

Stability analysis of reactive sputtering process with variable sticking coefficients

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Abstract

In reactive sputtering, the introduction of reactive gas would create a hysteresis transition from metal to compound mode in both the target and the substrate. The hysteresis transition is characterized by a sudden change in partial pressure, sputtering rate and fraction of compound formation, etc. Therefore, the stability is an important issue of process control. In this paper, a mathematical model with variable sticking coefficients based on surface kinetics is introduced to study the process stability. The variable sticking coefficient represents different mechanisms for surface reactions from the type of Langmuir to precursors. To facilitate the analysis, several nondimensional parameters are introduced and used for formulation. Results show that, when the chemical reaction on a substrate is moderate, a higher sputtering yield of the compound leads to a more stable steady-state at lower inflow rates. However, when the ratio of sputtering yield (compound/metal) is zero, there is no hysteresis transition because of the deposition of pure metal (single phase) on the substrate. For different sticking mechanisms, the precursor type is found to make the surface easier to saturate with compound due to its higher default sticking coefficient and the lower pressure and inflow rate for the hysteresis transition.

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1. Introduction

Reactive sputtering is a very important PVD process in thin film deposition particularly for producing complex compound films such as oxides, nitrides or carbides. Due to tremendous applications of these films, the process is extensively used in manufacturing the semiconductor and display devices [1–3]. Numerous studies [4–7] have shown that the hysteresis transition between the metallic and compound modes at the target surface is one characteristic feature of the reactive sputtering process. This hysteresis behavior is due to the introduction of reactive gas and commonly described by an abrupt change in deposition rate, film composition, partial pressure of the reactive gas and cathode voltage [6–10]. The first trial to model this phenomenon was originally proposed by Berg et al. [11–

13]. In their studies, a mass balance for the reactive gas in the chamber including absorption and sputtering at the surfaces of target and substrate was considered at first. The deposition rate and film compositions were then calculated as a function of inflow rate of reactive gas. This model successfully depicts the hysteresis transition by some simple but sound physical effects. However, one assumption of constant sticking coefficients made for the surface reactions with reactive gas typically leads to an underestimate of real situations. It is therefore necessary to investigate the issue based upon the theory of surface kinetics for chemical reactions. A variable sticking coefficient as a function of compound fraction is then proposed and discussed thoroughly.

In this study, we first establish formulae for reactive sputtering based on Berg's model and then recast the non-linear ordinary differential equations in terms of several nondimensional parameters. The steady-state solutions are then solved in details with the variable sticking coefficients. Finally, the influence of different sticking mechanisms on the steady-state solutions is carefully examined.

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2. Rate equations based on Berg's model

2.1. Rate equations for pressure and compound fractions

A typical reactive sputtering system is schematically shown in Fig. 1 where A_i and θ_i is the area and surface fraction of compounds at the target (t) and substrate (s), respectively. For simplification, the uniform ion current density (J) and reactive gas flux (Φ_r) are assumed near the vicinity of the target and substrate surfaces. Based upon this simple system, three evolution equations can be developed simply using the overall mass balance for the reactive gas in the chamber and the compound fraction at the target and substrate, respectively [11–13]. First considering the reactive gas by the ideal gas law and assuming a uniform pressure in the chamber, the rate change of the reactive gas (partial pressure) can be expressed as

$$\frac{dp}{dt} = \frac{k_B T}{V} (q_{in} - (q_t + q_s + q_{pump})) \quad (1)$$

where k_B is the Boltzmann constant, T is temperature and V is the volume of chamber. q_{in} is the inflow rate of reactive gas, q_t and q_s are, respectively, the consumption rates at the target and substrate surfaces, and q_{pump} is the outflow rate by the vacuum pump. Units for these quantities are all in (number of molecules/time). Notice that the gettering effect of the chamber walls is neglected here because the gettering area of the target and substrate is usually much larger than that of walls [11].

The consumption rates at the target or substrate surfaces can be expressed as following [7,11–13]

$$q_i = \Phi_r \alpha_i (1 - \theta_i) A_i \quad (2)$$

where the subscript i is either t or s and α_i is the sticking coefficient which represent the probabilistic feature of the gettering effect. A detailed discussion regarding the sticking

coefficient will be given later. The outflow rate by the vacuum pump is followed by

$$q_{pump} = \frac{ps}{k_B T} \quad (3)$$

where p is the (partial) pressure of reactive gas and s is the pumping speed (volume/time).

Note that the reactive gas flux can be found from kinetic theory by assuming a Maxwell distribution of molecular velocities. Skipping the derivations, the result is [7]

$$\Phi_r = \frac{p}{\sqrt{2\pi m k_B T}} \quad (4)$$

where m is the mass of reactive gas molecule.

The rate equations for compound formation at the target and substrate surfaces are given by the mass balance

$$\frac{d\theta_t}{dt} = \Phi_r \alpha_t (1 - \theta_t) A_t a_t - (J/e) \gamma_c \theta_t A_t, \quad (5)$$

$$\begin{aligned} \frac{d\theta_s}{dt} = & \Phi_r \alpha_s (1 - \theta_s) A_s a_s + (J/e) \gamma_c \theta_t A_t (1 - \theta_s) \\ & - (J/e) \gamma_m (1 - \theta_t) A_t \theta_s, \end{aligned} \quad (6)$$

where $a_t(a_s)$ is the stoichiometric number for compound formation (number ratio of compound molecules/reactive gas molecules) at the target (substrate), J is the ion current density (charges/area/time), e is the unsigned charge of an electron and $\gamma_c(\gamma_m)$ is the sputtering yield of the compound (metal) at the target (atoms sputtered/incident ion). Physically, the first term in Eq. (5) represents the reaction between the gas and metal at the target surface, which in turn would increase the amount of compound, while the second term represents the reduction in compound fraction due to sputtering by incident ions. Similar interpretation is applicable to Eq. (6) except that the third terms describe the reduction in compound fraction since the sputtered metal from the target could replace some fraction of the compounds at the substrate.

From Eqs. (5) and (6), the sputtering rate at the target surface can also be found from the unbalance of mass at the target

$$R = (J/e) [\gamma_c \theta_t + \gamma_m (1 - \theta_t)] A_t. \quad (7)$$

2.2. Nondimensionalized rate equations

To further simplify our analysis, it is necessary to introduce nondimensional quantities for pressure, pumping speed and time respectively as [16]

$$\begin{aligned} P = \frac{\Phi_r}{(J/e)} = \frac{p}{(J/e) \sqrt{2\pi m k_B T}}, \quad S = \frac{s \sqrt{2\pi m}}{A_t \sqrt{k_B T}}, \\ \tau_1 = \frac{pV}{k_B T} \left(\frac{\Phi_r}{A_t} \right), \quad \tau_2 = \frac{e}{J A_t} \end{aligned} \quad (8)$$

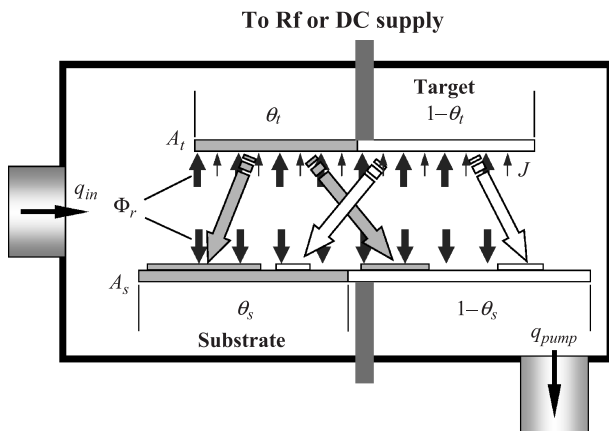


Fig. 1. Schematic drawing of Berg's model for reactive sputtering.

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