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Short communication

Simulation of sputtering from an isolated conductor surrounded by a dielectric during plasma etching

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ABSTRACT

We investigate the action of ion flows from a plasma onto the surface of a flat conductor lying on an insulator, with width less than the plasma Debye length. The model allows study of the processing with a steady state or pulsed potential on the microwire. The shape of pulses has been synthesized to provide the most homogeneous distribution of the etching rate over the microwire surface.

Plasma technologies for surface treatment of materials (etching, deposition of thin films, implantation, and modification of the structure) are fundamentally important for modern solid-state electronics. With the ever-decreasing characteristic dimensions of the elements of integrated circuits, the plasma treatment processes must presently be controlled on nanometer scale sizes.

In the production of nanoelectronic devices, however, traditional plasma technologies face inevitable problems caused, among other effects, by the accumulation of charges on the surfaces being treated. Understanding of such charged surfaces on the plasma process at nanometer-scales and on the geometry and topology of the structures obtained through these processes is key for achieving a high level of control. Local charging of the surface caused by the different electron (isotropic) and ion (anisotropic) fluxes was analyzed through simulation for the first time in Ref. [1]. Subsequently, more complex and accurate models were developed to analyze the effect of charging during the plasma etching of structures [2–6].

Different ways exist of controlling the distribution function of ions acting to the isolated structure. So, for the plasma reactor based on beam plasma discharge [7], two methods were proposed of controlling the distribution function of the ions [8]. In the first case, the periodic pulse voltage was applied to the substrate holder; in the second case, the pulsed voltage was applied to the discharge collector, thus modulating the plasma potential. The comparison shows that the second method provides more efficient control of the distribution function of ions, acting on the treated substrate.

Now there has been growing interest in developing nanoelectronic devices including structures of "microwire on isolator"' kind (see for example [9–13]). Special attention comprises structures based on graphene because of its superior electrical properties [14–16]. Patterning graphene into a nanoribbon can open a bandgap that can be tuned by changing the ribbon width, imparting semiconducting properties. In particular, the effect of ribbon width on electrical transport properties of graphene nanoribbons (GNRs) was reported in Ref. [13], where reactive ion etching of graphene sheets was applied.

This research, which continues the investigations of [17,18], was initiated by experiments on low-energy etching of topological insulator nanoribbons in a beam-plasma reactor [9], similar to the method by which samples of two-layer graphene [19] were obtained. These experiments gave a negative result: the etching effect was observed at the energy of ions, acting on the initial strips, ≥70 eV, but the resulting strips were highly heterogeneous in thickness. (Because of the negative result, information about these experiments was not published). There was a natural assumption that the unevenness is caused by the inhomogeneity of the ion flow, which was confirmed by the results of qualitative computer modeling [17].

In Ref. [8] was shown that it is possible to exclude or weaken the negative charging effect by means of a pulse modulation of the

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conductor potential. To study the processes with a pulsed potential on a conductor, it is necessary to use a model that eliminates the effects of plasma depletion and keeps the main plasma parameters constant in an area sufficiently remote from the conductor.

In Refs. [17,18] the present authors reported using the PiC method implemented through the electrostatic option in the KARAT code, first published in Ref. [20] and widely used and under ongoing development, (see for example, [21–23]). The goal of that work was to study the effects of charging a dielectric surface in a complex configuration consisting of a microwire supported on an insulating substrate. To ensure clear identification of the effects, in Ref. [17] a simple initial condition was chosen with a collisionless plasma homogeneously filling the space above the microwire-dielectric structure. A limitation of this approach was that we could observe only transient processes when a potential was applied to the microwire: the analysis time was limited by the depletion of the plasma because of the arrival and neutralization of charges at the wall. Nevertheless, the main qualitative effect of charging was clearly shown: the formation of an electrostatic lens, leading to a substantial inhomogeneity in the profile of the ion beam acting on the microwire.

The goal of the present work is to refine the numerical model to determine the state of the plasma near a grounded surface that absorbs charged plasma particles. We consider the problem both under conditions of constant potential on the microwire, and with pulse modulation.

In simulating a plasma–surface interaction by the PiC method, the question arises of how one should maintain fixed (i.e. time independent) properties of the plasma beyond the sheath. If initially a plasma with fixed parameters is formed inside the simulation region, then the plasma will start to change, first near the surface, and the modified region will expand in the direction normal to the surface.

If one wishes only to investigate the physics over a relatively short period, then it would be sufficient to solve the problem over a region meaningfully greater that the sheath scale length. However, if one wishes to study the dynamics over an extended period of time then this will be limited by depletion of the background plasma resulting in growth of the sheath length. This requires a computationally expensive increase in simulation volume, and is not physical, since in an experiment the plasma is replenished.

In Ref. [17] we solved a similar question in the 1D formulation. In this paper we consider 2D XZ geometry.

Fig. 1 shows a representative variant of such a simulation domain. At X = 0.16 mm there is a 60 μm thick dielectric absorbing surface with dielectric permittivity ε = 5, covering a perfectly conducting substrate at zero potential, and an electrode of 80 μm width absorbing the incident charged particles. At a reasonable distance X = 2 mm a particle absorbing conducting surface is located defining the upper boundary for the simulation. This size 2 mm was chosen to have the maximum length much more the Debye length of this plasma. This inequality provides the possibility to simulate a plasma. Increasing this maximum size only increases the calculation time.

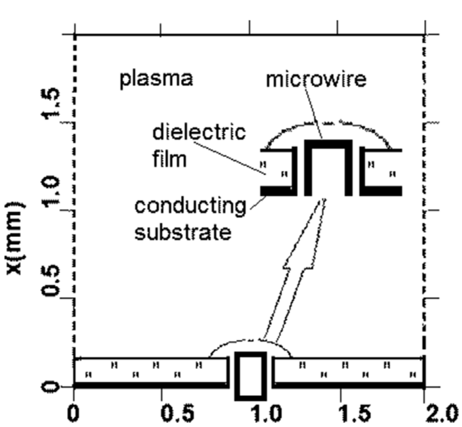

Fig. 1. Geometry of the simulated system.

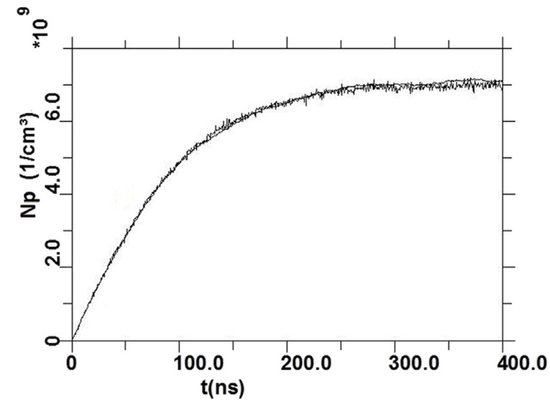

Fig. 2. Temporal evolution of electrons and ions densities in center of simulation region.

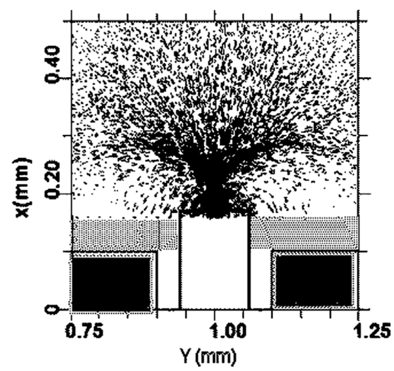

Fig. 3. The distribution of argon ions in the (X, Z) plane at a constant electrode potential of 70 V.

Along the Z direction, periodic boundary conditions are used. The electrode is insulated from the substrate. Its potential relative to the substrate may be chosen to be a constant voltage or a sequence of periodic pulses. In Ref. [8] was shown that the rectangle pulse modulation of the surface potential is more effective for preventing a dielectric substrate charging relative to usually used sinusoidal modulation, thus we applied this modulation of the microwire potential in the represented calculations. The space from the upper surface to the dielectric (X = 2 mm) is filled by a plasma modelled by PiC macroparticles.

After considering various possible algorithms for maintaining the plasma parameters, we identified the following approach as the best compromise. In the initially empty simulation domain (or some part of it), pairs of electrons and ions, with Maxwellian distributions in velocity and randomly distributed in space, are generated. A difficulty with this algorithm is that, because of the limited space dimension, namely, XZ geometry, particles generated with a small *X* component of velocity will accumulate, and we will lose the desired isotropy of the plasma in velocity space. We can resolve this problem by including in the model elastic collisions of electrons with neutrals of sufficient density inside the maintaining region. This does not contradict to the physical model of the plasma as we use a mean free path length much more than the Debye length.

The next issue to be addressed is the inclusion of a density-limiting mechanism, which may be realized by allowing recombination in the model. To realize this element of the model, the particle density and the corresponding recombination probability are computed periodically in the simulation region. A simple model is used with a constant

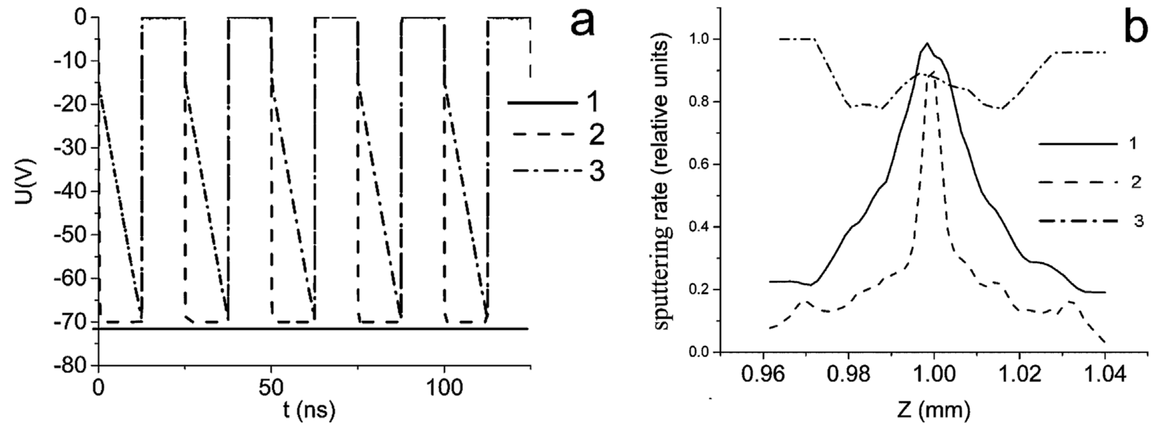

Fig. 4. The sputtering rate vs. the position across the conductor on the electrode (b) for various shapes of the conductor potential in time (a). 1 – DC bias on the conductor; 2 - rectangular voltage pulses; 3 - trapezoidal voltage pulses.

recombination coefficient α, such that the recombination events N_R per unit time and per unit volume is used [24]:

$$N_R = \alpha \cdot n^{+} \cdot n^{-} , \tag{1}$$

where n^+ and n^- are ion and electron densities.

In accordance with this simple model in our algorithm, at each time step, in each node of the simulation region, the recombination probability is calculated from the particle densities. If it is greater than a random number selected from the range from 0 to 1 with a uniform probability distribution, then the ion and electron nearest to the given point are found, and they are eliminated. Fig. 2 shows the history of the electrons and ions densities in a simulation region under the conditions for plasma formation and regulation described above. Equilibrium value of plasma density is equal to $7{*}10^9\ \mathrm{cm}^{-3}$ and temperature 0.3 eV.

A grid of 100 * 100 was used, which provides a space step much smaller than the Debye size of the plasma and other characteristic dimensions of the system. We select argon as the plasma-forming gas for which the mass of ions is $M \approx 80000m$, where m is the electron mass.

Thus, the chosen algorithm ensures the formation and maintenance of the background plasma. The plasma sustained using this algorithm can be used to study the plasma's response to various physical objects immersed in the plasma, for example, Langmuir probes.

In this paper, we consider the reaction of a plasma to a flat thin electrode, to which a potential is applied, and the corresponding sputtering of the material of this electrode. This design allows us to restrict ourselves to a 2D XZ geometry, where the XZ plane is perpendicular to the electrode. The electrode passes through a gap in a grounded substrate covered with a dielectric layer (see Fig. 1). We consider scattering of the electrode material under the influence of the ions incident on it, with the objective of studying the shape of the voltage pulse, which ensures the most uniform distribution of sputtering in Z.

To model the sputtering of electrode material we use the information describing the scattering of Ni atoms with Ar ions [25]. We approximated that information by the formula

$$Y = 10^{-4} \cos\theta {*} (W[\mathrm{eV}] / 30)^9, \tag{2}$$

where Y is the number of atoms scattered from the target per incident argon ion, $W < 200$ eV is the energy of an incident ion, and θ is the angle of incidence. In addition, it is critical to note that there is a threshold for the energy of the ion: at an energy of less than 30 eV there is no sputtering. For the calculation of sputtering, these data are combined with the calculated energy of the Ar ion and its angle of incidence on the electrode to provide the probability of an atom being released from the surface.

In a series of simulations, a number of features of this process of importance for applications were identified.

However, our expectations were not confirmed. The sputtering was seen to be maximal at the center, with an even stronger, sharper profile when compared to that predicted for a constant potential applied to the electrode, and with an order of magnitude variation in the sputtering across the width of the electrode.

Thus, the simulation revealed that the shape of the electrostatic lens (see Fig. 3) essentially depend on the ion energy. This led to a natural assumption about the possibility of smoothing the etching profile by temporal variation of the energy of incident ions. (A similar method of ion energy control at semiconductor etching by the way of patterning the substrate bias voltage was published in Ref. [23]).

We supposed that applying a simplest shape of potential variation during the bias pulse, which is trapezoidal form, more homogeneous distribution of the sputtering rate along the conductor width could be provided. This assumption is based on the results of [14], where different shapes of To test this assumption, simulations were carried out with trapezoidal voltage pulses with a different slope on the trailing edge and retaining the 25 ns period and duty factor of 0.5.

In Fig. 4 (line 3) results are shown when the pulse has the form of a trapezoid with a voltage drop from −20 V until −70 V along the pulse length (12.5 ns), while the sputtering is predicted to have a satisfactory uniformity.

The results presented show that the sputtering rate of the electrode atoms can have maxima at the center and\or at the edges. This is primarily determined by the position of the focus (see Fig. 3) of the ion flux above the surface of the electrode. The position and further scattering of the flow along Z is determined by the size of the Child-Langmuir region, which in turn depends on the bulk Debye length in the plasma. With the chosen plasma parameters, we could reach an intensity change of less than 10–20% across an electrode of width 0.08 mm.

Thus, we have shown that, for a surface plasma treatment of structures of the "connector on insulator" type for modern solid-state electronics application of the connector voltage in the shape of periodical trapezoidal pulses allows to achieve electrode size and plasma parameters to choose the potential temporal variation such that a heterogeneity of the electrode material scattering by the ion flux reaches a value less than 10–20%.

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