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Particle-in-cell simulation of an electron shock wave in a rapid rise time plasma immersion ion implantation process

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A one-dimensional Monte Carlo collision–particle-in-cell plasma computer code was used to simulate plasma immersion ion implantation by applying a negative voltage pulse to the substrate while the reactor wall is grounded. The results presented here show the effect of short rise time pulses: for rise times shorter than the electron plasma period (typically 5 ns/kV), an electron shock wave is observed where a rapidly expanding sheath heats the electrons up to high energies. Many of these fast electrons are expelled from the plasma leading to a high plasma potential and thus to a high surface electric field on the earthed electrode which could give rise to non-negligible electron field emission. © *2005 American Institute of Physics*. [DOI: 10.1063/1.1872894]

I. INTRODUCTION

In plasma immersion ion implantation (PIII), a plasma containing species to be implanted into a substrate is generated by an external plasma source or by the negative bias applied to the substrate.[1,2] After the negative bias is applied, electrons are repelled away from the surface leaving the heavy ions forming an ion matrix sheath. These positive ions will subsequently be accelerated by the electric field inside the ion sheath and be implanted to the substrate surface. The ion implantation energy and depth profiles after PIII have been investigated by theoretical models[3] and numerical simulations[4–6] since the early 1990s. If the time scale for the expansion of the sheath is long compared to the inverse of the plasma frequency, electron inertia effects can be neglected[5] and therefore the electrons can be supposed to be in Boltzmann equilibrium. Under these conditions, the electron transport can be described by fluid equations rather than treating the motion of each electron leading to significant saving in computing time. It has been shown that the low energy component of the ion implantation is related to the rise time of the negative biased pulse[6] and, in principle, an ideal square pulse with zero rise time would remove most of the low energy ions. In the previous numerical[4] studies, the electrons were assumed to be in thermal equilibrium and described by a Boltzmann relation despite the use of zero rise time pulses. This assumption smoothes out any temporal fluctuations less than the plasma frequency. In this work, a Monte Carlo collision–particle-in-cell (MCC-PIC) simulation of both ions and electrons is used to investigate the effect of fast rise times on the electron distribution (i.e., no assumption is made on the electron transport).

II. MODEL DESCRIPTION

A one-dimensional Monte Carlo collision–particle-in-cell[7,8] plasma computer code was used here to simulate very short rise time PIII processes. A PIC simulation is a purely kinetic representation of a system containing ions and electrons, which move under the influence of their own self-consistent electric field. Each particle is actually a macroparticle which represents billions of real particles. Neutral charged particle collisions are handled by a MCC scheme including the null collision method.[9] The particular PIC simulation developed here consists of a bounded plasma where the left boundary represents the substrate on which the negative pulse is applied and the right boundary represents the grounded reactor wall. Our aim is to measure the ion implantation energy after a negative pulse. Before starting the "implantation phase," a steady-state plasma is created by heating the electrons by applying rf electric field of 10 Mhz. A classical capacitive coupling[10–12] where a rf voltage of some hundreds of volts is applied to one of the boundaries would lead to an average rectified plasma potential which is the order of half the rf amplitude and therefore the order of the pulse voltage. Hence, the steady-state plasma is created by heating the electrons by applying a uniform rf electric field perpendicular to the axis of the simulation.[13] This

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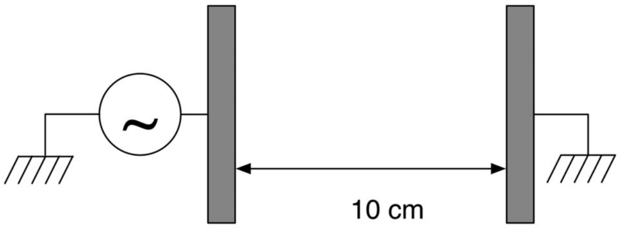

FIG. 1. Plasma immersion ion implantation: schematic of the simulation setup.

scheme is intended to model an inductive excitation without solving electromagnetic field equations and was thought to be more appropriate for our study. The plasma is considered to be in steady state when its characteristics (density, electron temperature etc.) are constant in time.

Figure 1 shows a schematic of the experimental setup: a series of numerical experiments was performed with a grid of 1000 cells and a total simulation length of 10 cm. Before the negative pulse, the plasma density was 3×10^{15} m^{-3}, the electron temperature 5 eV, the plasma potential 20 V, and the argon neutral pressure 1 mTorr. The negative pulse potential of -2 kV was applied with different rise times (from 0 to 500 ns) and had a total duration of 6 μs. The simulation time step was 0.1 ns. In the following, the time origin ($t=0$) is the instant at which the pulse is applied.

III. RESULTS

A. Zero rise time pulse

A steady-state numerical plasma was created with the parameters above and a zero rise time pulse of -2 kV was then applied to the substrate (left boundary) of the simulation. Figure 2 shows snapshots of plasma potential as a function of space for the first 5 ns (very beginning of the "implantation phase"). At $t=0$, before the plasma has not had time yet to react, the plasma can be seen as a dielectric where the charges do not move, hence the sudden wall potential creates an electric field of 20 kV/m across the whole system. This electric field starts accelerating the electrons toward the grounded wall and the ions toward the substrate. The plasma potential remains negative for 2 ns and in the following 1 ns it charges up to a positive potential everywhere. During this short period (3 ns) a very fast moving sheath appears and pushes the electrons toward the right-hand earthed wall at an average velocity of 6×10^{6} m/s, which is almost five times the thermal velocity of 1.3×10^{6} m/s. Hence it seems reasonable to call this phenomenon an electron shock wave since it is much faster than the electron thermal velocity.

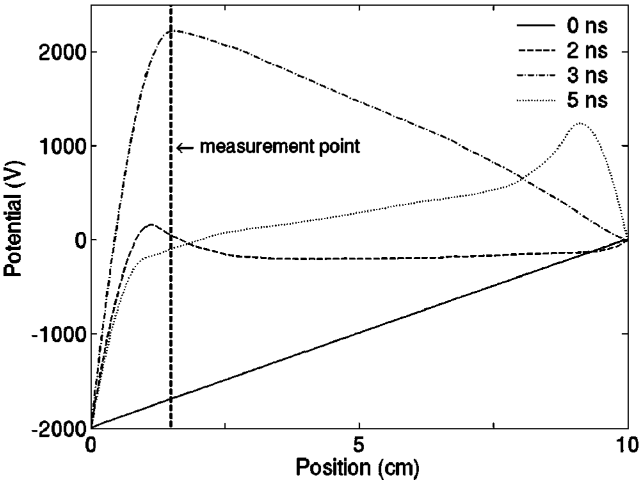

FIG. 2. Snapshots of the plasma potential profile at 0, 2, 3, and 5 ns after a zero rise time pulse of -2 kV. The bold dashed line (--) represents the point where the potential was measured as a function of time (Fig. 3).

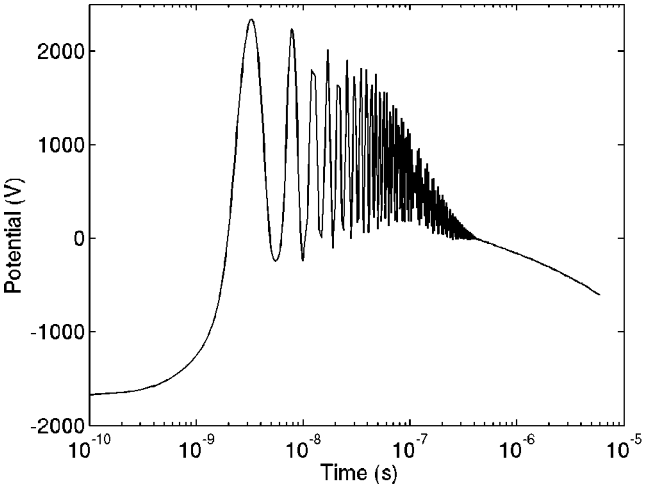

FIG. 3. Time evolution of the plasma potential after a zero rise time pulse of -2 kV the plasma potential is measured 1.5 cm away from the substrate (see the measurement position in Fig. 2).

Figure 3 shows the evolution of the plasma potential 1.5 cm from the substrate (the measurement point is shown on Fig. 2). This point was chosen to show the evolution of the plasma potential since it is the region where the plasma potential and its fluctuations are the most important. Figure 3 shows that the measurement point potential is almost -1.7 kV at $t=0$. After only 3 ns the plasma potential has risen to a positive potential greater than +2.1 kV reflecting the loss of electrons from the system onto the right-hand earthed wall. At this point, the plasma potential starts oscillating with an amplitude greater than 1 kV at approximately the electron plasma frequency until 100 ns and remains greater than 100 V until 300 ns when it drops rapidly to a few volts at 600 ns, after that we can consider that a "steady-state" is reached.

Figure 4 shows the evolution of the spatially averaged electron density versus time when the pulse is applied. The first thing that should be noted is that although the electron density presents the same oscillations as the plasma potential, these oscillations are smoothed out by the average in space and are not visible in Fig. 4. Four different periods are noticeable. First of all the electron density is observed to remain constant for almost 1 ns, which is possibly the minimal time that the plasma needs to react in the presence of a shock wave. Then a very fast decrease of the electron density is observed between 1 and 3 ns where almost 10% of the electrons are expelled in less than 2 ns. This is due to the very fast moving sheath accelerating the electrons to the

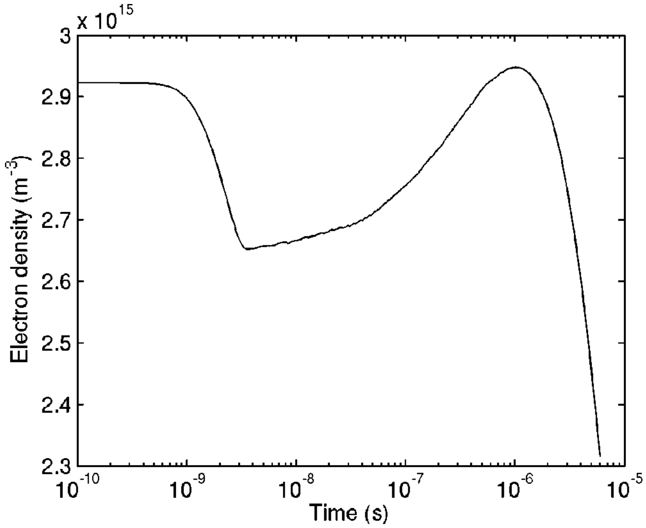

FIG. 4. Time evolution of the spatially averaged electron density after a zero rise time pulse of −2 kV.

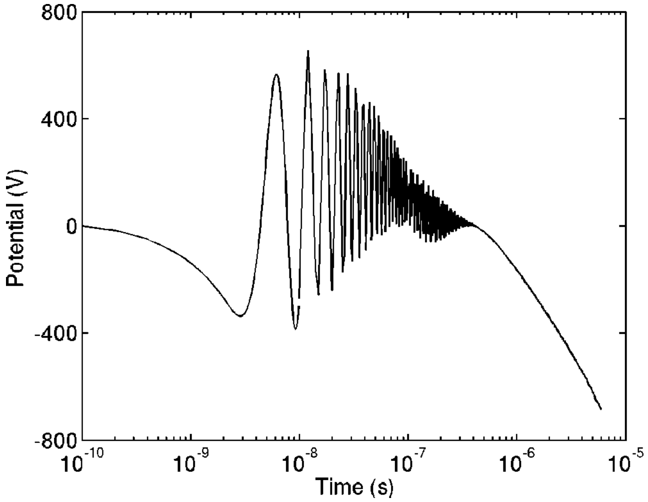

FIG. 6. Time evolution of the plasma potential after a 10 ns rise time pulse of −2 kV: the plasma potential is measured 1.5 cm away from the substrate.

right-hand wall (first very fast increase of the potential at the measurement point). After 3 ns an increase in the electron density is observed. This is due to the positive plasma potential preventing the slowest electron from escaping, also to the significant number of ionizing collisions resulting from electrons heated by the shock and possibly the large oscillations in the plasma potential. Finally, the electron density once again decreases, suggesting that in the absence of the large oscillations the electrons cool down.

Figure 5 shows that for the zero rise time case (black bars), some ions have an impact energy greater than the pulse itself (2 keV) as a result of the high positive potential (more than 1 kV) which exists for more than 100 ns. In previous numerical studies[4] Boltzmann electrons were assumed to describe zero rise time pulses and to evaluate the energy spectrum of the accumulated doses. It has been shown here that this assumption is not valid for such fast rise time pulses.

B. 10 ns rise time pulse

Figure 6 shows the evolution of the plasma potential (once again at 1.5 cm from the substrate) when a 10 ns rise time negative pulse is applied. The positive excursion of the potential oscillations commences at more than 600 V is about 100 V at 200 ns and is negligible at about 500 ns. The average velocity of the electrons pushed by the expanding sheath is very close to the thermal velocity, therefore in this case no electron shock wave is created. Under these circumstances, it is likely that the electrons could be represented by a Boltzmann equilibrium and therefore can be described as such by a numerical fluid simulation.

Figure 7 shows the evolution of the electron density versus time when the 10 ns rise time pulse was applied and

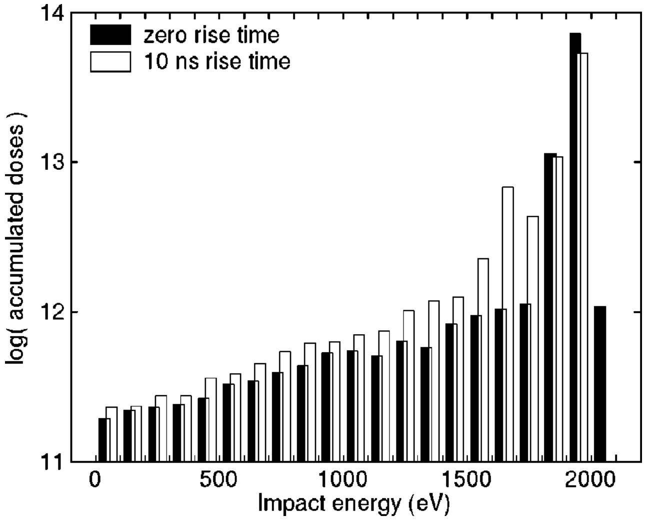

FIG. 5. Comparison between the natural logarithm of the accumulated doses (measured in m^{-2}) after a −2 kV pulse of 6 μs having a zero rise time and a 10 ns rise time.

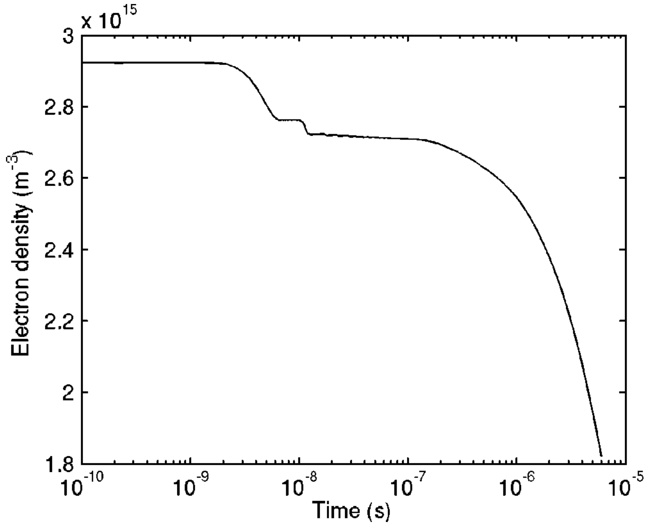

FIG. 7. Time evolution of the spatially averaged electron density after a 10 ns rise time pulse of −2 kV.

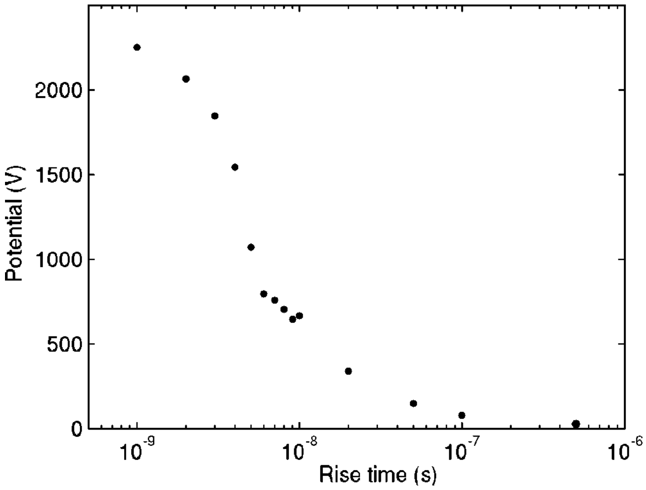

FIG. 8. Maximal plasma potential reached after a −2 kV pulse as a function of rise time.

different periods are noticeable. Initially, the electron density remains constant for 2 ns, which is once again probably the minimal time that the plasma needs to react in the absence of a shock wave. This is followed by two fast decreases of the electron density separated by a period of constant density which are observed between 2 and 10 ns. This is due to the two first oscillations of the plasma potential that occur during the rise time. During this period 7% of the electrons are expelled. Subsequently, the electron density decreases slowly as a linear function of time since not enough energy is introduced into the plasma to sustain it.

C. Condition of formation of an electron shock wave

It has been shown that an electron shock wave is generated for an ideal square pulse with zero rise time and that no shock wave was observed for a 10 ns rise time pulse. A number of simulations were then conducted for the same pulse length but varying rise times (from 0 to 500 ns). Figure 8 shows the maximum plasma potential reached after applying a −2 kV pulse as a function of rise time. For rise times shorter than 2 ns this maximum plasma potential is greater than 2 kV. This maximum value drops below 1 kV when the rise time becomes greater than 2–3 ns, which corresponds to the electron plasma period for these conditions ($T=2\pi/\omega_p=2$ ns with $\omega_p=3\times10^9$ rad/s). Several series of runs were then carried out with different plasma densities, and hence plasma frequencies which showed that if the pulse rise time becomes greater than the electron plasma period, no electron shock wave is observed.

IV. CONCLUSION

In this paper, it has been shown that an electron shock wave exists when a negative pulse is applied with rise time shorter than the electron plasma period. Modern pulsed high voltage power supplies can achieve a voltage slew rate of around 10 ns/kV which is near the values discussed in this paper. Rise times will likely become even shorten in the future. The previous numerical study[4] did not take into account nonlinear phenomena that occur when a negative pulse is applied with a null rise time, since the electrons were assumed to be in Boltzmann equilibrium.

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