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SIMULATION OF Si AND SiO$_2$ ETCHING IN CF$_4$ + H$_2$ PLASMA

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The reactive ion etching of silicon and silicon oxide in $CF_4 + H_2$ plasma is considered by the proposed model, which includes processes of adsorption, chemical reactions, desorption, sputtering, and stochastic mixing. The etching rates are calculated as functions of concentrations of chemically active and inactive plasma components and ion bombardment parameters. The chemical composition of $CF_4 + H_2$ plasma is calculated to achieve the goal. It is found that the reaction products and CF_2 radicals cover the silicon surface. CF_2 radicals penetrate in the bulk and form an altered layer in the near-surface region. At high H_2 content in the feed (>30%), the deposition of fluorocarbon polymer takes place. Meanwhile, the concentrations of adsorbed layer components are low during SiO_2 etching in $CF_4 + H_2$ plasma.

Keywords: $CF_4 + H_2$ plasma, Si, SiO_2, reactive ion etching

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1. Introduction

Selective etching of silicon oxide over silicon or silicon nitride in fluorocarbon plasmas is widely used in integrated circuit manufacture. Fluorocarbon plasmas produce CF_x ($x \leq 3$) radicals that polymerize on surfaces in contact with the plasma. Oxygen from the SiO_2 surface, aided by ion bombardment, prevents the build-up of polymer and allows net etching. The lack of oxygen, on the other hand, permits polymer deposition on the silicon surface and promotes selectivity [1–3].

The fluorocarbon layer is formed on both SiO_2 and Si surfaces during etching in $CF_4 + H_2$ plasma. The thickness of the fluorocarbon layer on SiO_2 is much smaller than on Si for comparable discharge conditions [4, 5]. During Si etching in $CF_4 + H_2$ plasma the adsorption of CF_2 radicals on the Si surface is enhanced by ion bombardment, i. e. the sticking coefficient of CF_2 radicals on the Si surface is increased in the presence of ion bombardment [6]. Meanwhile, the fluorocarbon film is thin on the SiO_2 surface as adsorbed CF_x ($x \leq 3$) radicals react with surface oxygen to form volatile CO, CO_2, and COF_2 molecules. These phenomena are used in the selective etching of SiO_2 layers on a Si surface. As the SiO_2 layer is etched, the underlying Si is etched slowly. In this way, the fixed depth trenches and contact holes are formed.

In this work, the main reactions occurring in $CF_4 + H_2$ plasma are considered and the concentrations of plasma components are calculated by extrapolation from experimental data. Using the derived composition of the flux of particles from the plasma, reactive ion etching (RIE) of Si and SiO_2 is investigated. It is found that CF_2 radicals penetrate in silicon bulk and form an altered layer in the near-surface region. Low SiO_2 surface coverage by the reaction products and CF_2 radicals is confirmed.

2. Modelling of Si and SiO$_2$ etching in CF$_4$ + H$_2$ plasma

2.1. *Modelling of chemical composition of CF$_4$ + H$_2$ plasma*

The chemical composition of $CF_4 + H_2$ plasma is considered. Specific reactions in $CF_4 + H_2$ plasma are reactions of CF_x ($x \leq 3$) radicals with H atoms [7–9]. In order to reduce the number of frequency probabilities only the main reactions are included in the model:

$$CF_4 + e \rightarrow CF_3 + F + e, \tag{1.1}$$

$$H_2 + e \rightarrow 2H + e, \tag{1.2}$$

$$F + H_2 \rightarrow HF + H, \tag{1.3}$$

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$$CF_3 + F + M \rightarrow CF_4 + M, \quad (1.4)$$

$$CF_3 + H \rightarrow CF_2 + HF, \quad (1.5)$$

$$H + F + M \rightarrow HF + M, \quad (1.6)$$

$$2H + M \rightarrow H_2 + M. \quad (1.7)$$

Reaction rates are characterized by frequency probabilities of dissociation G_i and reaction R_{ij}:

$$G_1 = \frac{g_1[\mathrm{e}]}{N}, \quad (2.1)$$

$$G_2 = \frac{g_2[\mathrm{e}]}{N}, \quad (2.2)$$

$$R_{25} = k_3, \quad (2.3)$$

$$R_{35} = \frac{k_4[\mathrm{M}]}{N}, \quad (2.4)$$

$$R_{36} = k_5, \quad (2.5)$$

$$R_{56} = \frac{k_6[\mathrm{M}]}{N}, \quad (2.6)$$

$$R_{66} = \frac{k_7[\mathrm{M}]}{N}, \quad (2.7)$$

where g_i is the dissociation rate constant of the ith reaction, N is the total neutral particle concentration in the plasma, k_i is the reaction rate constant of the ith reaction, and M is a third particle or the wall of the reactor. Let us assume that frequency probabilities of dissociation and reaction do not depend on H_2 content in the feed.

It follows that seven chemical species exist in the plasma: CF_4, H_2, CF_3, CF_2, F, H, and HF, with relative concentrations $n_1 = [CF_4]/N$, $n_2 = [H_2]/N$, $n_3 = [CF_3]/N$, $n_4 = [CF_2]/N$, $n_5 = [F]/N$, $n_6 = [H]/N$, and $n_7 = [HF]/N$, respectively. The following system of rate equations describes the kinetics of chemical composition of CF_4 + H_2 plasma:

$$\frac{\mathrm{d}n_1}{\mathrm{d}t} = I_1 - G_1 n_1 + R_{35} n_3 n_5 - E n_1, \quad (3.1)$$

$$\frac{\mathrm{d}n_2}{\mathrm{d}t} = I_2 - G_2 n_2 - R_{25} n_2 n_5 + R_{66} n_6^2 - E n_2, \quad (3.2)$$

$$\frac{\mathrm{d}n_3}{\mathrm{d}t} = G_1 n_1 - R_{35} n_3 n_5 - R_{36} n_3 n_6 - E n_3, \quad (3.3)$$

$$\frac{\mathrm{d}n_4}{\mathrm{d}t} = R_{36} n_3 n_6 - E n_4, \quad (3.4)$$

$$\frac{\mathrm{d}n_5}{\mathrm{d}t} = G_1 n_1 - R_{25} n_2 n_5 - R_{35} n_3 n_5 - R_{56} n_5 n_6 - E n_5, \quad (3.5)$$

$$\frac{\mathrm{d}n_6}{\mathrm{d}t} = 2G_2 n_2 + R_{25} n_2 n_5 - R_{36} n_3 n_6 - R_{56} n_5 n_6 - 2R_{66} n_6^2 - E n_6, \quad (3.6)$$

$$\frac{\mathrm{d}n_7}{\mathrm{d}t} = R_{25} n_2 n_5 + R_{36} n_3 n_6 + R_{56} n_5 n_6 - E n_7, \quad (3.7)$$

where $I_i = \Phi_i/(V_0 N)$ is the injection rate of the ith component of gas mixture, E is the frequency probability of exhaust, Φ_i is the flow rate of the ith component, and V_0 is the volume of the reactor.

2.2. *Modelling of Si etching*

The RIE of a Si substrate in CF_4 + H_2 plasma is considered. The relative concentrations of plasma components calculated from the previous model of plasma composition are used for the calculation of the etching rates. The main reactions taking place on the surface are the following:

$$Si + 4F \rightarrow SiF_4, \quad (4.1)$$

$$2Si + 2CF_3 \rightarrow SiF_4 + SiF_2 + 2C, \quad (4.2)$$

$$Si + 2CF_2 \rightarrow SiF_4 + 2C, \quad (4.3)$$

$$Si + CF_2 \rightarrow Si - CF_2, \quad (4.4)$$

$$CF_2(s) + CF_2 \rightarrow CF_2 - CF_2(s). \quad (4.5)$$

Reactions (4.1)–(4.3) are characterized by reaction rate constants k_1, k_2, and k_3, and reactions (4.4) and (4.5) by sticking coefficients α_{43} and α_{44}. The relative flux of ith type plasma species to the surface is equal to $S_{i,0} = J_{i,0}/C$, where $J_{i,0} = n_i N[kT/(2\pi m_i)]^{1/2}$ is the flux of ith type species, k is the Boltzmann constant, T is temperature, m_i is the mass of ith type species, and $C = 1.36 \cdot 10^{19}\ \mathrm{m}^{-2}$ is the concentration of surface atoms. Let us assume that C atoms produced during reactions (4.2) and (4.3) do not stick on the surface or form clusters that occupy small surface area [10].

The reaction products desorb and are sputtered by incident ions. The frequency probability of removal of

ith adsorbed layer component ω_i consists of frequency probabilities of desorption and sputtering:

$$\omega_i = \omega_{i,\mathrm{d}} + \omega_{i,\mathrm{s}} = \nu_0 \exp\left(-\frac{E_{i,\mathrm{d}}}{kT}\right) + \frac{Y_i I_0}{C}, \tag{5}$$

where ν_0 is the frequency of oscillation of atoms in the solid, and $E_{i,\mathrm{d}}$ is the desorption activation energy of ith type molecules, Y_i is the sputtering yield of the ith component, I_0 is the ion flux. Let us assume that ions have the same energy and strike the surface perpendicularly. As the processes of adsorption and removal take place simultaneously, the stochastic mixing between monolayers (ML) occurs. When a particle is adsorbed on the surface, a particle of kth monolayer is transferred into $(k+1)$th monolayer, and when a particle is removed from the surface, a particle of kth monolayer is transferred into $(k-1)$th monolayer.

Chemically neutral components produced during reactions on the surface are included in the adsorbed layer of one-monolayer thickness. It follows that two components exist in the adsorbed layer: SiF_2 and SiF_4, with relative concentrations $c_1 = [\mathrm{SiF_2}]/C$ and $c_2 = [\mathrm{SiF_4}]/C$; two components exist on the surface: Si and CF_2, with relative concentrations $c_3 = [\mathrm{Si}]/C$ and $c_4 = [\mathrm{CF_2}]/C$. The relative concentrations of surface components must fulfill the condition $c_1 + c_2 = 1$. The following system of equations includes rate expressions of different processes [11, 12] and describes the kinetics of component concentrations in the adsorbed layer and in the near-surface region:

$$\frac{\mathrm{d}c_1}{\mathrm{d}t} = \frac{k_2 \beta c_3^{(1)} n_3}{2} - \omega_1 c_1, \tag{6.1}$$

$$\frac{\mathrm{d}c_2}{\mathrm{d}t} = k_1 \beta c_3^{(1)} n_5^4 + \frac{k_2 \beta c_3^{(1)} n_3}{2} + k_3 \beta c_3^{(1)} n_4^2 - \omega_2 c_2, \tag{6.2}$$

$$\frac{\mathrm{d}c_3^{(1)}}{\mathrm{d}t} = \omega_4 c_3^{(2)} - \alpha_{43} \beta c_3^{(1)} n_4, \tag{6.3}$$

$$\frac{\mathrm{d}c_3^{(k)}}{\mathrm{d}t} = -(V_\mathrm{A} + V_\mathrm{S}) c_3^{(k)} + V_\mathrm{A} c_3^{(k-1)} + V_\mathrm{S} c_3^{(k+1)}, \quad k \geq 2, \tag{6.4}$$

where $\beta = 1 - \Theta$ is the fraction of the surface not covered with adsorbate, $\Theta = \sum_{i=1}^{4} c_i$ is the surface coverage, and n_i is the relative concentration of the ith plasma component, $V_\mathrm{A} = \alpha_{43} c_3^{(1)} n_4 + \alpha_{44} c_4^{(1)} n_4$ is the adsorption rate, and $V_\mathrm{S} = \omega_1 c_1 + \omega_2 c_2 + \omega_4 c_4^{(1)}$ is the removal rate. The etching rate V is proportional to the difference of removal and adsorption rates:

$$V = h_0 (V_\mathrm{S} - V_\mathrm{A}) \tag{7}$$

where $h_0 = 2.72$ Å is the monolayer thickness, which is estimated using the expression $h_0 = [M_\mathrm{Si}/(\rho_\mathrm{Si} N_\mathrm{A})]^{1/3}$, where $M_\mathrm{Si} = 2.809 \cdot 10^{-2}$ kg/mol is the atomic weight of Si, $\rho_\mathrm{Si} = 2330$ kg/m^3 is the density of Si, and N_A is Avogadro's number.

2.3. Modelling of SiO_2 etching

The RIE of a SiO_2 film in CF_4 + H_2 plasma is considered. The relative concentrations of plasma components calculated from the previous model of plasma composition are used for the calculation of the etching rates. The main reactions taking place on the surface are the following:

$$2\mathrm{SiO_2} + 2\mathrm{CF_3} \to \mathrm{SiF_2} + \mathrm{SiF_4} + 2\mathrm{CO_2}, \tag{8.1}$$

$$\mathrm{SiO_2} + 2\mathrm{CF_2} \to \mathrm{SiF_4} + 2\mathrm{CO}. \tag{8.2}$$

These reactions are characterized by reaction rate constants k_1 and k_2, respectively. Chemically neutral components produced during reactions on the surface are included in the adsorbed layer of one monolayer thickness. It follows that four components exist in the adsorbed layer: SiF_2, SiF_4, CO, and CO_2, with relative concentrations $c_1 = [\mathrm{SiF_2}]/C$, $c_2 = [\mathrm{SiF_4}]/C$, $c_3 = [\mathrm{CO}]/C$, and $c_4 = [\mathrm{CO_2}]/C$, where $C = 8.90 \cdot 10^{18}$ m^{-2} is the concentration of surface molecules. The following system of equations includes rate expressions of different processes [11, 13] and describes the kinetics of component concentrations in the adsorbed layer:

$$\frac{\mathrm{d}c_1}{\mathrm{d}t} = k_1 \beta n_3^2 - \omega c_1, \tag{9.1}$$

$$\frac{\mathrm{d}c_2}{\mathrm{d}t} = k_1 \beta n_3^2 + k_2 \beta n_4^2 - \omega c_2, \tag{9.2}$$

$$\frac{\mathrm{d}c_3}{\mathrm{d}t} = 2 k_2 \beta n_4^2 - \omega c_3, \tag{9.3}$$

$$\frac{\mathrm{d}c_4}{\mathrm{d}t} = 2 k_1 \beta n_3^2 - \omega c_4. \tag{9.4}$$

The surface concentrations of components under steady-state conditions are equal to

$$c_{1,\mathrm{St}} = \frac{k_1 n_3^2}{4k_1 n_3^2 + 3k_2 n_4^2 + \omega}, \qquad (10.1)$$

$$c_{2,\mathrm{St}} = \frac{k_1 n_3^2 + k_2 n_4^2}{4k_1 n_3^2 + 3k_2 n_4^2 + \omega}, \qquad (10.2)$$

$$c_{3,\mathrm{St}} = \frac{2k_2 n_4^2}{4k_1 n_3^2 + 3k_2 n_4^2 + \omega}, \qquad (10.3)$$

$$c_{4,\mathrm{St}} = \frac{2k_1 n_3^2}{4k_1 n_3^2 + 3k_2 n_4^2 + \omega}. \qquad (10.4)$$

The etching rate is proportional to the removal rate of formed SiF_2 and SiF_4 molecules. According to Eqs. (10.1) and (10.2) the etching rate under steady-state conditions is equal to

$$V_{\mathrm{St}} = \frac{h_0 \omega (2k_1 n_3^2 + k_2 n_4^2)}{4k_1 n_3^2 + 3k_2 n_4^2 + \omega}, \qquad (11)$$

where $h_0 = 3.35$ Å is the monolayer thickness.

3. Results and discussion

3.1. Chemical composition of CF_4 + H_2 plasma

The experimentally measured dependences of relative concentrations of H_2 and HF molecules in CF_4 + H_2 plasma on H_2 content in the feed [7] are used for calculating the chemical composition of CF_4 + H_2 plasma. This experiment is chosen because of mass spectrometry measurements of plasma composition. It is assumed that the flow rate of gas mixture is 30 sccm, the pressure is 133 Pa, the reactor volume is $1.3 \cdot 10^{-4}$ m^{-3}, and the plasma temperature is 500 K. The total gas injection rate of 5.47 s^{-1} is estimated using the expression $I = \Phi/(V_0 N)$, where $N = 1.93 \cdot 10^{22}$ m^{-3} is the total neutral particle concentration, and the flow rate Φ is measured in molecules/s.

Experimental [7] and theoretical dependences of the relative concentration of H_2 and HF molecules in the plasma on H_2 content in the feed calculated using Eq. (3) under steady-state conditions are shown in Fig. 1. The following values of frequency probabilities of dissociation and reaction are used: $G_1 = 3.7$ s^{-1}, $G_2 = 2.0$ s^{-1}, $R_{25} = 1.0 \cdot 10^4$ s^{-1}, $R_{35} = 100$ s^{-1}, $R_{36} = 2.0 \cdot 10^4$ s^{-1}, $R_{56} = 1.0 \cdot 10^4$ s^{-1}, $R_{66} = 100$ s^{-1}, $E = 5.47$ s^{-1}. These values were determined by extrapolation from experimental results [13, 14].

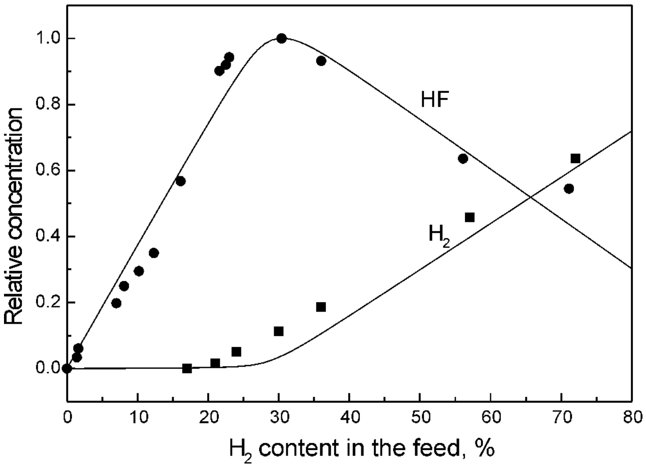

Fig. 1. Experimental [7] (points) and theoretical (curves) dependences of the relative concentrations of H_2 and HF molecules on H_2 content in the feed.

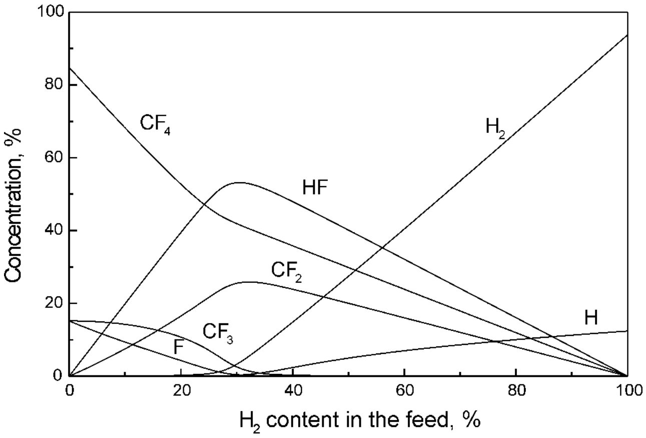

Fig. 2. The chemical composition of CF_4 + H_2 plasma as a function of H_2 content in the feed.

The chemical composition of CF_4 + H_2 plasma as a function of H_2 content in the feed calculated using Eq. (3) under steady-state conditions is shown in Fig. 2. The concentration of HF molecules with increase of H_2 content in the feed increases at first due to the reactions of H atoms with F atoms and CF_3 radicals (Eqs. (1.5) and (1.6)). As the concentration of HF molecules approaches the maximum value, almost all F atoms and CF_3 radicals have reacted (Fig. 2). With further increase in H_2 content in the feed the concentration of HF molecules starts to decrease in proportion to the amount of injected CF_4 molecules. At H_2 content in the plasma >30%, the concentration of CF_2 radicals is about 10 times higher than that of CF_3 (Fig. 2) or CF radicals [8, 9]. This indicates that the reaction of H atoms with CF_3 radicals is intensive. Due to intensive

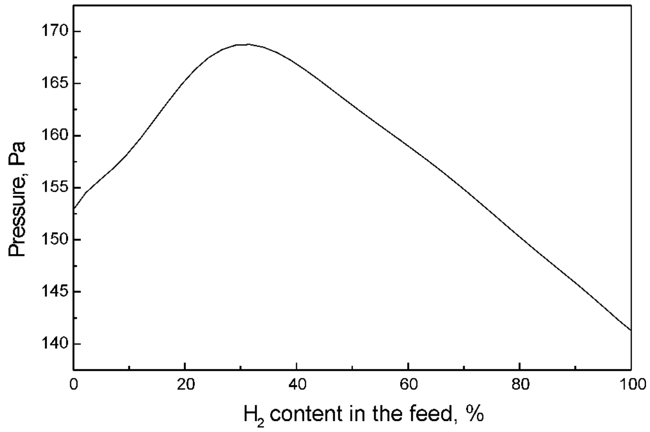

Fig. 3. The dependence of pressure on H_2 content in the feed.

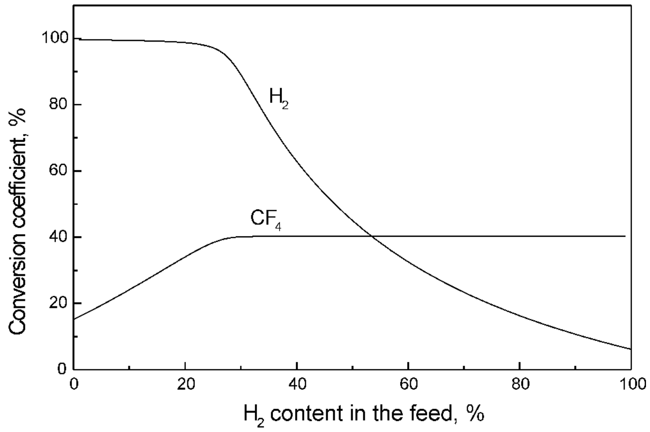

Fig. 4. The dependences of the conversion coefficients of CF_4 and H_2 molecules on H_2 content in the feed.

reactions taking place in $CF_4 + H_2$ plasma the pressure in the reactor increases (Fig. 3).

The conversion coefficient of the ith component of the gas mixture indicates the part of molecules converted to reaction products and is equal to

$$\eta_i = 1 - \frac{En_i}{I_i}. \tag{12}$$

The dependences of the conversion coefficients of CF_4 and H_2 molecules on H_2 content in the feed are presented in Fig. 4. At H_2 content in the feed $<30\%$, all H_2 molecules are converted to reaction products. The conversion coefficient of CF_4 molecules increases due to the dissociation reaction (1.1) and subsequent reaction (1.5) of H atoms with CF_3 radicals. At high H_2 content the conversion coefficient of CF_4 molecules is constant, and conversion of H_2 molecules decreases due to dilution of CF_4 gas.

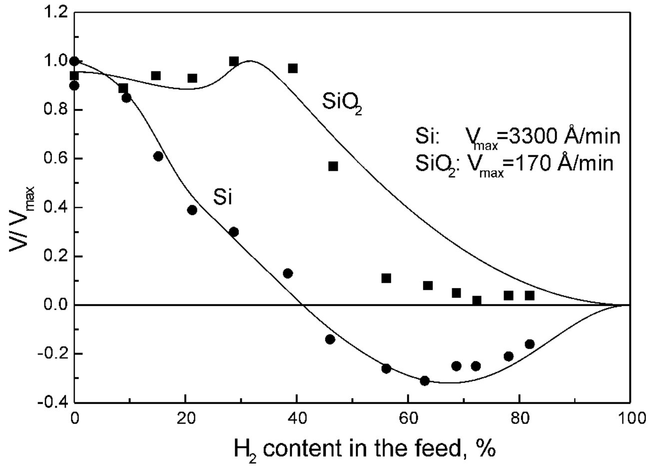

Fig. 5. Experimental [15] (points) and theoretical (curves) dependences of RIE rates of Si and SiO_2 on H_2 content in the feed.

3.2. Si etching

The experimentally measured dependence of the RIE rate of Si on H_2 content in the feed [15] is used in the model in order to calculate etching rates. Let us assume that the Si etching rate in the absence of H_2 in the feed is equal to a value measured during experiment [16]. Experimental [15] and theoretical dependences of RIE rates of Si on H_2 content in the feed calculated using Eq. (7) are shown in Fig. 5. The following values of reaction rate constants, sticking coefficients, and frequency probabilities of removal are found by extrapolation: $k_1 = 5.0{\cdot}10^7\ \mathrm{s}^{-1}$, $k_2 = 8.0{\cdot}10^4\ \mathrm{s}^{-1}$, $k_3 = 5.0{\cdot}10^4\ \mathrm{s}^{-1}$, $\alpha_{43} = 39\ \mathrm{s}^{-1}$, $\alpha_{44} = 4.0{\cdot}10^4\ \mathrm{s}^{-1}$, $\omega_1 = \omega_2 = 1200\ \mathrm{s}^{-1}$, $\omega_4 = 14\ \mathrm{s}^{-1}$. The etching rate approaches the steady-state regime within 1 s. It is important to note that the sticking coefficient of CF_2 radicals from the plasma on CF_2 radicals on the surface is three orders higher than on Si atoms. Due to preferential sticking the concentration of CF_2 radicals on the surface is low (Fig. 6), and the etched surface is rough. The obtained results are in agreement with the experimental measurements [17].

The dependences of the concentrations of adsorbed layer components on H_2 content in the feed are shown in Fig. 6. The minimum is observed in the dependence of concentration of SiF_4 molecules on H_2 content in the feed. It is a result of simultaneous formation of SiF_2 and SiF_4 molecules (Eq. (4.2)). Concentrations of CF_2 radicals in the near-surface region at different H_2 content in the feed are shown in Fig. 7. It is observed that the thickness of the altered layer increases with the increase of H_2 content in the feed due to increased flux of CF_2 radicals to the surface. The concentration of CF_2 radi-

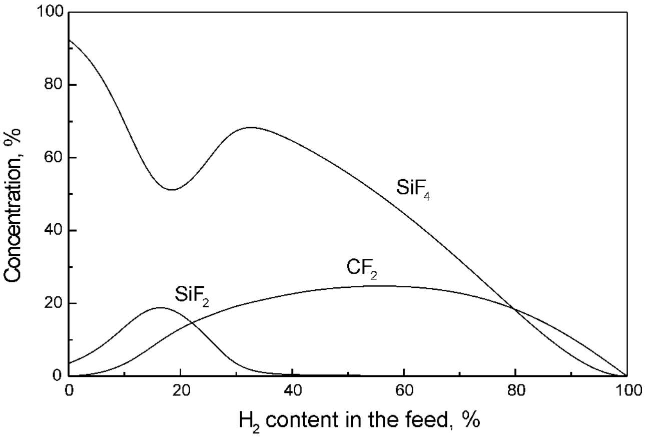

Fig. 6. The dependences of the concentrations of adsorbed layer components on H_2 content in the feed during RIE of silicon in $CF_4 + H_2$ plasma.

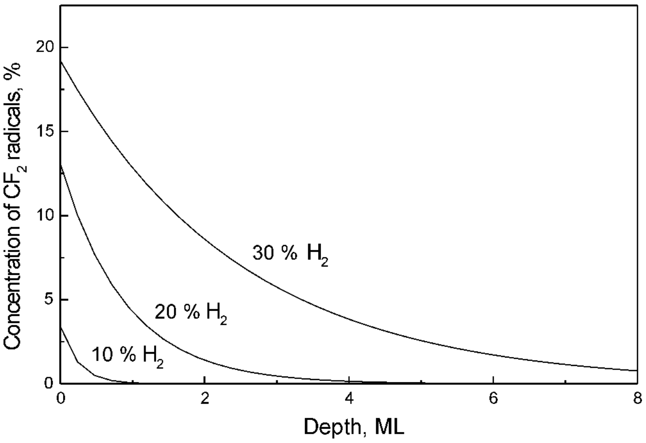

Fig. 7. Concentrations of CF_2 radicals in the near-surface region at different H_2 content in the feed.

cals in the near-surface region does not change during the deposition of the fluorocarbon film.

3.3. SiO_2 etching

The experimentally measured dependence of the RIE rate of SiO_2 on H_2 content in the feed [15] is used in the model in order to calculate etching rates. Let us assume that the SiO_2 etching rate in the absence of H_2 in the feed is equal to a value measured during experiment [16]. Experimental and theoretical dependences of RIE rates of SiO_2 on H_2 content in the feed calculated using Eq. (11) are shown in Fig. 5. The following values of reaction rate constants and frequency probability of removal are used: $k_1 = 19$ s^{-1}, $k_2 = 14$ s^{-1}, $\omega = 10$ s^{-1}. These values were determined by extrapolation from experimental results [13].

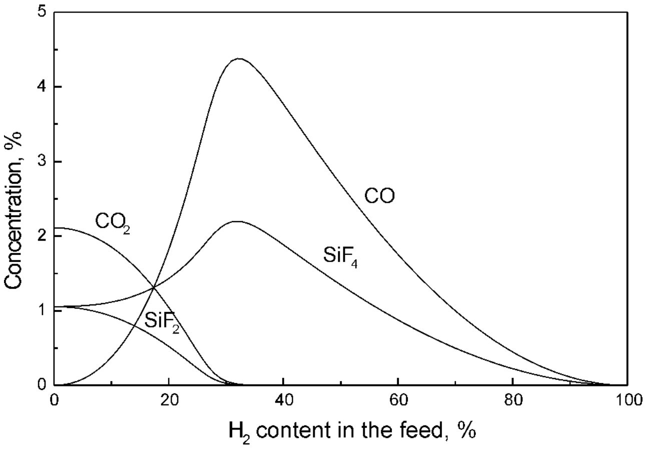

Fig. 8. The dependences of the concentrations of adsorbed layer components on H_2 content in the feed during RIE of SiO_2 in $CF_4 + H_2$ plasma.

The dependences of the concentrations of adsorbed layer components on H_2 content in the feed are shown in Fig. 8. It is observed that the concentrations of adsorbed layer components are low. The dependences of concentrations of CO_2 and SiF_2 molecules are similar to the dependence of the concentration of CF_3 radicals in the plasma. It is influenced by the same reaction of CF_3 radicals with SiO_2 molecules (Eq. (8.1)). The maxima of the concentrations of CO and SiF_4 molecules are achieved at the maximum concentration of CF_2 radicals in the plasma. The obtained results are in agreement with the experimental measurements [6, 18].

4. Conclusions

1. In $CF_4 + H_2$ plasma at H_2 content in the feed $<30\%$, all H_2 molecules are converted to reaction products. It is a result of intensive dissociation and subsequent reaction of H atoms with CF_3 radicals.

2. During RIE of Si in $CF_4 + H_2$ plasma CF_2 radicals penetrate in the bulk and form an altered layer in the near-surface region. The thickness of the altered layer increases with the increase of H_2 content in the feed due to increased flux of CF_2 radicals to the surface.

3. During RIE of SiO_2 in $CF_4 + H_2$ plasma the concentrations of adsorbed layer components are low.

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Si IR SiO_2 ĖSDINIMO $CF_4 + H_2$ PLAZMOJE MODELIAVIMAS

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Santrauka

Išnagrinėtas silicio ir silicio oksido reaktyvus joninis ėsdinimas $CF_4 + H_2$ plazmoje. Pasiūlytame modelyje atsižvelgta į įgerties, cheminių reakcijų, atvirkštinės gerties, dulkėjimo ir stochastinio maišymo vyksmus. Ėsdinimo spartos vertės apskaičiuotos kaip chemiškai aktyvių ir neaktyvių plazmos sandų koncentracijų bei joninio apšaudymo parametrų funkcija. Tikslui pasiekti apskaičiuota $CF_4 + H_2$ plazmos cheminė sudėtis. Rasta, kad reakcijos produktai ir CF_2 radikalai dengia silicio paviršių. CF_2 radikalai prasiskverbia į tūrį ir sudaro pakeistą sluoksnį. Esant dideliam H_2 kiekiui įleidžiamame mišinyje (>30%), susidaro fluorokarboninis polimeras. Tačiau silicio oksido ėsdinimo $CF_4 + H_2$ plazmoje metu įgerto sluoksnio sandų koncentracijos yra mažos.