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Influence of the asymmetry of the metal mask arrangement on the matching of the lower electrode with a high-frequency displacement generator during reactive-ion etching of massive substrates

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The effect of the degree of asymmetry in the arrangement of metal masks on the matching of the lower electrode with a high-frequency displacement generator during selective reactive-ion etching of massive substrates in plasma-forming gas mixtures based on freon-14 is studied theoretically and experimentally. Theoretically, the absence of the influence of the asymmetry of the mask location on the specific reactive power is shown. It is shown that at the edge of the substrate, especially with a mask, there is a sharp increase in the RF current density, which proves mainly the surface (end) nature of its flow. The influence of the mask location on the behavior of the electric charge density, which correlates with the distribution of the RF current density in the near-surface layer of the substrate, is established. No redistribution of the charge density of the chemically active plasma particles at the edge of the mask was detected. In accordance with the theoretical results obtained, it is experimentally shown that metal masks with a side length ratio of 36/0 mm reduce the power reflection coefficient within 5%.

Keywords: diffractive optical element, reactive ion etching, inductively coupled plasma, contact mask, lower electrode, simulation Multiphysics.

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1. Introduction

Techniques for fabrication of diffractive optical elements (DOEs) by reactive-ion etching (RIE) in inductively coupled plasma performed to establish a periodic relief structure in a substrate are now gaining momentum [1–7]. High-energy and reactive particles interact and react with surface atoms on the substrate in the process of plasma etching. Simulations attract ever-increasing attention as tools for examining the behavior of plasma and optimizing the plasma etching processes. Models of inductively coupled plasma chambers for RIE setups with high-frequency (HF) bias voltage applied to the lower electrode with a substrate installed on it have already been developed and tested [8–11].

In certain cases, high optical characteristics of DOEs (e.g., wavefront stability) are required; relatively massive substrates are then needed to fabricate such elements [12,13]. However, the influence of dimensional parameters of substrates on matching of a high-frequency generator (HFG) with the lower electrode is neglected in current models. Simulations in COMSOL multiphysics performed in [14] revealed that an increase in the surface area and thickness of a substrate translates into a considerable enhancement of specific reactive power, which, in turn, implies an increase in the power reflection coefficient at the lower electrode connected to an HFG. The results of these simulations were verified experimentally. The growing power reflection coefficient exceeds the limit rated values, and the material etching rate then decreases sharply, making further processing infeasible. A substrate holder designed to address this problem has been constructed and tested with success.

A two-stage procedure with additional metal masks is normally used to fabricate DOEs [2,15,16]. At the first stage, the desired microrelief is transferred via a photoresist layer to a metal film, which serves as a selective contact mask at the second stage of microrelief transfer to the substrate. The use of this two-stage process is necessitated by the fact that the rate of etching of the photoresist layer is significantly higher than the rate of etching of the material in which the microrelief is to be created, potentially making a direct transfer of the relief structure infeasible. It was demonstrated in [17] that metal masks with almost any practically relevant coefficient of substrate coverage are beneficial to the matching of the lower electrode with an HFG and reduce the power reflection coefficient by up to 15%. However, the influence of asymmetry of positioning of metal masks relative to the substrate center on the matching of the lower electrode with an HFG has not been examined in [17]. In actual practice, the topological pattern of an element is often arbitrary (e.g., when several small-size DOEs need to be fabricated on a single base). The entire substrate is then subjected to etching for the purpose of microrelief formation. In the present study, the influence of the degree of positioning asymmetry of metal masks on the surface of large-scale circular substrates in a special holder on the matching of the lower electrode with an HFG in RIE setups is examined by conducting a numerical experiment in COMSOL Multiphysics.

2. Modeling

A numerical experiment was carried out in COMSOL Multiphysics v.5.2. The project made use of the Inductive Coupled Plasma and AC/DC Electric Current software modules. These modules allow one to simulate an HF induction discharge in the working chamber of the setup with an HF bias applied to the lower electrode.

The diagram of the modeled system is shown in Fig. 1 in [14]. A specialized coil (inductor) generates and sustains plasma under a gas pressure of 0.01–10 Pa. The substrate is placed onto the lower electrode. Ions are accelerated by the electrode and bombard the substrate. With chemical reactions and ion-impact reactions, etching proceeds on the substrate, and desorbed atoms are pulled out of the plasma domain.

Since the problem needed to be solved in the present case for the entire substrate surface, simulations were performed in the two-dimensional (2D) symmetry mode. Contact masks had different degrees of positioning asymmetry. The dimensions of the main structure elements were as follows: the chamber diameter was 300 mm, the lower electrode diameter was 200 mm, and the inductor with an insulator was 14×50 mm in size. Figure 1 presents the modeled substrate with aluminum metal masks. The mask thickness is 40 nm. The substrate holder, which has already been examined in [14], is a metal frame that covers all faces of the substrate except for the working one. Calculations were performed using the Frequency–Transient software module at time point $t = 1$ ms when plasma is steady-state. The chamber design and the domain properties are in exact accordance with [14].

Distributions of the specific reactive (at capacitive load) power, which characterize the power reflection coefficient for the lower electrode, and other important parameters characterizing the physical processes in inductive plasma were obtained as a results of simulations.

The simulation in [14] was performed for a substrate with a diameter of 120 mm and a thickness of 15 mm positioned on the lower electrode. However, it turned out to be impossible in the present study to obtain a solution in the symmetric mode for such a substrate and a metal mask covering $> 30\%$ of its diameter due to an increasing divergence in calculations. Therefore, the numerical experiment was performed for substrates 120×12 mm in size and a metal mask covering 30% of their diameter. These calculations yielded a stable result.

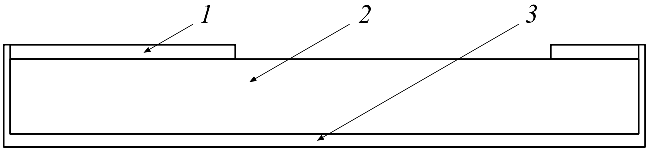

Figure 1. Modeled substrate, which is mounted within a substrate holder, with an asymmetrically positioned metal mask [14]: *1* — mask, *2* — substrate, *3* — substrate holder.

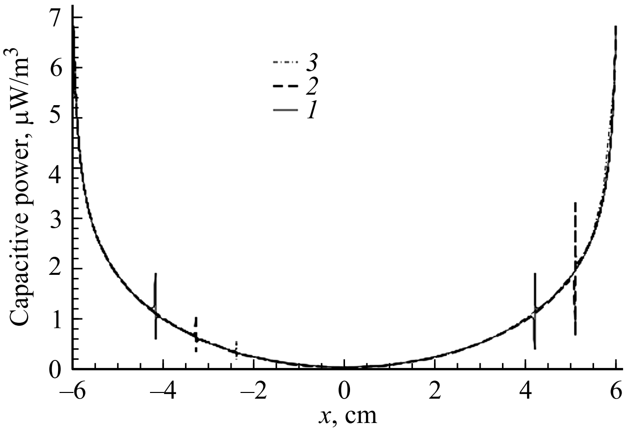

Figure 2. Calculated distribution of the specific reactive (at capacitive load) power over the surface of a substrate (120 mm in diameter and 12 mm in thickness) along radial coordinate x. The side length ratio of the mask, mm: *1* — 18/18, *2* — 27/9, *3* — 36/0; $t = 1$ ms.

Figure 2 shows the calculated dependence of the specific reactive power on the side length ratio of the mask (the parameter characterizing asymmetry) in the case with a substrate holder. The displacement of the mask relative to the substrate center does not produce any unusual effects in this instance. The only thing of note is the power jump, which increases in magnitude toward the substrate edge, in the edge part of the mask, but it has already been observed in our earlier studies. Variations of the side length ratio of the mask do not induce any additional enhancement of the values at the substrate edge.

We have made an assumption in [17] that the specific reactive power jump at the mask edge and its dependence on the distance to the substrate edge are related to the surface nature of flow of HF current through the substrate and the lower electrode and the resulting redistribution of the density of plasma particles in a confined space. This hypothesis was put forward in view of the fact that numerical experiments for smaller substrates revealed an insignificant influence of the corona effect (another probable cause). The involvement of the corona effect appears even less probable if one remembers that it is typically manifested under high gas pressures. Additional studies were carried out to test the suggested hypothesis. Figure 3 presents the calculated distribution of the charge density (Q_ρ) of

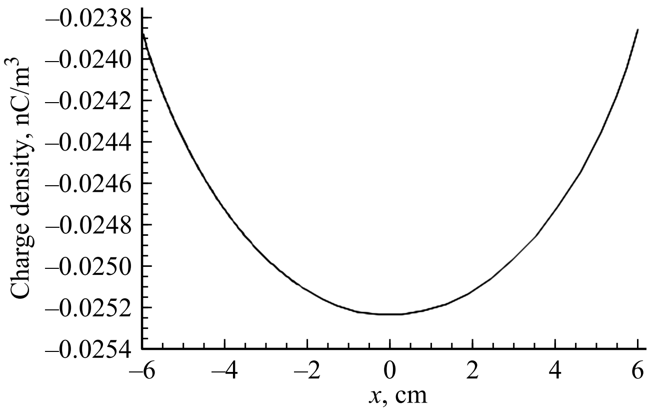

Figure 3. Calculated distribution of the charge density of plasma CAPs at the substrate surface for a mask with a side length ratio of 36/0 mm; $t = 1$ ms.

chemically active particles (CAPs) in plasma at the substrate surface with the greatest mask positioning asymmetry. The left (relative to coordinate $x = 0$) part of the curve corresponds to the masked region; the right part, to the unmasked region. It is evident that the charge density of CAPs varies symmetrically from 0.0252 at the center to 0.0238 nC/m^3 at the substrate edge and does not reveal any deviations at the mask boundary. This implies that the charge density of CAPs is not affected by the presence of a mask, is not the cause of the effect in question, and may account for it, in some degree, only at the substrate edge. The specific reactive power jump may also be caused by a sharp change in the values of impedance load at the mask–substrate interface induced by the emergence of additional inductive components and resonance circuits that exist in long lines with mismatched and partially matched load [18]. Additional studies were conducted to probe this issue further.

Figure 4 shows the dependences of current density J at the substrate surface with the greatest mask positioning asymmetry. The current density in the unmasked substrate region (right curve part) remains almost unchanged up to $x = 50$ mm and starts to increase at the very edge of the substrate, reaching a value of -1500 kA/cm^2, which is ~ 3 times higher than the density at point $x = 0$. At the interface with the mask, the current density undergoes a jump with a magnitude of -2000 kA/cm^2. The value of J then increases and reaches -3000 kA/cm^2 at the substrate edge. This verifies the hypothesis that the increase in specific reactive power at the substrate edge is related to the surface nature of current flow. The current density at the masked edge of the substrate is, in general, ~ 2 times higher than the one at the opposite edge; this is attributable to the enhancement of conduction current by the metal mask.

Figure 5 presents the calculated distributions of the spatial density of electric charges in the surface substrate layer. When the mask is positioned symmetrically (curve *1*), the spatial density of electric charges also varies symmetrically. At the interface with the mask, the spatial density of electric charges increases sharply. This is followed by a rapid reduction with a magnitude of $\sim 100\,\mu$C/m^3 and a no less steep increase to $450\,\mu$C/m^3 at the substrate edges. Notably, the density of electric charges in the region covered with the metal mask is 2 orders of magnitude higher than the density in the unmasked region.

The pattern changes drastically if the mask is asymmetric to a certain extent (curve *2*). The polarity of charges changes in this case. Although the mask is displaced in the right part, the charge density does not vary up to the interface with the mask, remaining at a near-zero level. However, the jump at the interface with the mask is $\sim 10\%$ larger in magnitude than the corresponding jump at the opposite side. At the substrate edges, the charge density is as high as $500\,\mu$C/m^3. This value is 10% higher than the density corresponding to the symmetric mask positioning.

The distribution of the density of electric charges with the greatest mask positioning asymmetry (curve *3*) is essentially the same as the one corresponding to partial displacement.

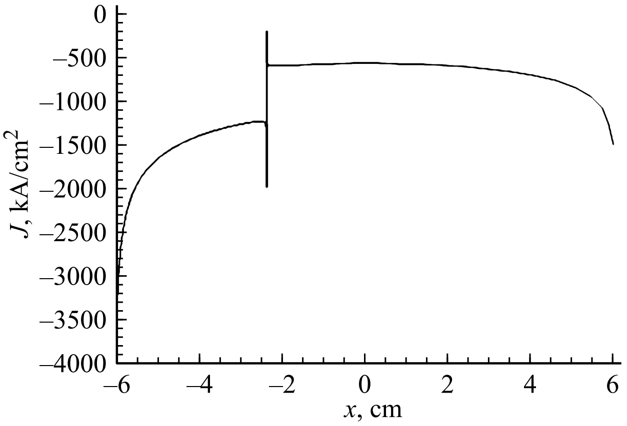

Figure 4. Calculated distribution of current density J at the substrate surface for a mask with a side length ratio of 36/0 mm; $t = 1$ ms.

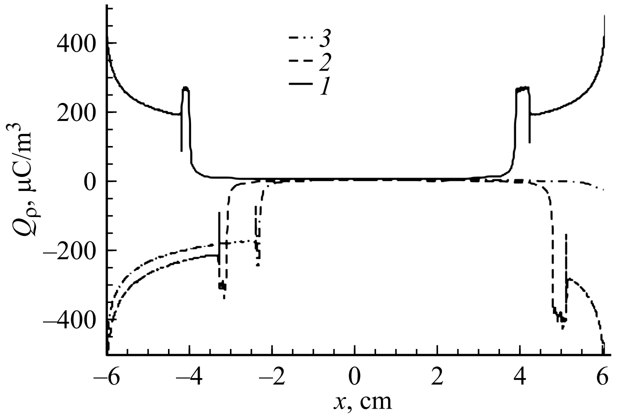

Figure 5. Calculated distributions of the spatial density of electric charges in the surface substrate layer. The side length ratio of the mask, mm: *1* — 18/18, *2* — 27/9, *3* — 36/0; $t = 1$ ms.

Power reflection coefficients at the lower electrode for a Caroline PE15 RIE setup with different gases and a substrate holder with and without an aluminum mask

Substrate	$P_{\text{refl}}/P_{\text{inc}}$, %			
	CHF_3/Ar	CF_4/Ar	SF_6/Ar	Ar
With a symmetric mask	30	24	18	19
With an asymmetric mask	28	22	17	18

Note. The inductor power is 400 W, the argon flow is 0.6 L/h, the freon flow is 1.0 L/h, and the mask thickness is 40 nm.

However, the density in the unmasked region remains constant at $10\,\mu$C/m^3, reaching a value of $25\,\mu$C/m^3 only at the substrate edge.

The presented data indicate that the density of electric charges increases sharply in the masked region; this enhancement correlates with the behavior of the HF current density.

3. Experiment

Experiments were carried out to verify the obtained theoretical results and estimate the influence of an aluminum mask with a side length ratio of 36/0 mm on the matching of an HFG with the lower electrode. A Caroline PE15 [19] RIE setup and freon-based plasma-forming media were used in these experiments. The mask was formed by magnetron deposition. The matching quality was estimated by measuring the coefficient of reflection ($P_{\text{refl}}/P_{\text{inc}}$) of HF power from the HFG incident on the electrode. The substrate 120 mm in diameter and 15 mm in thickness was mounted within the substrate holder and placed on the circular lower electrode with a diameter of 200 mm. The argon and freon flows were set in accordance with the results obtained in [14]. The rim of the substrate holder was set so that its projection was aligned with the substrate surface subjected to the influence of plasma. This ensures electric contact between the mask and the holder. An additional layer of foil was introduced between the rim projection and the mask to make the contact more reliable and uniform. The experimental results are presented in the table. It can be seen that the mask reduces the power reflection coefficient, although the magnitude of this reduction is insignificant (no higher than 5%). With the curves in Fig. 2 being identical, the obtained experimental result may be attributed to the fact that the magnitude of a specific reactive power jump at the mask boundary decreases at the approach to the substrate edge.

4. Conclusion

Theoretical and experimental results of studies into the influence of the degree of positioning asymmetry of metal masks on the process of RIE of massive substrates in plasma-forming gas mixtures based on various freons were presented.

The discovered increase in HF current density at the substrate edge is attributable to an enhancement of conduction current by the metal mask. Coupled with the discontinuous jump at the substrate–mask interface, this effect basically verifies the proposed idea of a surface (end) nature of current flow and its relation to the phenomenon in question. Data on the density distribution of electric charges in the near-surface substrate layer, which correlate with the behavior of the HF current density, also provide evidence in favor of the mentioned hypothesis. In addition to that, an intriguing effect of polarity change of electric charges in the case of asymmetric positioning of a metal mask was discovered theoretically. No redistribution of the charge density of plasma CAPs at the mask edge was observed. Thus, the effect of an abrupt change in specific reactive power at the substrate–mask interface apparently does not extend to plasma and is related to the specifics of current flow through the substrate and the lower electrode.

The results of calculations revealed that the behavior of the specific reactive power distribution does not depend on the degree of asymmetry of the mask positioning (with the sole exception of the magnitude of a jump at the interface with the substrate). However, experiments demonstrated that metal masks with a side length ratio of 36/0 mm reduce the power reflection coefficient by up to 5%. This essentially agrees with the presented theoretical results (Fig. 2). Therefore, compared to symmetrically positioned masks, asymmetric masks are expected to produce an additional slight improvement of matching of the lower electrode with an HFG in etching of massive substrates with an arbitrary topological pattern.

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Conflict of interest

The authors declare that they have no conflict of interest.

References

[1] D.L. Flamm, V.M. Donelly. VLSI Electron. Microstructure Sci., **8**, 190 (1985).
[2] S.B. Odinokov, G.R. Sagatelyan, M.S. Kovalev, K.N. Bugorkov. J. Opt. Technol., **86** (5), 317 (2019). DOI: 10.1364/JOT.86.000317.
[3] V.S. Pavelyev, S.A. Borodin, N.L. Kazanskiy, G.F. Kostyuk, A.V. Volkov. Opt. Laser Technol., **39** (6), 1234 (2007). DOI: 10.1016/j.optlastec.2006.08.004

[4] N.L. Kazanskiy, V.A. Kolpakov. *Optical materials: Microstructuring surfaces with off-electrode plasma* (CRC Press, 2017). DOI: 10.1201/b21918.

[5] *Methods for Computer Design of Diffractive Optical Elements,* ed. by Victor A. Soifer (John Wiley & Sons, Inc., 2002).

[6] V. Korolkov, D. Belousov. *Int. Conf. Information Technol. and Nanotechnol.* (*ITNT*), (2020) p. 1. DOI: 10.1109/ITNT49337.2020.9253171

[7] N.M. Lebedeva, T.P. Samsonova, N.D. Il'inskaya, S.I. Troshkov, P.A. Ivanov. JTF, **65** (6), 957 (2020). DOI: 10.1134/S1063784220060195]

[8] B. Zhang, X. Zhang. Vacuum, **174**, 109215 (2020). https://doi.org/10.1016/j.vacuum.2020.109215

[9] C. Jia, J. Linhong, Z. Yu, S. Yixiang. J. Semicond., **31** (3), 032004 (2010). DOI: 10.1088/1674-4926/31/3/032004

[10] T. Xiao, D. Ni. Chem. Eng. Res. Des., **164**, 113 (2020). https://doi.org/10.1016/j.cherd.2020.09.013

[11] A.O. Brezmes, C. Breitkopf. Vacuum, **109**, 52 (2014). http://dx.doi.org/10.1016/j.vacuum.2014.06.012

[12] P.A. Nosov, A.F. Shirankov, R.S. Tret'yakov, A.G. Grigor'yants, A.Ya. Stavertii. Izv. Vyssh. Uchebn. Zaved., Priborostr., **59** (12), 1028 (2016) (in Russian). DOI: 10.17586/0021-3454-2016-59-12-1028-1033.

[13] N.L. Kazanskiy, G.V. Uspleniev, A.V. Volkov. Proc. SPIE, **4316**, 193 (2000). DOI: 10.1117/12.407678

[14] S.D. Poletayev, A.I. Lyubimov. JTF, **66** (4), 639 (2021). DOI: 10.1134/S1063784221040150]

[15] E.T. Lim, J.S. Ryu, C.W. Chung. Thin Sol. Films, **665**, 1 (2018). https://doi.org/10.1016/j.tsf.2018.08.046

[16] M.A. Butt, S.N. Khonina N.L. Kazanskiy. Computer Optics, **43** (6), 1079 (2019). DOI: 10.18287/2412-6179-2019-43-6-1079-1083

[17] S.D. Poletayev, A.I. Lyubimov. Tech. Phys. Lett., **47** (8), 569 (2021). DOI: 10.21883/PJTF.2021.11.51008.18717

[18] I.E. Efimov, G.A. Ostan'kovich. *Radiochastotnye linii peredachi* (M., Svyaz', 1977) (in Russian).

[19] E. Berlin, S. Dvinin, L. Seidman. *Vakuumnaya tekhnologiya i oborudovanie dlya naneseniya i travleniya tonkikh plenok* (M., Tekhnosfera, 2007) (in Russian).