakdown threshold set to 2.5% of the maximum electric field value for a model with reduced width to 1cm from the original 2cm. This was done to investigate the voltage oscillation in this direction. If the oscillation frequency increases to 30GHz (the expected frequency for a 1cm width), then the voltage oscillation is likely unphysical and due to the PMC boundary conditions.

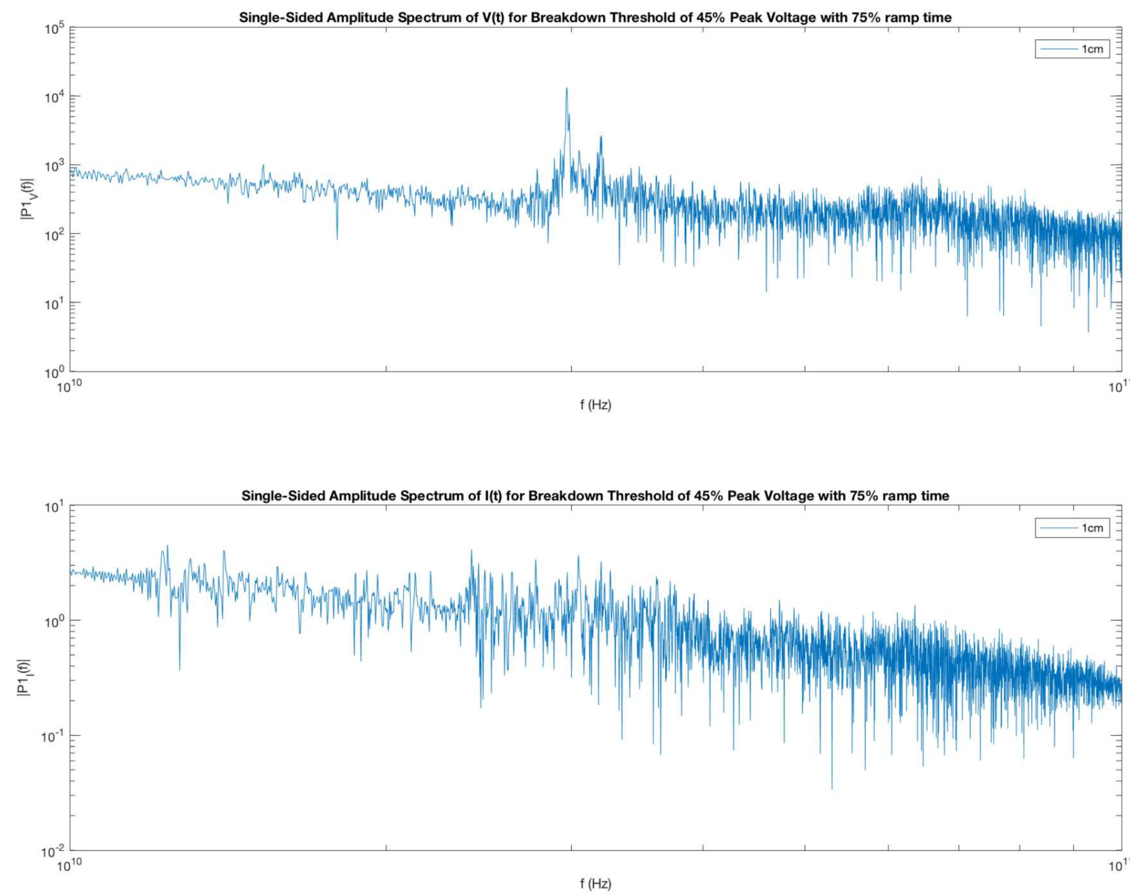


Fig. 13. FFT of the signals in Figure 12, for a model of reduced width to 1cm. The voltage oscillation moves to 30GHz, exactly what is expected for an oscillation in a 1cm gap.

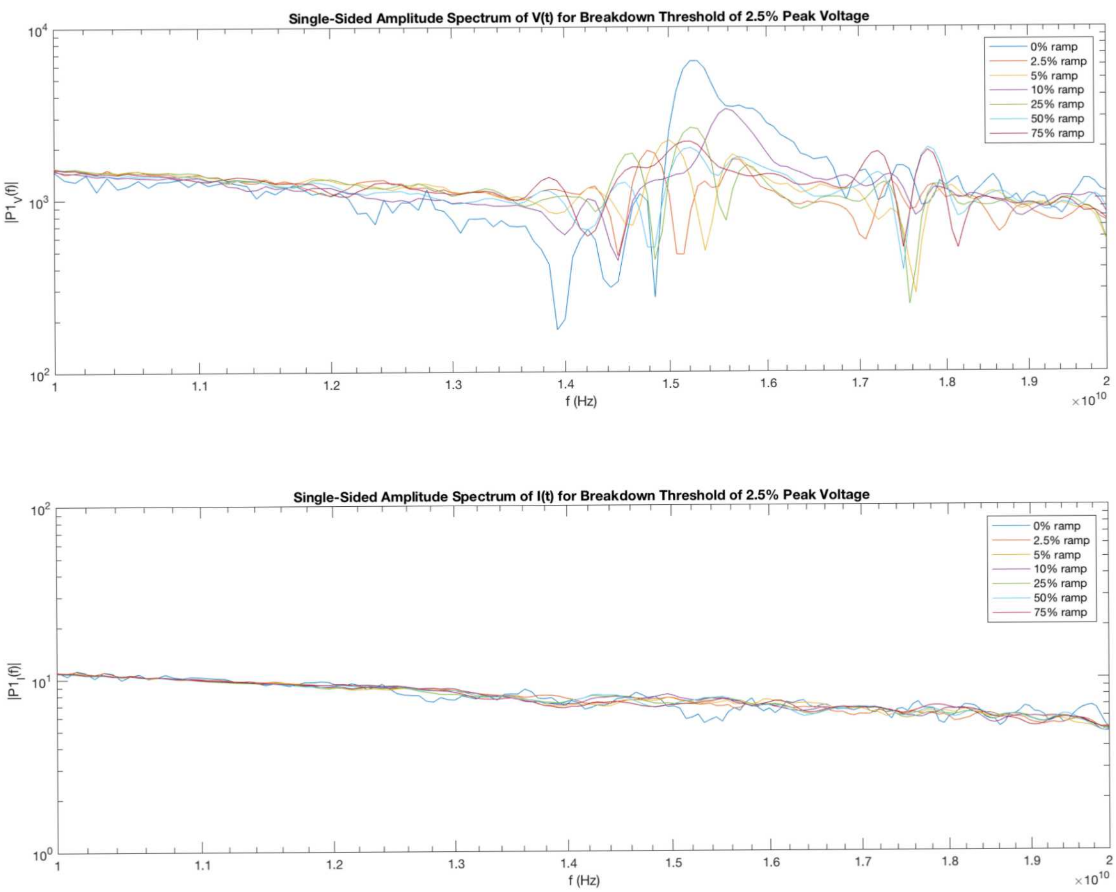


Fig. 14. FFT of the signals in Figure 8, cutting off the sample window at 15ns. Cutting off the sample window is a simple way to compare the growth of the steady-state oscillation.

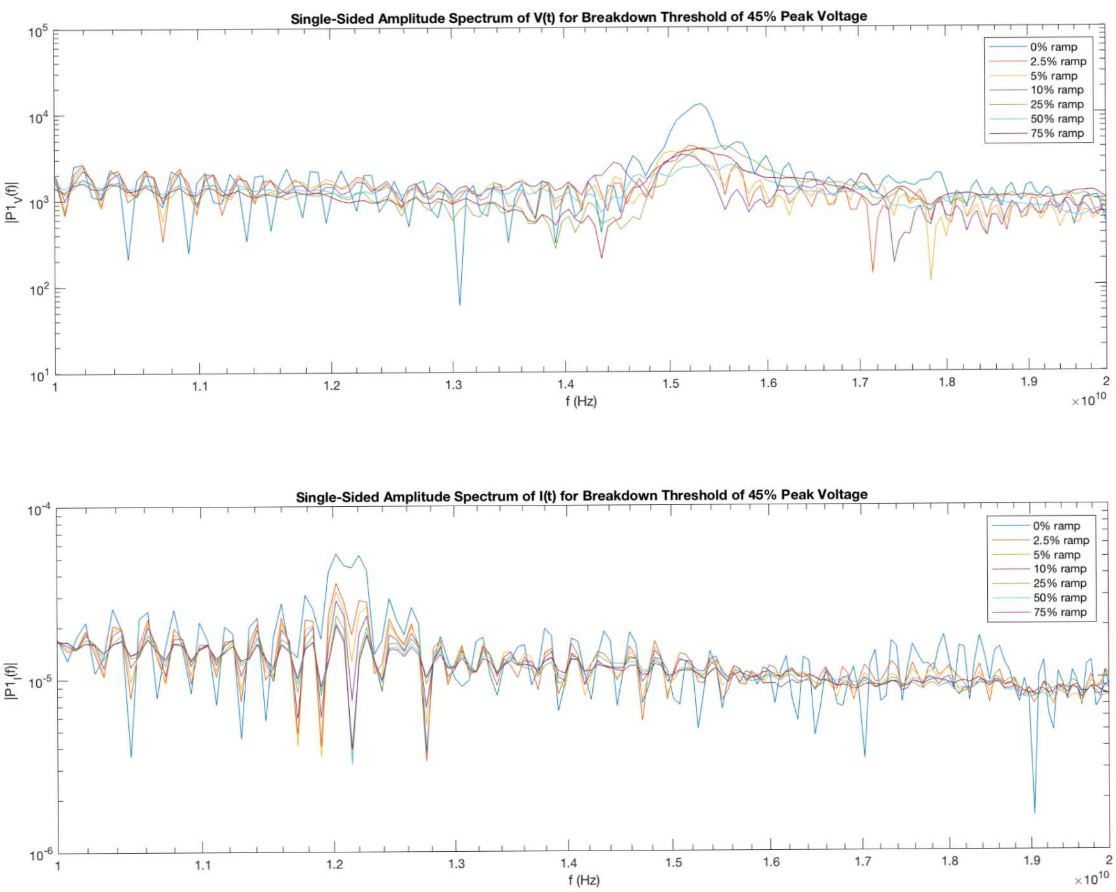


Fig. 15. FFT of the signals in Figure 9, cutting off the sample window at 15ns. Cutting off the sample window is a simple way to compare the growth of the steady-state oscillation.

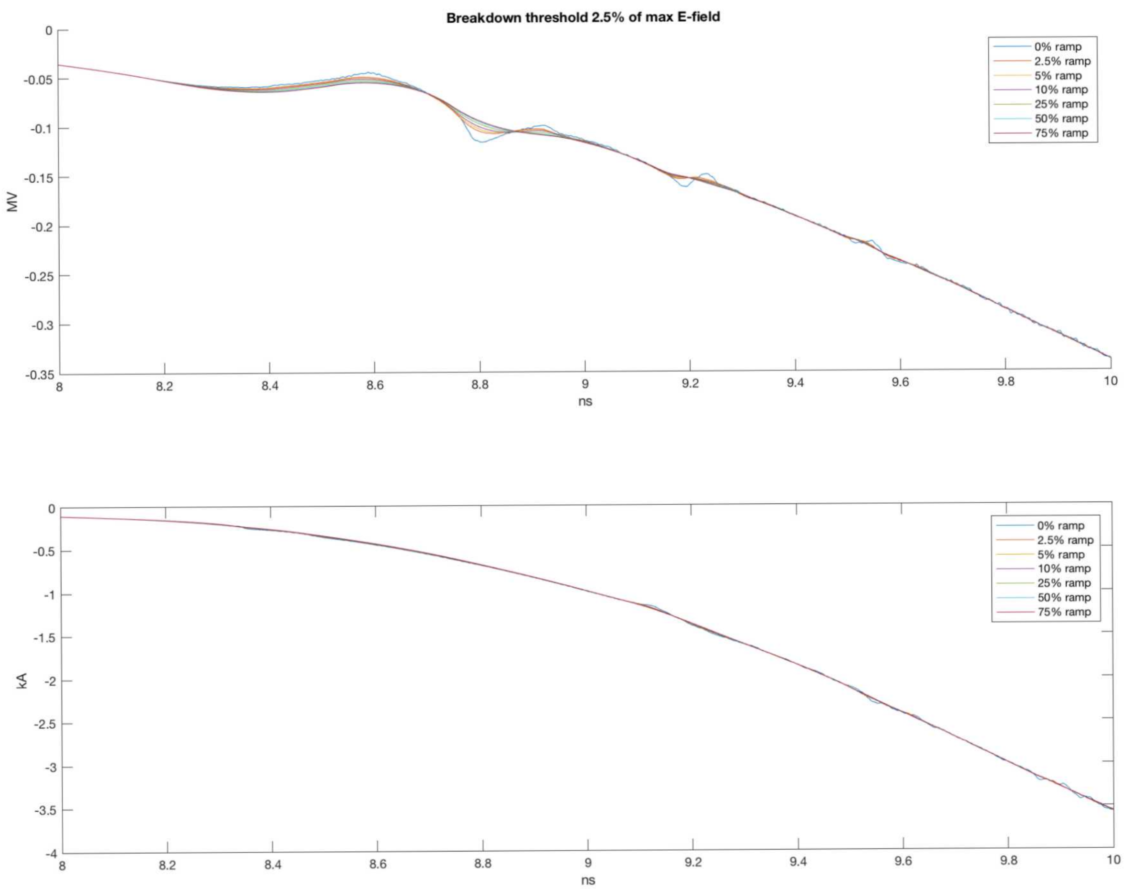


Fig. 16. Varying ramp time with breakdown threshold set to 2.5% of the maximum electric field value plotted near the breakdown of the diode to illustrate the direct effect of the smoothing due to the ramp time parameter.

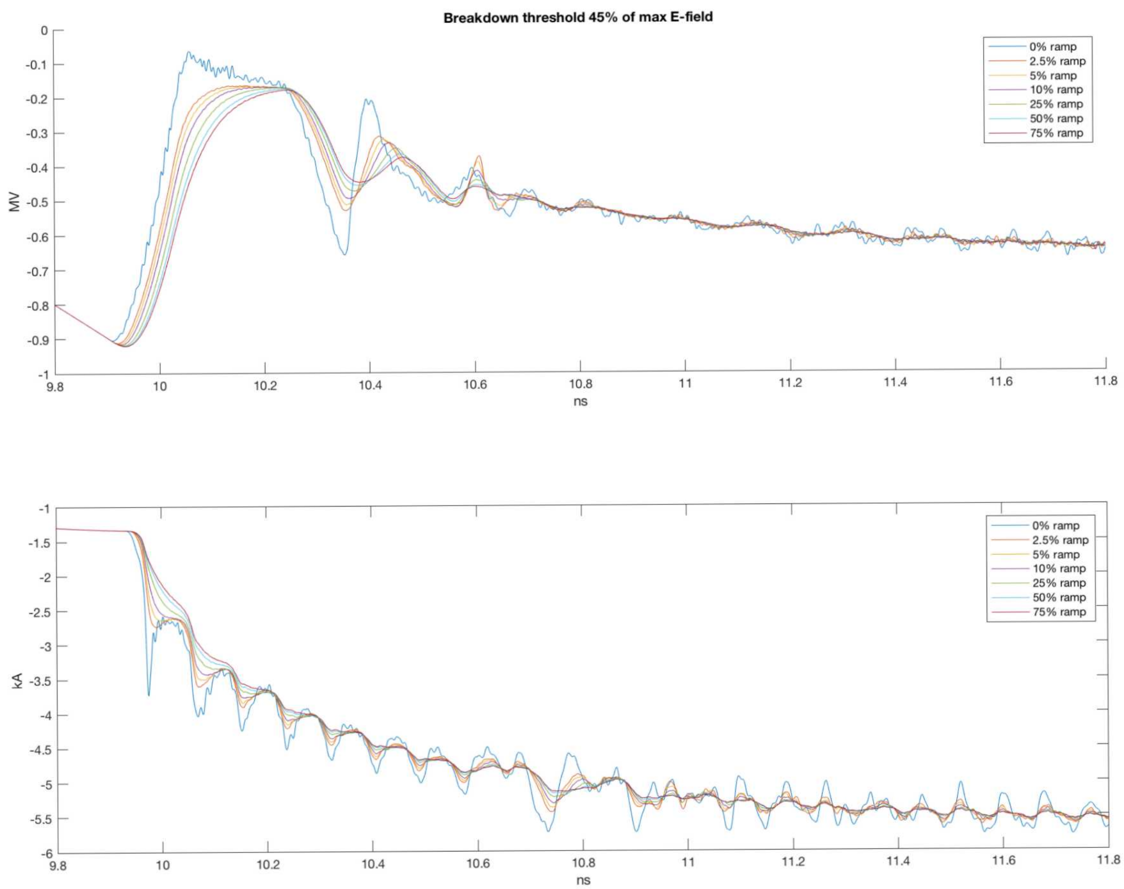


Fig. 17. Varying ramp time with breakdown threshold set to 45% of the maximum electric field value plotted near the breakdown of the diode to illustrate the direct effect of the smoothing due to the ramp time parameter.