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Charging Effect in Plasma Etching Mask of Hole Array*

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Abstract It has already been found that the round shape of holes can be changed into hexagonal shape during plasma etching processes. This work aims to understand the mechanism behind such a shape change using particle simulation method. The distribution of electric field produced by electrons was calculated for different heights from the mask surface. It is found that the field strength reaches its maximum around a hole edge and becomes the weakest between two holes. The field strength is weakened as moving away from the surface. The spatial distribution of this electric field shows obvious hexagonal shape around a hole edge at some distances from the surface. This charging distribution then affects the trajectories of ions that fall on a mask surface so that the round hole edge is etched to become a hexagonal hole edge. The changing of this hole shape will again alter the spatial distribution of electric field to enhance the charging effect dynamically.

Keywords: plasma etching, charging effect, hole array

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1   Introduction

Along with the remarkable development of microelectronics industry, integrated circuit density keeps rising, which leads to the emergence of a fact that characteristic dimension has entered the under-submicron range. The extent of micro-processing technology achieved is one of the most important decisive factors for producing integrated circuits of such an extremely small characteristic dimension. In micro-processing technology, making high-resolution holes or trenches in thin layers using plasma etching technology is a basic and important step. In etching process, the sheath region formed by plasma on a wafer surface has considerable research significance [1~6]. Because the sheath electric field (E-field) established by self-bias voltage directly control the energy distribution and incidence angle distribution of ions bombarding the wafer, it can really affect the plasma etching process. Low-energy ions entering the sheath with Bohm velocity accelerated by sheath E-field bombard wafer nearly vertically. On one hand, this ion physical bombardment can assist chemical reaction taking place between neutral free radicals and molecules on wafer surface by transferring the kinetic energy of ions to surface molecules; increasing number of molecules whose energy is higher than the activation energy thus accelerates the etching progress. On the other hand, it is also able to remove polymers deposited on the wafer surface. Velocity of electrons in sheath region basically obeys Maxwell distribution; its

direction is isotropic and its magnitude is much larger than that of ions due to small mass of an electron. However, it is this huge difference of velocity distributions between ions and electrons that causes a problem, i.e. charging effect, which needs to be solved in industrial applications.

In 1983, YOSHIDA and WATANABE [7] first reported charging phenomenon. From then on, more and more studies have been focused on this issue [8~24]. Charging effect commonly leads to profile defects such as tilt [16,17], notching [18,19], bowing [20] and shouldering [21] and these defects will get worse with increasing demand on high aspect ratio. Up to now, many investigations including numerical simulations [8~10,23,24] and experimental studies [15,22] have already revealed the mechanism that leads to charging phenomena in various degrees. Now, it is currently considered that the difference of velocity distributions between ions and electrons is the root cause for this issue. Because electrons arrive at the trench surface first, and then they set up an electric field distribution, trajectories of tardy ions will be directly affected by the field. The charging then leads to etching of unexpected places or vice versa, so it seriously influences the end result of etching.

So far, nearly all the studies focus on the charging effect on the profile of a trench. Yet in some experiments, it has already been found that charging on the top surface of the mask also influences etching process. For instance, when a mask is made of round holes aligned in hexagonal array, the round shape of holes can be

changed to hexagonal shape during etching process. It is harmful to the ultimate etching result of wafer. This is because, with etching progress goes on the shape of mask holes is gradually changed, meanwhile the mask material itself is also reduced under ion bombardment and the mask thickness becomes smaller. Under the influence of this new mask of hexagonal holes, the etched shape for wafer will become hexagonal. However, there is no research report on the mechanism of charging effect on the top surface of mask. The aim of this paper is to use a particle simulation method to investigate the spatial charging phenomenon on the top of a mask made of hexagonal array of round holes; the calculation explains the mechanism underlying the shape changing of holes during etching process.

2   Experiment

Fig. 1(a) and (b) show the scanning electron microscopy (SEM) photographs of a mask of round holes aligned in hexagonal array before and after etching, respectively. All etching experiments were accomplished on Primo D-RIE of AMEC with two radio-frequency (RF) sources of 60 MHz and 2 MHz. The mask material was carbon. The composition of etching gases was C_4F_6, O_2 and Ar. Obviously, the initial round holes has changed into hexagonal holes after etching.
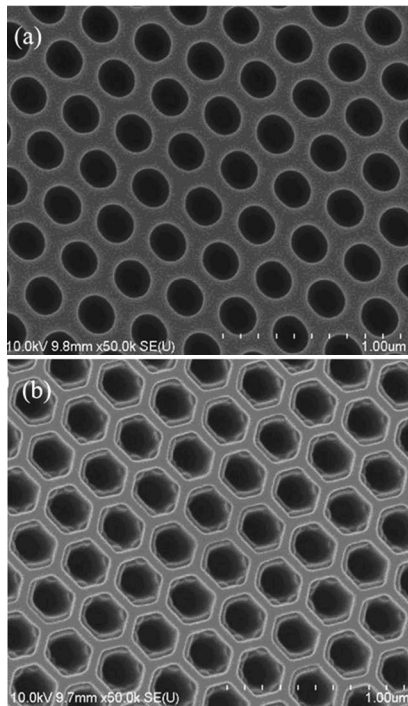

Fig.1   SEM photograph of a mask of round holes aligned in a hexagonal array: (a) Before etching, (b) After etching

3   Calculation model

The real size of the mask is several hundred square millimeters, and holes are extremely abundant. By the periodicity of mask pattern, the environment around

each hole can be regarded as equivalent. In this paper, only a circle with radius of 1.1 μm which contains 37 holes (Fig. 2(a)) was considered as the system under study. The diameter of the holes, D_1, is taken as 0.2 μm and the spacing between the holes, D_2, is 0.1 μm. The hole in the center of the circle can approximately stand for all holes in a real mask due to local periodicity and the boundary effect should be small. The purpose of setting up a circle is that the circle boundary does not destroy the six-fold rotation symmetry of the center hole. Some reasonable assumptions for simplification are as follows. **a.** Only electrons and positively charged ions are taken into consideration in a plasma source. In this simulation, Ar^+ was used. **b.** By plasma characteristics, RF bias voltage on top surface of the mask can only act on electrons and ions in sheath region. However, the frequency of low RF source used to control the bombarding ion energy is 2 MHz which is much greater than the plasma frequency, so ions actually cannot respond to the rapid variation of RF bias voltage. They are subjected to a time-averaging potential only, and are thus accelerated to bombard wafer under the influence of negative DC self-bias voltage, V_{dc}. Additionally, movements of electrons are assumed to depend only on their hot kinetic energy due to their small mass and fast speed. **c.** Electron thermal energy equals to 3 eV and electrons have an isotropic angular distribution and Maxwellian velocity distribution everywhere. Ions entered the sheath edge from plasma source with Bohm velocity, $\sqrt{kT_e/m_i}$, where T_e is the electron temperature and m_i is the ion mass. And $V_{dc} = 3 \times 10^3$ V from an experimental measurement. **d.** Both the mean
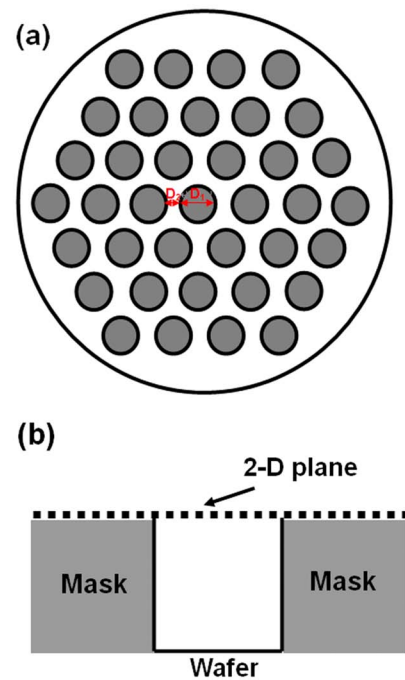

Fig.2   (a) Calculation region made of 37 holes aligned in hexagonal array and contained within a circle with radius of $D_1 = 1.1$ μm. The spacing between holes is $D_2 = 0.1$ μm; (b) The 2D plane (dashed line) for the simulation of particle impinging on

free paths of electrons and ions are usually as large as the thickness of sheath under low pressure, the collision between electrons and ions is then ignored. In addition, the interaction of electrons and ions is also ignored due to such fast speed of electrons and such high self-bias voltage. **e.** The particles impinging on the surface of a mask are considered to remain at the impact sites. For our aim of studying charging effect on the top of mask surface, only the 2D plane that particles impinging on is considered (Fig. 2(b)). **f.** Because of Debye shielding effect, the particles beyond the RF sheath cannot be affected by the mask surface electric field. The RF sheath was therefore set as the whole computation region. This sheath thickness was obtained by the modified Child-Langmuir equation [4].

The computation flowchart and sketch are shown in Fig. 3(a) and (b), respectively. At the beginning, both electrons and ions are randomly distributed at the sheath edge and start to move toward the wafer with their own speeds. The sheath space including the 2D plane of mask surface is divided into many square grids. When an electron falls on a square grid of 2D plane, the charge value of the grid point is subtracted by one; correspondingly, the value is added by one for an ion.
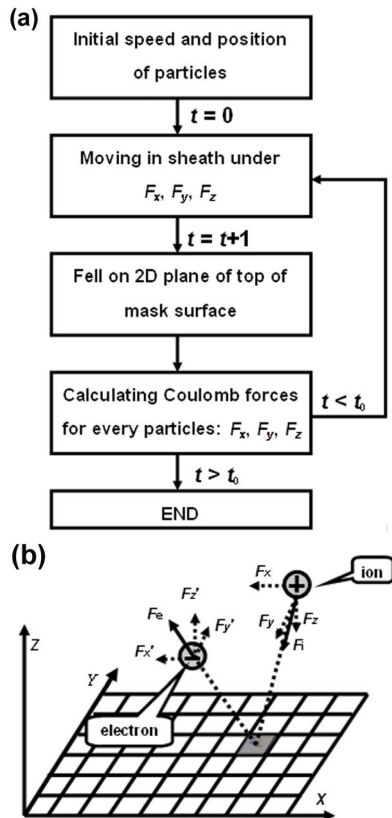

Fig.3 (a) Computation flowchart, (b) Sketch of the process of one ion and electron moving under the electric field on mask top 2D surface according to Newton equation and Cartesian coordinates of particle trajectory. F_i is the force taken by falling ion, F_x, F_x, and F_z, are the three components of F_i; F_e is the force taken by falling electron, F_x', F_y' and F_z', are the three components of F_e

The reason for this deign is that the surface of carbon mask material was covered by silicon dioxide, so the charge can be accumulated. Therefore neutralization of charge is considered. After a certain time, each grid point at 2D plane accumulates a net charge; the charge value and polarity are then considered to calculate the Coulomb interaction force acting on every later coming electrons and ions on their way falling down. Decomposing the force into three components, F_x, F_y and F_z, a particle will move under the force according to Newton equation, and Cartesian coordinates of the particle trajectory are then calculated. In other words, the distribution of electric field on the top of the mask can be obtained by calculating electric field of space grid points. After time long enough for accumulating charge the electric field distribution is then established. However, in this work we have not considered the electric field distribution inside the mask hole and those particles that fall into the hole are ignored; any charge inside the hole would not intensively deflect trajectories of ions that damage top surface of the mask.

4 Results and discussion

4.1 Electric field distribution

As a result of their fast and isotropic character of velocity, electrons arrive at mask surface within a very short time and ions have not yet moved approximately at that moment. The electric field on top surface of a mask established by electrons plays a key role in the deflection of ion trajectories. First, we have simulated a distribution of electric field strength, $E = \sqrt{E_x^2 + E_y^2 + E_z^2}$, for a round hole with a diameter of 1 μm in a 2D plane in negative charges (Fig. 4). Here E_x and E_y are the horizontal components of electric field, and E_z is the vertical component. Fig. 4(a) and (c) illustrate profiles of electric field strength in vertical direction, and, in horizontal plane from a certain height above the top surface of a hole, respectively. Fig. 4(b) and (d) are their corresponding contour maps. It can be seen that the electric field gradually decreases with the height in vertical direction and with the distance away from hole edge in horizontal plane. Then, ions will be likely to bombard on the hole edge at a faster speed in a closer distance to the surface. Because only the horizontal components, E_x and E_y, of this electric field are responsible for the deflection of trajectories of ions, Fig. 5(a)~(c) show the distribution of electric field strength in horizontal plane, $\sqrt{E_x^2 + E_y^2}$, at different heights above the surface, 0.0 μm, 0.5 μm, 1.0 μm, respectively. The insets in these figures display the electric field distribution at the circular boundary. From Fig. 5, it is obviously that the electric field strength has maximum value around holes edge and is weaken away from a holes at different heights. At height of 0.0 μm, this is particular obvious and the electric field is the strongest compared with that at other

heights. The overall distribution of electric field also displays a hexagonal array, being consistent with the mask pattern. Along with the rise of height, the electric field strength presents a reasonable trend of decreasing. Remarkably, the maximum field strength around each hole outer edge approaches a hexagonal shape; meanwhile the weakest field strength at the mid between the holes exhibits an exact hexagonal shape. The fact then clearly implies that ions may likely to impact on the holes edge rather than on the round hole center and the hexagonal mid between holes. At the circular boundary, it presents an obviously different field strength distribution from those around the center hole. The boundary filed strength is higher than any other places at a certain height above the wafer surface. This means that ions actually bombard the boundary most intensively. But this boundary effect is not in our concern here.
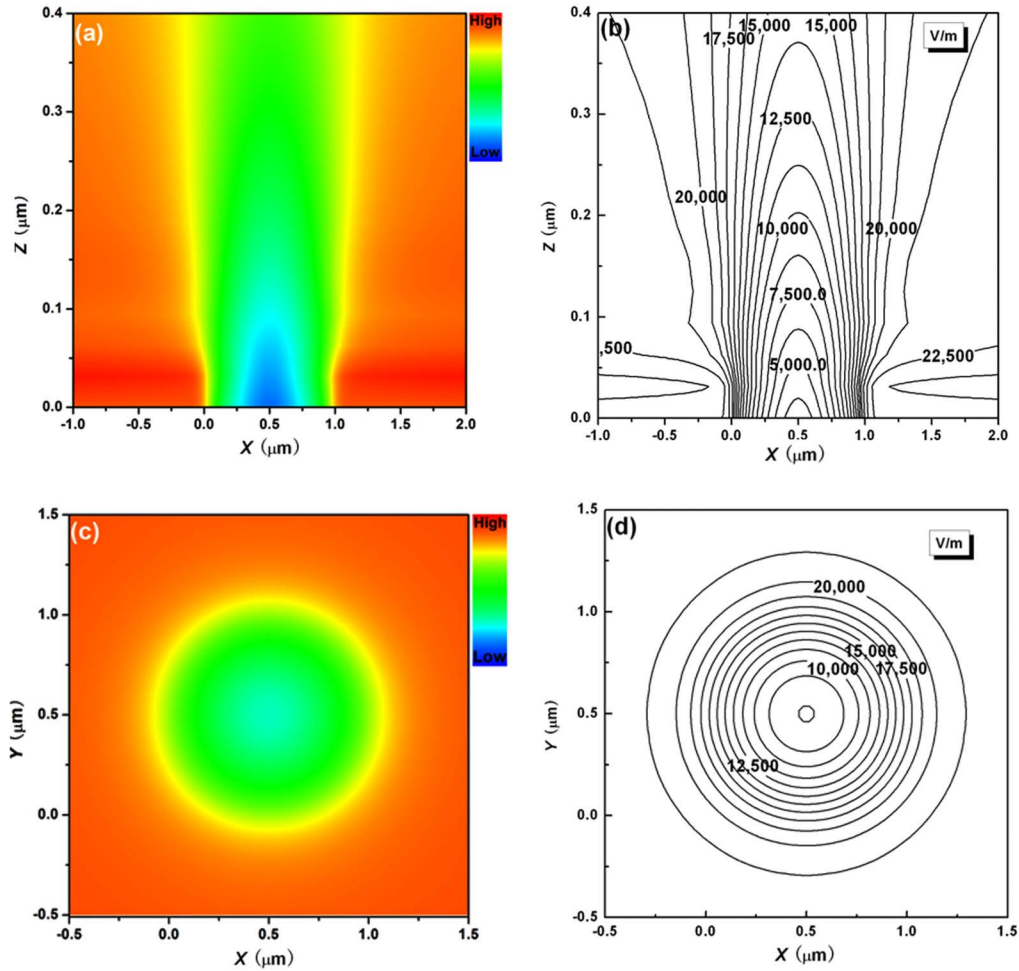

Fig.4 The distribution of electric field strength, $E = \sqrt{E_x^2 + E_y^2 + E_z^2}$, for a round hole with diameter of 1 μm in a 2D plane in negative charges: (a) Profile of electric field strength in vertical direction, (b) The contour map of (a), (c) Profile of electric field strength in horizontal plane at a certain height, 0.15 μm, above the top surface of a hole, (d) The contour map of (c). The values on (b) and (d) are relative values of the electric field strength (color online)
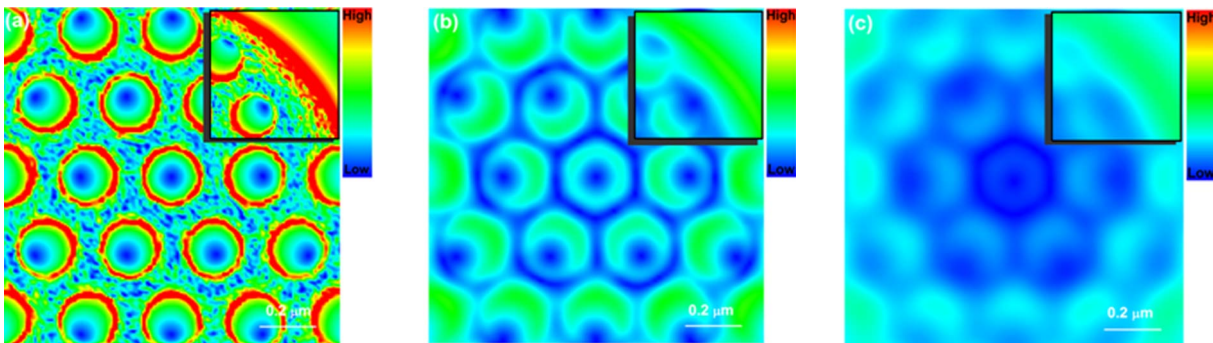

Fig.5 The distribution of electric field strength in horizontal plane, $\sqrt{E_x^2 + E_y^2}$, at different heights above the surface of mask: (a) 0.0 μm, (b) 0.5 μm, (c) 1.0 μm. The insets in these figures display the electric field distribution at the circular boundary (color online)

The above observation is especially clear for the center hole edge at a large height of 1.0 μm. Because of the limited boundary size in simulation, the center hole here actually represents the true holes in a real mask; the effect of boundary size becomes larger with increasing height. The hexagonal shape at outer edge becomes more and more obvious with the rise of height. The reason for this is that when the height is 0 μm, the field strength on mask surface is sensitive only to the local charge which has a roughly constant distribution on the surface except for holes. Therefore, the hexagonal distribution does not appear in a very short distance from the surface. With the increase of the height, the field strength has more contribution from nearby charges and the array effect begins to appear. At a far distance from the surface, the field strength around the center hole is contributed by charges distributed between many holes; thus, the distribution of electric field at the hole edge takes a hexagonal shape. This suggests that ions have already been affected by the hexagonal field distribution as they start to fall from the sheath edge. And also, their trajectories have a trend of being hexagonally distributed in horizontal cross section.

Fig. 6 shows the distribution of electric field strength in horizontal plane, $\sqrt{E_x^2 + E_y^2}$, at 0.5 μm heights above the surface of the mask for different spacing values between the holes. Obviously, with increasing spacing value the electric field strength distribution around the central hole transforms gradually to a non-hexagonal shape due to a decreasing effect of the mask pattern of hexagonal array.

4.2 Ion distribution

The physical bombardment of heavy ions not only acts on the wafer, but also changes the shape of the mask holes, especially the holes edge. The ion bombardment site on the 2D plane on top of the mask surface then determines the final shape of the hole edge. In this paper, the evolution of holes edge shape under ion bombardment with etching time is not included, but instead we study the 2D distribution of ion bombardment site evolved with time. It is worth noting that although the 2D distribution of electric field produced by electrons takes a hexagonal shape and it is also the cause for the deflection of ion trajectories, but with

the falling down of the ions the electrons on the mask surface are neutralized. More electrons can be then accumulated on. The charging effect can be weakened or strengthened with time. This is a dynamic process; the influence of field on tardy ions is different from the first coming ions. Fortunately, in this paper, the simulation method mentioned above has already included the neutralization effect. Hence, the dynamic distribution of ions falling down on the 2D plane of mask surface can represent real damage of mask surface under ion bombardment.

Fig. 7(a)∼(c) illustrate respectively the simulated ion density distribution on the mask surface at different times: 40, 60 and 80 in unit of 2×10^{-11} s. As shown in Fig. 7(a), in the first step ions fall in the mid region between the holes by composed electric field around edges. As time goes on, ions fall into holes more and more. Hexagonal etching pattern should appear in this stage in Fig. 7(b). At the time of 80 units, there is an indistinct hexagonal distribution around the hole and later on the steady etching stage comes. The reason for that relates tightly with the electric field distribution. Ions at first are affected by horizontal hexagonal distribution of weak field and their trajectories tend to be hexagonally distributed. In the falling process of ions, the horizontal field strength increases gradually but the distribution deviates from hexagonal one; furthermore, the speed of ions becomes faster and faster. The influence of electric field hardly changes the later ion trajectories as it approaches the surface. The hexagonal distribution trend of trajectories will be maintained until they finally hit the surface. As the time goes on neutralization occurs, and the field is dynamically weakened. Then more ion trajectories are not affected by the field and fall into holes. However, it is also worth discussing that this result may be different for different experiment parameters. The sheath thickness is the major factor which is determined by DC self-bias voltage, plasma density and so on [4]. The sheath thickness directly affects the dynamic process of ions falling. If the sheath thickness is much smaller than the distance between holes, the number of ions which is affected by mask surface electric field is smaller. What is more, the ion trajectories are almost affected only by local electric filed around each individual hole. Therefore, the round shape of holes may not be changed to hexagonal shape.
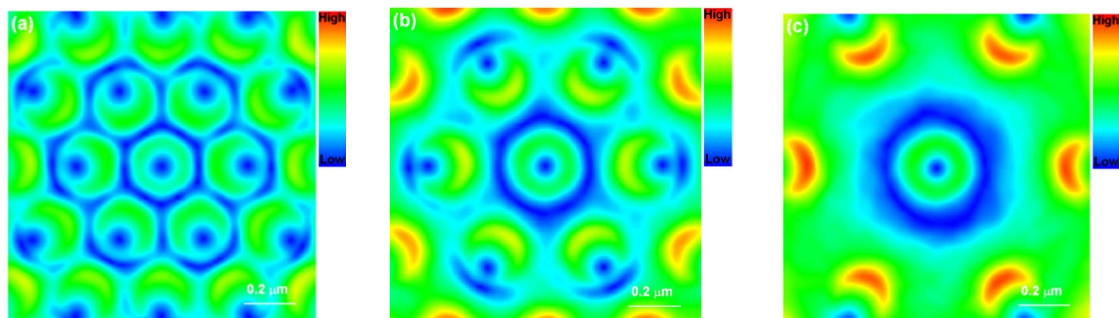

Fig.6 The distribution of electric field strength in horizontal plane, $\sqrt{E_x^2 + E_y^2}$, at 0.5 μm heights above the surface of mask for different spacing values between holes: (a) D_2=0.1 μm, (b) D_2=0.2 μm, (c) D_2=0.4 μm (color online)
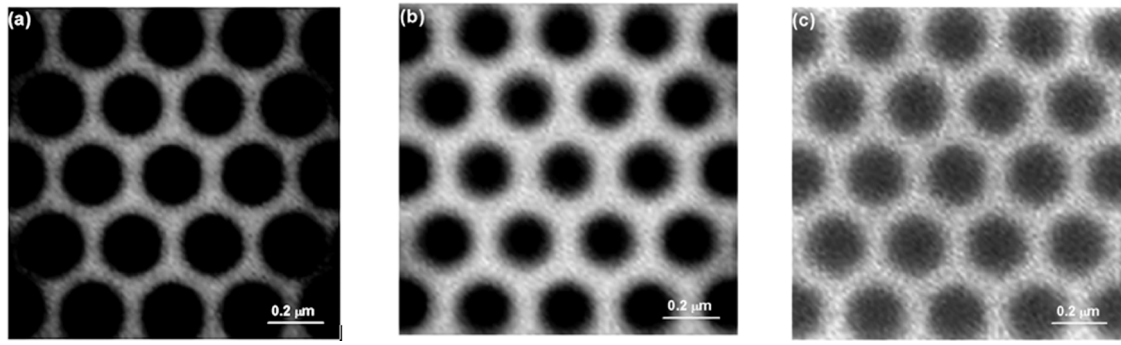
Fig.7 The simulated distribution of ion falling on a 2D plane on top of the mask surface at different time units: (a) 40 time units, (b) 60 time units, (c) 80 time units

Although it seems that the ion distribution around the hole does not present an obvious hexagonal shape in Fig. 7, however, it must be considered that in a practical experimental situation the shape of a hole edge gradually develops into a hexagonal one under ion bombardment, while such a dynamical change of hole edge shape is not considered in the present simulation. The variation of holes edge shape can further strengthen the hexagonal field distribution. This is because the next coming electrons will establish the field distribution based on the varied holes shape. It is therefore speculated that the etching is a positive feedback process with time until the final hexagonal shape is formed. In order to demonstrate this, we have performed another simulation for a mask pattern in which the holes shape is originally perfect hexagonal. This corresponds to a steady etching process when the round holes shape has already become hexagonal after certain time period of etching. Fig. 8 shows the density distribution of ions falling on surface at 100 time units. Quite obviously, there is a hexagonal distribution around the hole edge. This indicates that when the round hole shape becomes hexagonal, the hexagonal shape may still be kept in later etching process.
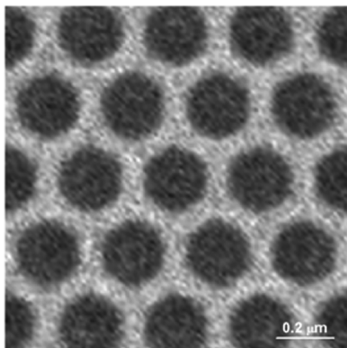

Fig.8 The distribution of ions falling on a 2D plane on top of the mask surface, of which the holes shape is originally hexagonal at 100 time units

5 Conclusion

In this paper, a particle simulation method has been used to study the charging effect on the top surface of a mask made of round holes aligned in a hexagonal array. The distribution of electric field produced by electrons is calculated at different heights from the surface. It is observed that the horizontal field strength develops to display a hexagonal pattern because of the charge accumulation in a far region which contains nearby holes. The influence of the mask pattern on electric field distribution then gradually extends to the density distribution of ions falling on the mask surface. Dynamical etching process generates the final hexagonal hole edge shape at the steady etching stage. According to these results, the changing of the hole shape is largely related to the mask pattern and feature size.

Acknowledgments

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