Theoretical Analysis of Silicon Surface Roughness Induced by Plasma Etching

R. K. Tyagi

Department of Mechanical Engineering, Amity School of Engineering and Technology, Amity University Uttar Pradesh, Noida, India, e-mail: tyagi_rk1@rediffmail.com

A theoretical study of single-crystal silicon surface roughness induced by SF_6 plasma has been carried out by means of atomic force microscopy. Plasma which contains the velocity shear instability has been used to study the relation between the plasma parameters and subsequent surface roughness. The surface roughness has been examined in the dependence on experimental parameters. The results obtained by theoretical calculations are identical to the experimental ones. The present paper has quantified the influence of a DC electric field values on plasma parameters such as the ratio of ion flux to the neutral reactant flux (J^+/J_F), exposure time, DC electric field, magnetic field and inhomogeneity. Theoretical investigation shows that the roughness of silicon surface increases with the increase of the values of J^+/J_F, exposure time, of magnetic field, of inhomogeneity in a DC electric field and decreases through increasing the value of a DC electric field.

УДК 533.9

INTRODUCTION

The understanding of the contact mechanism between surfaces is important for the study of both electrical and mechanical properties of bonded interfaces. Such mechanical and electrical properties include the true contact area, bond strength, contact resistance, i.e. conductivity and reliability. Surface roughness plays a crucial role in the contact and friction of surfaces. In order to describe the roughness of a surface, statistical parameters for the distribution function of the roughness height such as the root mean square (*rms*) height, slope and radius curvature of asperity, have been used in several works. Those parameters can be directly related to the density of asperity, forms of asperity, and the standard deviation of the roughness height [1].

According to P. Verdonck [2], in general, plasma etching is a chemical etching, not a physical etching. This means that a chemical reaction takes place between a solid atom (from the film to be etched**)** and gas atoms to form a molecule, which is removed from the substrate. Because of the existing DC bias, there is always some sputtering, which is insignificant and in most cases should not be taken into account. Nevertheless, the importance of other physical aspects of the etching is emphasized in the studies of other authors [Verdonck, 2006, and Flamm 1986]. As is noted in [2], the main steps in the etching process commented in more detail on the example of the etching of silicon using sulphur hexafluoride (SF_6) are:

i) Formation of the reactive particle;

ii) Arrival of the reactive particle at the surface to be etched;

iii) Adsorption of the reactive particle at the surface;

iv) Chemisorption of the reactive particle at the surface, i.e. a chemical bond is formed;

v) Formation of the product molecule;

vi) Desorption of the product molecule;

vii) Removal of the product molecule from the reactor.

For the similar idea regarding etching, see also [3].

As outlined in [4], the problem of interface roughness has received particular attention, especially the development of its theoretical base. This is due to its practical connection to the thin-film growth. However, rather little effort has been made so far to interpret experimental data in terms of kinetic roughening as can be done for the interaction of plasma with different materials. In this regard, it is worth noting here that an independent varying of plasma parameters is an advantage over conventional machining process. As a major result from [4], an empirical analytical form describing the surface roughness as a function of plasma parameters has been established.

As is known, for the integrated circuits with a decrease of their dimensions the roughness of compound material layers deposited on silicon at different steps of a device fabrication becomes so critical that it needs to be carefully assessed before and after etching. Thereby, it is evident that at such tiny dimensions the plasma etching of the surface cannot be considered being uniform. Thus, it is necessary to take into account roughness, which is closely connected with such plasma parameters as ion energy, ion current density, and the flow of the reacting species. As indicated in [5], the investigated range of roughness values is not amenable to conventional surface metrology techniques such as the scanning electron microscopy (SEM), profilometry, etc. The transmission electron microscopy (TEM) is quite a cumbersome technique to be routinely used since sample preparation takes up too much time. Moreover, a nondestructive sample analysis is not possible by the latter technique. The scanning tunneling microscopy (STM) and atomic force microscopy (AFM) have now become the up-to-date tools to carry out such measurements. The AFM provides a unique opportunity to study the extent of the silicon roughness produced at the SF_6 plasma etched silicon surfaces [5].

The central goal of patterning by plasma processing is to obtain any high rate, while preserving anisotropy, uniformity, and selectivity at the obtained rate. Significant advances in fundamental understanding of plasma-assisted processes have been reported in the recent past, although engi-neering development of a new system continues to rely heavily upon trial and error procedures [6]. Using a one-dimensional radial dispersion model, the authors [6] examine the role of physical factors such as etchant convection and diffusion, which are determined by the concentration of the etchant, and also present a detailed study of the etch rate of a polymer in an oxygen plasma as a function of pressure, power, and flow rate.

Further, mathematical model by Tyagi et al [7, 8] for the plasma containing velocity shear instability is presented and it is considered that the surface roughness is formed by impacts of ions. To analyse the obtained results the phenomenological power law for the heights of surface roughness from [4] is used.

MATHEMATICAL MODEL AND PLASMA GENERATION WHICH CONTAINS VELOCITY SHEAR INSTABILITY

Plasma generated in laboratory conditions contains both positive K^+ ions and negative SF_6^- ions. Potassium ions are produced by spraying potassium atoms onto a tungsten plate and SF_6^- ions are produced from the electrons released from another tungsten plate. The generation and control of the parallel velocity shear are achieved by individual biasing of each segment of the segmented ion source, i.e. a difference between voltages applied between two conjunctive segments. The generation of a parallel velocity shear instability can be achieved with an electrostatic energy analyzer and through the laser-induced florescence diagnostic technique. Negative ions are produced by introducing SF_6 gas into the potassium plasma. An SF_6 molecule has a great electron attachment cross-section for the electron energies less than 1 eV. This is why both negative and positive ions are formed in different layers, that have shear of velocity and density gradient in a respective layer. The detailed description of generation of velocity shear instability is described by the author of the present paper and his colleagues in [8].

Since ions are electrical charges, their trajectories and velocities are influenced by electric and magnetic fields**.** Using our earlier results [8], it is easy to obtain the expression for the group velocity of an electrostatic ion-cyclotron wave by assuming small perturbations of the electric field E_1, magnetic field B_1, and distribution function f_{s1}. For the perturbed values of the electric and magnetic fields the harmonic dependences as exp $i(kr\text{-}\omega t)$ are assumed. Considering the ion velocity v to be equal to the group velocity of the wave, i.e. to $\partial\omega_r/\partial k$, and using the expression for the real frequency ω_r of the wave incident on the workpiece surface, equation (15) from our earlier work [8] can be written as:

$$\frac{\overline{\omega'}}{\Omega_i} = -\frac{b_1}{2a_1}\left[1 \pm \sqrt{\left(1-\frac{4a_1c_1}{b_1^2}\right)}\right] \tag{1}$$

where:

$$a_2 = a_2\left(\frac{\Omega_i}{k_{||}\alpha_{||}}\right)^2, \quad b_1 = \frac{\Omega_i}{k_{||}\alpha_{||i}}b_2 - \frac{2k_\perp\Delta'}{k_{||}^2\alpha_{||i}^2}a_2\Omega_i,$$

$$a_2 = \frac{\eta_e}{\eta_i}\frac{T_{\perp i}}{T_{||i}} + \frac{T_{\perp i}}{T_{||i}} - \Gamma_n(\mu_i)\frac{T_{\perp i}}{T_{||i}},$$

$$b_2 = \frac{\Gamma_n(\mu_i)k_\perp}{2k_{||}}\varepsilon_n\rho_i\frac{\alpha_{\perp i}}{\alpha_{||i}} - \frac{\Gamma_n(\mu_i)k_\perp}{2k_{||}} - \frac{\Gamma_n(\mu_i)k_\perp n\Omega_i}{2k_{||}^2\alpha_{||i}},$$

$$c_1 = \frac{\Gamma_n(\mu_i)T_{\perp i}}{2T_{||i}}\left(1-\frac{k_\perp}{k_{||}}A_i\right) - \frac{b_2k_\perp\Delta'}{k_{||}\alpha_{||i}} + \frac{k_\perp^2\Delta'^2}{k_{||}^2\alpha_{||i}^2},$$

$$\eta_i = 1-\frac{\overline{E_i'}(x)}{4\Omega_i^2}, \quad \eta_e = 1-\frac{\overline{E'_e}(x)}{4\Omega_e^2}, \quad \overline{\omega}' = \overline{\omega} - n\Omega_i,$$

$$E(x) = E_0\left(1-\frac{x^2}{a^2}\right), \quad \overline{E}(x) = \frac{e_sE(x)}{m_s},$$

$$\Omega_s = \frac{e_sB_0}{m_s}, \quad \alpha_{\perp s} = \left(\frac{2k_BT_{\perp s}}{m_s}\right)^{1/2}, \quad \alpha_{||s} = \left(\frac{2k_BT_{||s}}{m_s}\right)^{1/2},$$

$$\xi = \frac{\overline{\omega} - (n+p)\Omega_s - k_\perp\Delta'}{k_{||}\alpha_{||s}}, \quad \Delta' = \frac{\partial\Delta}{\partial t},$$

$$\Delta = \frac{\overline{E}(x)t}{\Omega_s}\left[1+\frac{E''(x)}{E(x)}.\frac{1}{4}\left(\frac{v_\perp}{\Omega_s}\right)^2 \ldots\ldots\ldots\ldots\right],$$

$$A_s = \frac{1}{\Omega_s}\frac{\delta v_{oz}(x)}{\delta x}, \ \varepsilon_n = \frac{\delta \ln n_0(x)}{\delta x}, \ A_T = \frac{\alpha_{\perp s}^2}{\alpha_{\| s}^2} - 1,$$

$$\overline{\omega} = \omega - k_{\|} v_{oz}(x),$$

$$\Gamma_n(\mu_s) = \exp(-\mu_s) I_n(\mu_s), \ \mu_s = \frac{k_{\perp}^2 \rho_i^2}{2}, \ (s = i, e).$$

Here $\mathbf{E}(x)$ is the inhomogeneous DC electric field that is perpendicular to the external magnetic field B_0, which is parallel to ion flow. The detailed description of all variables, used in the given model, is considered in [8].

The dimensionless real frequency and ion velocity have been calculated by computer technique with the help of equation (1) for an inhomogeneous DC electric field. For an inhomogeneous DC electric field, the condition $x/a \le 1$ has been taken.

The kinetic energy of the charged particle under the action of voltage U is determined as:

$$E = eU = \frac{mv^2}{2} \tag{2}$$

Evidently, the metal removal rate is dependent upon the generated voltage U, which defines the depth of the ion penetration in the workpiece. The thickness of its surface layer (for the free penetration of electrons) is defined by the Shenland's relation [9]

$$\delta \approx 2.2 \cdot 10^{-12} \cdot \frac{U^2}{\rho} \ \text{[cm]} \tag{3}$$

where ρ is the workpiece material density, in g/cm^3 and U is the acceleration voltage, in V.

The detailed description of ion penetration and effect of plasma factors on ions penetration is described by the author of the present paper and his colleagues in [7].

Using an atomic force microscope, the topographical maps of the surface have been recor-ded. The root mean square value of the roughness height was found to obey a power law. The empirical law for surface roughness (*rms*) was found to obey the following phenomenological power law, in which $\beta = 1$ and $\eta = 0.45$ [5]:

$$rms \propto \frac{1}{\sqrt{E}} \left(J^+ / J_F \right)^n t^{\beta} \tag{4}$$

where J^+ is the ion flux impinging on the substrate, E – the kinetic energy of the ion and J_F – the SF_6 atom flux and t – the exposure time.

RESULTS AND DISCUSSION

Numerical investigation with the help of mathematical formulation and computer technique by using the experimental data from [5] has been performed on the base of equations (1), (2), and (4). The generated plasma contains the SF_6^- ions are in majority. The mathematical model has the plasma factors from [5, 7].

Figure 1 shows the variations of surface roughness (nm) versus $k_{\perp}\rho_i$ for different values of the ratio of the ion flux to the neutral reactant flux (J^+/J_F), with other fixed parameters listed in the Fig. 1 caption. The surface roughness increases with the increase of the ratio of the ion flux to the neutral reactant flux (J^+/J_F). The maximum value of the surface roughness is 2.47 nm when the value of the ratio of the ion flux to the neutral reactant flux (J^+/J_F) is 60 and the minimum value is 1.32 nm for 20, with other fixed parameters listed in the Fig. 1 caption.

Figure 2 shows the variations of surface roughness (nm) versus $k_{\perp}\rho_i$ for different values of the exposure time, with other fixed parameters listed in the Fig. 2 caption, the value of surface roughness increases with the increase of the exposure time. The maximum value of surface roughness is 4.03 nm when the value of the exposure time is 8 minutes and the minimum value is 1.87 nm for 4 minutes, with other fixed parameters listed in the Fig. 2 caption.

Figure 3 shows the variations of surface roughness (nm) versus $k_{\perp}\rho_i$ for different values of the inhomogeneous DC electric field, with the value of surface roughness decreasing with the increase of the inhomogeneous DC electric field. The maximum value of surface roughness is 2.52 nm when the value of the inhomogeneous DC electric field is 16 V and the minimum value is 1.59 nm for 20 V, with other fixed parameters listed in the Fig. 3 caption.

Figure 4 shows the variations of surface roughness (nm) versus $k_{\perp}\rho_i$ for different values of the magnetic field, with the value of surface roughness increasing with the increase of the value of the magnetic field. The maximum value of surface roughness is 3.63 nm when the value of the magnetic field is 0.18 T and the minimum value is 1.87 nm for 0.10 T, with other fixed parameters listed in the Fig. 4 caption.

Figure 5 shows the variations of surface roughness (nm) versus $k_{\perp}\rho_i$ for different values of the inhomogeneity (x/a) in a DC electric field, with the value of surface roughness increasing with the increase of the value of inhomogeneity (x/a). The maximum value of surface roughness is 3.24 nm when the value of inhomogeneity (x/a) is 0.9 and the minimum value is 1.87 nm for 0.3, with other fixed parameters listed in the Fig. 5 caption.

The value of surface roughness was experimentally found out in [5]: the ratio of the ion flux to the neutral reactant flux (J^+/J_F) varied from 20 to 80, the exposure time varied from 2 minutes to 12 minutes,

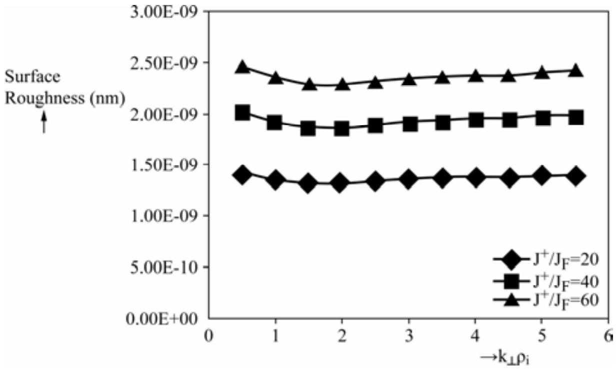

Fig. 1. Variations of surface roughness versus $k_\perp\rho_i$ for different values of J^+/J_F and other parameters: A_i = 0.5, T_e/T_i = 1, E_0 = 20 V/m, θ_1 = 88.5^0, A_T = 1.5, $\varepsilon_n\rho_i$ = 0, B_0 = 0.10 T, time = 4 min, x/a = 0.3.

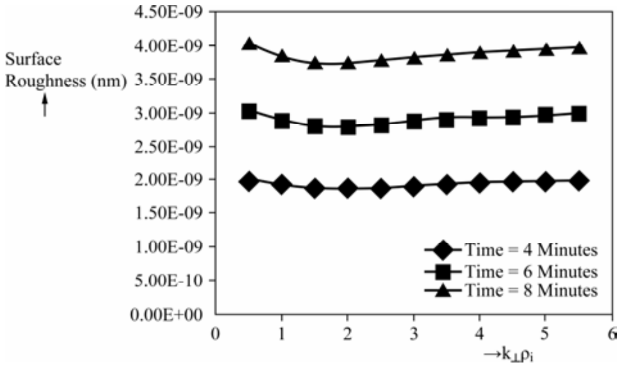

Fig. 2. Variations of surface roughness versus $k_\perp\rho_i$ for different values of time and other parameters: A_i = 0.5, T_e/T_i = 1, E_0 = 20 V/m, θ_1 = 88.5^0, A_T = 1.5, $\varepsilon_n\rho_i$ = 0, B_0 = 0.10 T, x/a = 0.3, J^+/J_F = 40.

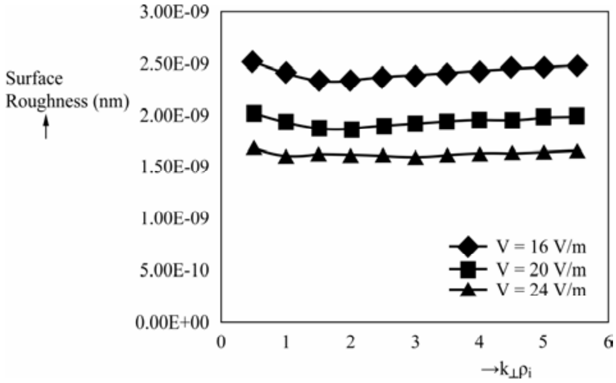

Fig. 3. Variations of surface roughness versus $k_\perp\rho_i$ for different values of electric fields and other parameters: A_i = 0.5, T_e/T_i = 1, θ_1 = 88.5^0, A_T = 1.5, $\varepsilon_n\rho_i$ = 0, B_0 = 0.10 T, x/a = 0.3, time = 4 min, J^+/J_F = 40.

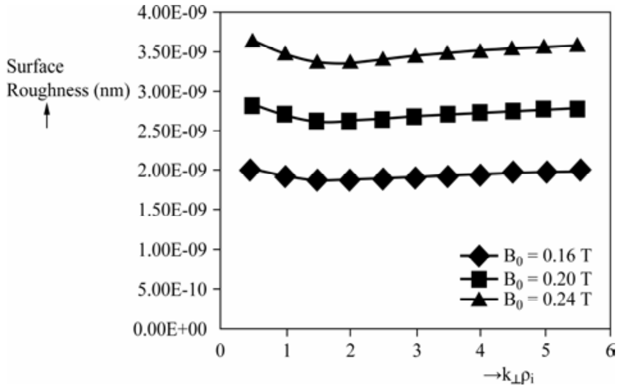

Fig. 4. Variations of surface roughness versus $k_\perp\rho_i$ for different values of magnetic field and other parameters: A_i = 0.5, T_e/T_i = 1, E_0 = 20 V/m , θ_1 = 88.5^0, A_T = 1.5, $\varepsilon_n\rho_i$ = 0, x/a = 0.3, time = 4 min, J^+/J_F = 40.

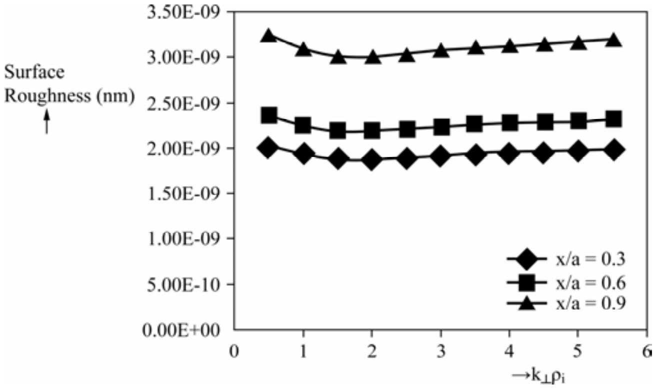

Fig. 5. Variations of surface roughness versus $k_\perp\rho_i$ for different values of inhomogeneity in DC electric field and other parameters: A_i = 0.5, T_e/T_i = 1, E_0 = 20 V/m, B_0 = 0.10 T, θ_1 = 88.5^0, A_T = 1.5, $\varepsilon_n\rho_i$ = 0, time = 4 min, J^+/J_F = 40.

the magnetic field was 0.10 T, the homogeneous DC electric field was 15 V, with other parameters also described in [5]. The value of the silicon surface roughness varied from 2 to 20 nm. The theoretical results obtained with the cited mathematical model and computer technique fit into the range of experimental results from [5].

CONCLUSIONS

This paper describes a mathematical model for valuation of the silicon surface roughness. In the framework of the given model for plasma with velocity shear instability, the ion velocity is obtained (and hence the ion kinetic energy). Then, using the pheno-menological power law for surface roughness heights from [4, 5], the dependences of the *rms* versus $k_\perp\rho_i$ for different parameters of the plasma model (magnitudes of electric and magnetic fields, inhomogeneity, etc.) were calculated and graphically plotted. The analysis carried out here shows the flexibility of using a magnetic field, an electric field and its inhomogeneity, the ratio of the ion flux to the neutral reactant flux (J^+/J_F), exposure time, as well as other parameters, so as to control the silicon surface roughness. The present study clarifies the microscopic mechanism of etching. The results of the present study can be useful for the design of a new silicon etching machine, which will work on the principle of velocity shear instability in plasma, or for increasing the effectiveness of existing machines.

ACKNOWLEDGEMENTS

I thank the reviewer for very useful suggestions and improvements in the manuscript, which have been incorporated at appropriate places.

REFERENCES

1. Greenwood J.A., Williamson J.B.P. Contact of Nominally Flat Surfaces. *Proceedings of the Royal Society of London, Series A*. 1966, **295**, 300–319.
2. Verdonck P., Plasma Etching, in *Oficina de Microfabricação: Projeto e Construção de CI´s MOS,* Swart J.W., Ed., Campinas (São Paulo, Brazil): UNICAMP, 2006, Chapter 10.
3. Flamm D.L. *Introduction to Plasma Chemistry. Plasma etching. An introduction,* D.M. Manos and D.L. Flamm, Eds., Boston-San Diego-New York: Academic press Inc., 1989. pp. 91–184.
4. Brault P., Dumas Ph. and Salvan F. Roughness Scaling of Plasma-etched Silicon Surfaces. *J. Phys.: Condens. Matter*. 1998, **10**(1), L27–L32.
5. Pétri R., Brault P., Vatel O., Henry D., André E., Dumas P., Salvan F. Silicon Roughness Induced by Plasma Etching. *J. of Applied Physics*. 1994, **75**(11), 7498–7506.
6. Economou D.J. and Alkire R.C. A Mathematical Model for a Parallel Plate Plasma Etching Reactor. *J. Electrochem.Soc.: Solid State Science and Technology*. 1988, **135**(11), 2786–2794.
7. Tyagi R.K., Srivastava K.K., Pandey R.S. Non Tradition Machining Processes by Means of Velocity Shear Instability in Plasma. *Surface Engineering and Applied Electrochemistry*. 2012, **48**(1), 64–68.
8. Tyagi R.K., Srivastava K.K., Pandey R.S. Analysis of Electrostatic Ion-cyclotron Instability Driven by Parallel Flow Velocity Shear. *Surface Engineering and Applied Electrochemistry*, 2011, **47**(4), 370–377.
9. Slătineanu L., Coteață M., Dodun O., Iosub A., Apetrei L. Impact Phenomena in the Case of Some Nontraditional Machining Processes. *Int. J. Mater. Form.* 2008, **1**(1), 1391–1394.

Received 19.03.12
Accepted 14.06.12

Реферат

Теоретическое исследование поверхности монокристаллического кремния с индуцированными SF_6 плазмой шероховатостями осуществлено с помощью атомно-силовой микроскопии. Плазма, содержащая неустойчивость сдвига скорости, была использована для изучения связи между параметрами плазмы и соответственно параметрами шероховатой поверхности. Шероховатость поверхности была исследована в зависимости от параметров эксперимента. Результаты, полученные в теоретических расчетах, совпадают с экспериментальными результатами. Количественно выполнен учет влияния таких параметров плазмы, как отношение потока ионов к нейтральному потоку реагента (J^+/J_F), время экспозиции, постоянное электрическое поле, магнитное поле и неустойчивость в DC электрическом поле. Теоретическое исследование показывает, что шероховатость поверхности кремния увеличивается при увеличении значения J^+/J_F, времени экспозиции, магнитного поля, неоднородности в постоянном электрическом поле и уменьшается при увеличении величины постоянного электрического поля.