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Effect of reactant transport on the trench profile evolution for silicon etching in chlorine plasmas

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ABSTRACT

A sheath is generated over the rf biased substrate in etching processes, its properties play an important role in determining the transport of reactant species including ions and neutrals toward the substrate, as well as the surface reactions, and as a consequence the evolution of the etching profile. In this work, a multi scale model including the global, sheath and trench model is applied to simulate dry etching processes in nano-patterned samples. First, the global model gives the discharge parameters in chamber. Sheath properties in terms of external discharge parameters are decided using the sheath model, the reactant transports in sheath to trench surface are then obtained. At last, based on the surface reaction model and cellular removal algorithm, the evolution of trench profile is simulated. Influences of different discharge parameters like pressure and bias voltage on microscopic non-uniformity generation during etching are studied for better understanding of etching mechanism. Results show that the profiles have different evolution processes under various discharge conditions. Specially, the directionality, charging induced distortion and reflection for ions determine the profile of micro-trenching. Besides, neutral coverage associated with pressure and pattern geometry can influence the local etch rate, further decide the formation of RIE lag, undercut and bowing.

1. Introduction

Plasma etching has been widely used in semiconductor industry as one of the key surface processes. Because the nano- and micro-electronic devices demand increasing shrinkage of the critical dimension (CD) in integrated circuit (IC) fabrication, further understanding of the etching progress for better pattern transfer fidelity in the anisotropy etching procedure is required. As the complexity of the multi-scale, the synergistic effects between physical and chemical processes in etching, numerical simulations have been an effective tool to achieve better understanding, realize optimization of processing and design reactors with less cost.

In recent decades, lots of experimental and numerical works have been done to study the etching progress in feature scale. Early works gave perspectives into the surface kinetic reactions of the ion enhanced etching processes [1–3]. Coburn *et al.* studied the ion enhanced gas-surface chemical reaction exposed to halogen containing radicals with beam experiment [1]. Chang *et al.* performed the beam scattering for silicon etching under chlorine plasma and studied the etch yield in dependence of the ion impact energy, incident angle and neutral-to-ion flux ratio [3]. In order to study the intrinsic nature and mechanism of various factors involved in the surface reaction, Monte-Carlo (MC) or Molecular Dynamics (MD) methods were developed [4–7]. While for the feature scale profile evolution study, with the surface reaction models, different surface advancement calculations like string [8,9], level set [10], cell represent [5,6,11,12], and even atomic scale [13,14] methods were developed. In addition, microscopic mechanisms like ion scattering [5,6,11,15–17], charging [18] were coupled to consider the control of pattern profile morphology. Mahorowala *et al.* gave a detailed description on the feature charging calculations capable of both insulating and resistive features [18]. In a recent work, Saussac *et al.* proposed a robust cell removal method to achieve the profile simulation where a Gaussian angular distribution was assumed, the computational cost was acceptable [11].

Besides the surface chemical reactions, ion energy and angular distributions and reactant fluxes arriving at the etched material are also very important for the value of etching rate, and consequently they can influence the pattern profile evolution progress.

In the anisotropy etching, in order to achieve high anisotropy, ions are preferred to have less dispersive angular distributions. The energetic ions can activate and enhance the surface reaction by influencing the adsorption and desorption of the neutral radicals at the surface layer, stripping off the etched material with depletion of

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neutrals there. Thus, they determine the selectivity, etch rate, and finally the pattern profile. Therefore, the transport of ions and neutrals through the sheath to feature, or the ion energy, ion angle, neutral energy, and neutral angle distributions (IEDs, IADs, NEDs and NADs), these distributions and also the ion and neutral fluxes arriving at the feature surface are crucial for etching profile evolution.

The reactant fluxes are mainly decided by the discharge parameters in chamber, while energy and angular distributions to the feature for reactant species are determined mainly by the time varying sheath properties, which are decided by discharge parameters in chamber, and also, the external discharge conditions. Therefore, we have to combine reactor, sheath, and trench scale model together in order to study the evolution progress in consistent with the discharge parameters.

We notice only a few studies combined the ion energy and angular distributions derived from a sheath or reactor scale model with the etching profile evolution simulator [10,16,19–21]. Hoekstra *et al.* coupled a Monte-Carlo feature profile model [20] to the HPEM model (Hybrid Plasma Equipment Model) to study etching profiles with subwafer and superwafer topography. And in their later work [16], the micro-trenching caused by specular reflection was studied. But influences of factors like charging, local surface coverage had not been discussed yet. Vyvoda *et al.* coupled a string-type feature model to a reactor scale model to study the ion scattering behavior, however, the local charging was neglected [17].

In this paper, transport of reactant particles including ions and neutrals in both sheath and trench are considered to predict the trench profile evolution progress, and the discharge parameters in reactor are given by a global model. The global and sheath model are first used to consider the fluxes, energy and angular distributions for reactants arriving at the substrate. Their motions and distributions at feature surface are further simulated in trench model, where charging to the insulating mask surface is coupled to consider ion trajectory distortion in local electric field. Finally, by combining a surface reaction model including the consideration of the neutral coverage with a cell removal method, we simulated the profile evolution progress under different discharge parameters for silicon etching in chlorine based plasmas.

The paper is organized as follows: the detailed model descriptions are presented in next section. The results and discussion are shown in Sec. 3 and conclusions are given in Sec. 4.

2. Model descriptions

2.1. Global model

In this paper, we study the etching of poly-silicon masked by the insulating photoresist under fluxes of chlorine ions and neutral radicals. As the trench dimension we considered is much smaller than the sheath thickness, which is also small compared to the reactor scale in a typical low pressure, high density plasma rector. The combination of 0D (0 dimensional) reactor scale model, the 1D sheath model and 2D trench model is sufficient to simulate the trench profile evolution.

From 1990s the global model have been gradually developed into a convenient choice for reactor scale modeling with considering the chemical reactions in chamber, the spatial and temporal averaged species densities and electron temperature can be solved by numerical methods for multi species gas discharge [22,23,26]. Thorsteinsson *et al.* used the global model to conduct a serious of studies considering varied gas or electrical modulate, here we mainly use the method described in detail in Refs. [24] for the chlorine discharge. But we neglected the vibration excited state for molecular chlorine.

The particle balance and the power balance equations are solved using numerical methods, the volume averaged reactant densities and electron temperature are solved. And we further derive parameters having direct influences on the sheath and trench simulation. The species fluxes at plasma-sheath edge are important for the simulation of the sheath properties, as well as the trench etching. They are decided not only by the volume averaged densities, but also the edge-to-center density ratios for ions. Besides, the ion temperature has influences on the ion directionality as the temperature can reach up to 0.5 eV in low pressure condition. There are also other factors such as electronegativity at sheath edge, the gas temperature and so on. In this paper we choose a typical inductively coupled plasma (ICP) reactor as the source for chlorine plasma.

2.2. Sheath model

In order to achieve independent control of plasma generation and ion bombardment in low pressure, high density plasma sources, a separate rf bias is usually applied to the substrate electrode. At the adjacent area of the substrate placed on the bias electrode, there will be a sheath formed in which ions get the energies for surface processing. Ion transport in sheath is important for the ion fluxes and velocities arriving at the substrate, and thus further influence the processing of etching or deposition.

In this section, a hybrid sheath model in combination of a fluid method with Monte-Carlo method is described. First, the fluid model is used to calculate the spatial and temporal profiles for variables like electric potential, sheath thickness, electron density, and ion density in the sheath. With the derived results, the Monte-Carlo method is applied to consider the ion neutral collisions and we get the energy and angular distributions for ions.

2.2.1. Fluid equations

In electronegative plasmas, one of the key parameters describing the negativity is the density ratio of negative ions to electrons defined as $\alpha_s \equiv n_-/n_e$ another parameter is the temperature ratio of electrons to ions which is defined as $\gamma = T_e/T_i$. These variables under various discharge conditions need to be given from a reactor scale model, which is the global model in this study.

For either positive or negative ions, as the thermal velocity is much smaller than the drifting velocity in sheath region, ion velocity $u(x,t)$, ion density $n(x,t)$ and the electric potential $V(x,t)$ satisfy the cold fluid equations including the continuum and momentum balance equations:

$$\frac{\partial u_\alpha}{\partial t} + u_\alpha \frac{\partial u_\alpha}{\partial x} = -\frac{e}{m}\frac{\partial V}{\partial x} - \nu u_\alpha \tag{1}$$

$$\frac{\partial n_\alpha}{\partial t} + \frac{\partial (n_\alpha u_\alpha)}{\partial x} = 0 \tag{2}$$

where subscript α represents either positive when $\alpha \equiv +$ or negative chlorine ions when $\alpha \equiv -$, ν is the collision frequency between ion and neutrals.

For electrons, we assume that they have sufficient collisions so that we apply the isotropic thermal equilibrium condition: the velocity satisfies the Maxwellian velocity distributions and the electron density $n_e(x,t)$ satisfies the Boltzmann relation:

$$n_e(x,t) = n_0 \exp\left(\frac{eV(x,t)}{k_B T_e}\right) \tag{3}$$

where n_0 is the density of bulk plasma, e is the element charge, k_B is the Boltzmann constant and T_e is the electron temperature.