MODELING AND STABILITY ANALYSIS OF THE NONLINEAR REACTIVE SPUTTERING PROCESS

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ASBSTRACT

The model of the reactive sputtering process has been determined from the dynamic equilibrium of the reactive gas inside the chamber and the dynamic equilibrium of the sputtered metal atoms which form the compound with the reactive gas atoms on the surface of the substrate. The analytically obtained dynamical model is a system of nonlinear differential equations which can result in a histeresis-type input/output nonlinearity. The reactive sputtering process has been simulated by integrating these differential equations. Linearization has been applied for classical analysis of the sputtering process and control system design..

Keywords: reactive sputtering process, dynamical modeling, linearization, steady state operating point, stability.

1. Introduction

Mathematical models may be developed along two methods: the analytical and the experimental way to get the dynamical model. Development of the analytical dynamic model does not necessarily involve any experimentation on the actual system. The other way towards mathematical modeling is directly based on experimentation, and this method is generally referred to as "system identification". The analytically obtained dynamical model generally is a system of nonlinear differential equations.

When faced with an engineering problem of a nonlinear system, the first approach usually is the linearization; in other words, trying to avoid the nonlinear aspects of the problem. In this paper we present one simple linearization method of the analytical model of the reactive sputtering process. The linearized model is valid just in a small region of the selected operating point.

The linearization is useful in model analysis and on the other hand we can specify the system stability in the given operating point. The reactive sputtering is a highly nonlinear process, which frequently exhibits stability problems. The mathematical model itself is nonlinear, with a hysteresis-type input-output nonlinearity.

2. Modeling the reactive sputtering process

A very sensitive aspect of the reactive sputtering process is the dynamic equilibrium of the reactive gas inside the chamber and of the metal atoms which form the compound with the reactive gas atoms on the surface of the substrate. The components of this rather complex balance are schematically shown in fig. 1. The phenomena on both the surfaces of the target and of the substrate include sputtering and gettering of the reactive gas atoms.

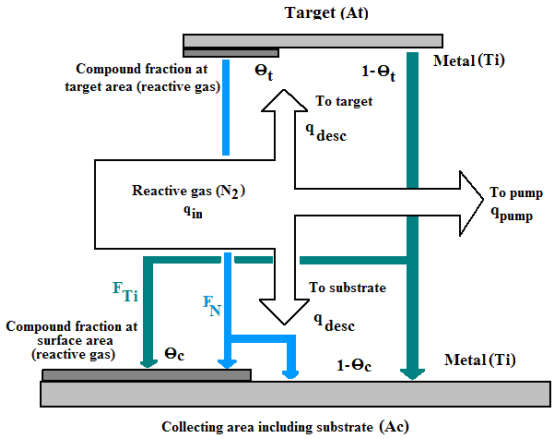

Fig.1 – Schematic representation of the reactive gas balance and of the main particle fluxes on the target and substrate surfaces.

The larger the surface of elemental nonreacted metal, the stronger the flux of sputtered metal atoms which further reduces the reactive gas concentration by forming compound on the surface of the substrate. The reactive gas consumption increases when the fractional coverage with compound is smaller. It results that the reactive sputtering process is strongly nonlinear. The main type of nonlinearity is hysteresis, which can be observed both from theoretical results (obtained from simulation using the mathematical model), and from practical measurements.

The mathematical model developed is based on the hypotheses and formulation used by S. Berg [1] [2] [3] as follows:
- the partial pressure of the reactive gas has uniform distribution in the processing chamber;
- the secondary electron emission due to the ionic bombardment of the target surface is uniform and independent of the surface fraction covered by compound;
- the glow discharge takes place in a mixture of inert gas and reactive gas (ex. Ar and 2…3% of N_2)
- the contribution of the reactive gas ions to the bombarding ion flux is negligible due to the small concentration of the reactive gas;
- no reactive gas is consumed at the fraction of the target surface that is already covered by compound;
- homogenous sputtering rate is assumed on the whole surface of the target.

These hypotheses are based on widely accepted research results in the field of PVD by reactive magnetron sputtering; respectively provide a reasonably correct description of the process by a model which is simple enough to be considered for stability analysis and process controller design [7]. The dynamic model of the reactive magnetron sputtering process is defined by the system of equations (1):

$$\begin{aligned}
&\frac{dp_N}{dt} = k_1 \cdot (q_{in} - q_p - (\alpha_{tM} \cdot F_N \cdot (1-\theta_t) \cdot A_t + \alpha_{cM} \cdot F_N \cdot (1-\theta_c) \cdot A_c) \\
&\frac{d\theta_t}{dt} = \frac{1}{N_{Ti}} (2 \cdot \alpha_{tM} \cdot F_N \cdot (1-\theta_t) - J \cdot \eta_N \cdot \theta_t) \\
&\frac{d\theta_c}{dt} = \frac{1}{N_{Ti}} (J \cdot \eta_N \cdot \theta_t \cdot \left(\frac{A_t}{A_c}\right) \cdot (1-\theta_c) + 2 \cdot \alpha_{cM} \cdot F_N \cdot (1-\theta_c) - \\
&\quad - J \cdot \eta_M \cdot (1-\theta_t) \cdot \left(\frac{A_t}{A_c}\right) \cdot \theta_c)
\end{aligned} \tag{1}$$

In this mathematical model the following notation has been used:
p_N- the partial pressure of reactive gas (nitrogen) in the sputtering chamber;
θ_t- the fractional surface of the target covered by compound molecules;
θ_c- the fraction of the condensation area covered by compound molecules;
F_N- the flux of reactive gas molecules (N_2) on the target or on the substrate;
q_{in}- the input reactive gas flow;
q_p- the gas flow evacuated by the vacuum pump;
A_t- the target area;
A_c- the substrate (condensation) area (including the substrate and the chamber);
m_N- mass of the reactive gas molecule (28 a.u. ($1 a.u. = 1.66 \cdot 10^{-27} kg$));
m_{Ti} - mass of the metal (47.9 a.u.);
η_M- sputtering yield of the elemental metallic material (titanium);
η_N- sputtering yield of the compound (titanium nitride);
α_{tM}, α_{cM}- sticking coefficients for the nitrogen molecule (to the titanium target or to the covered part);
N_{Ti}- the superficial density of the titanium atoms on the surface of the metallic target;
J- the particle density of argon ions on the surface of the target, which can be calculated using the relationship:

$$J = I_d / (A_t \cdot e) \tag{2}$$

e- the charge of electron ($1.6 \cdot 10^{-19} C$);
I_d –the intensity of the discharge current;
k_1- proportional coefficient, calculated in function of temperature and chamber volume.

$$k_1 = \frac{R \cdot T}{N_A \cdot m_N \cdot V}; \tag{3}$$

R – ideal gas constant ($8314 J / molK$);
N_A – Avogadro's number ($6.022 \cdot 10^{23} mol^{-1}$);
T – temperature;
V – volume of the sputtering chamber.

This mathematical model in state space representation (1) has three state variables (p_N, θ_t and θ_c) two input signals (q_{in} and I_d) and for the output signal we can choose between the fractional surface of the target covered by compound molecules θ_t or the sputtering rate (R_p) defined by the relationship (4):

$$R_p = J \cdot [\eta_N \cdot \theta_t + \eta_M \cdot (1-\theta_t)] \tag{4}$$

3. Modeling results

The reactive sputtering process has been simulated employing a Runge-Kutta step control algorithm. The sampling time was typically set to 0.01 sec. The parameters used for simulation are listed in table 1.

Table 1. Parameters used for simulation

Notation	Value
T	300K
V	$75 \cdot 10^{-3} m^3$
η_M	1.5
η_N	0.3
N_{Ti}	$140 \cdot 10^{-12} m^2$
A_t	$0.84 \cdot 10^{-2} m^2$
A_c	$0.22 m^2$
α_{tM}, α_{cM}	1

The steady-state analysis of the process yields very nonlinear characteristics defining the steady-state relation between the input reactive gas quantity and the state variables from equations (1). For simulation we considered the reactive gas flow as input, different time variations of the input signal, used in our experiments, are presented in fig. 2 [4][5].

The fractional coverage of the target (θ_t) in function of the input N_2 quantity (q_{in}) is shown in fig. 3, where the bombarding particle density of argon ions (J) is calculated for constant discharge current intensity (I_d=1.125 A). These results obtained by simulation using the dynamic model (1) put in evidence the hysteresis loop described in the plane

defined by θ_t and q_{in} (fig. 3.) at different variation speeds of the input reactive gas flow in accordance with fig. 2.

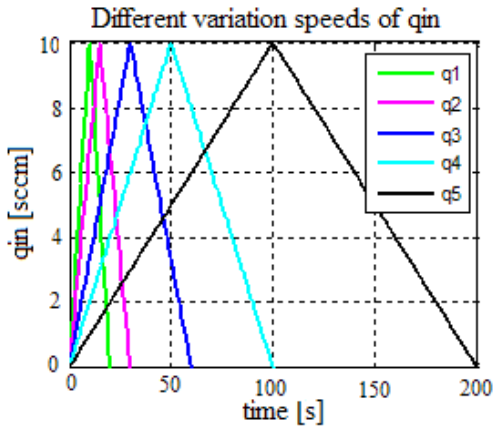

Fig. 2 – Variation in time of the reactive gas flow in case of different variation speeds

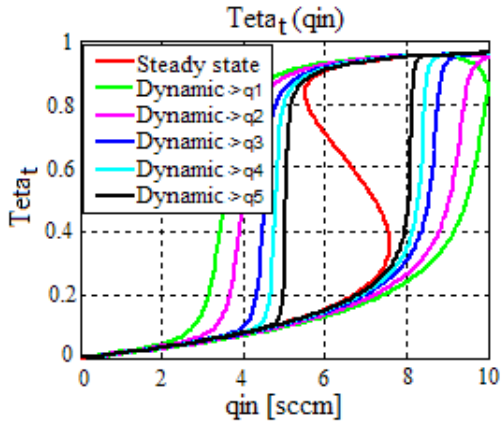

Fig. 3 – The steady-state relation between the fractional surface coverage of the target and the input reactive gas flow, respectively the hysteresis loops obtained in case of different variation speeds of the input reactive gas flow

4. Linearization with Taylor series approximation method

The object of linearization is to derive a linear model the response of which agrees closely with that of the nonlinear model. Numerous technological dynamic processes can be analytically modeled by means of differential equations, which in the state representation have the form:

$$\begin{cases} \dot{\underline{x}}(t) = \underline{f}(\underline{x}(t), \underline{u}(t), t) \\ \underline{y}(t) = \underline{g}(\underline{x}(t), \underline{u}(t), t) \end{cases} \quad (5)$$

where the input signal $\underline{u}(t)$ is an independent m x 1 variable, $\underline{y}(t)$ is the output vector (p x 1) and $\underline{x}(t)$ is the state vector (n x 1).The number of input signals is m, the number of output signals is p and the number of state variables is n. The aim of linearization methods is to determine a linear mathematical model, which has the general form in state space representation:

$$\begin{cases} \dot{\underline{x}}(t) = \underline{A}(t) \cdot \underline{x}(t) + \underline{B}(t) \cdot \underline{u}(t) \\ \underline{y}(t) = \underline{C}(t) \cdot \underline{x}(t) + \underline{D}(t) \cdot \underline{u}(t) \end{cases} \quad (6)$$

where the matrices of the system are: $\underline{A}(t)$ (n x n), $\underline{B}(t)$ (n x m), $\underline{C}(t)$ (p x n) and D(t) (p x m).

The linearization approach presented in this section is based on the small signal linearization method. For the linearization of the equations the Taylor series approach has been applied. According to this method, a nonlinear continuous function $F(t)$ can written as:

$$F(x) = F(x_k + \delta x_k) = F_k(\delta x_k) = \sum_{q=0}^{\infty} \frac{\delta x_k^q}{q!} \cdot \left(\frac{d^q F}{dx^q} \right)_k \quad (7)$$

where x_k represents the pivot moment at the sequence k and δx_k is the perturbation, considered small enough. The index k is used here for the functions specification at the x_k. This relation is possible to apply if the right side members of the equation (5) are continuous, differentiable functions and the initial conditions are considered known. If we ignore the higher order members (q>1), for the linearized model we can use following relationship:

$$\begin{cases} \frac{d}{dt} \delta \underline{x}_k = \underline{A}_k \cdot \delta \underline{x}_k + \underline{B}_k \cdot \delta \underline{u}_k \\ \delta \underline{y}_k = \underline{C}_k \cdot \delta \underline{x}_k + \underline{D}_k \cdot \delta \underline{u}_k \end{cases} \quad (8)$$

where the matrices are:

$$\underline{A}_k = \left(\frac{\partial \underline{f}}{\partial \underline{x}} \right)_k ; \quad \underline{B}_k = \left(\frac{\partial \underline{f}}{\partial \underline{u}} \right)_k ; \quad \underline{C}_k = \left(\frac{\partial \underline{g}}{\partial \underline{x}} \right)_k ; \quad \underline{D}_k = \left(\frac{\partial \underline{g}}{\partial \underline{u}} \right)_k . \quad (9)$$

For the discrete-time model, we can apply methods with polynomial approximation and numerical integration, and the model becomes:

$$\begin{cases} \delta \underline{x}_{k+1} = \underline{\Phi}_k \cdot \delta \underline{x}_k + \underline{\Gamma}_k \cdot \delta \underline{u}_k \\ \delta \underline{y}_k = \underline{C}_k \cdot \delta \underline{x}_k + \underline{D}_k \cdot \delta \underline{u}_k \end{cases} \quad (10)$$

where $\underline{\Phi}_k$, $\underline{\Gamma}_k$, $\underline{C}_k$ and D_k are the matrices of the linearized discrete time system with adequate dimensions.

The results of linearization are valid just in a small region around the selected operating point. The responses of the linear and nonlinear models do not agree exactly and may differ significantly under some conditions. Generally there exists a set of inputs and initial conditions for which the agreement will be satisfactory.

5. Stability analysis of the nonlinear process and the results of linearization

The linearization of the dynamic model of the reactive sputtering process has been performed for different operating points. In fig. 4 there is presented the steady state relation between the fractional surface coverage of the target and the input reactive gas flow with three selected operating points P_1, P_2 and P_3. Stability analysis of a dynamical system helps us to understand what is going to happen with the state variables after perturbation. Stability properties of a physical system refer to the way the system responds to some perturbation of initial states; whether the system can recover on its own after being perturbed

or it has an unpredictable behavior. In fig. 5, 6 and 7 we show the variation of states after perturbation for different operating points.

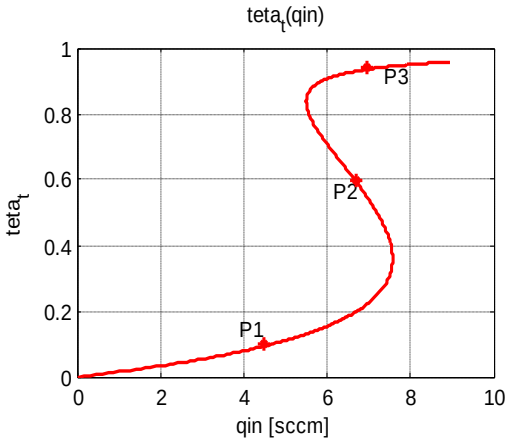

Fig. 4 – The steady-state relation between θ_t and q_{in} with three selected operating points

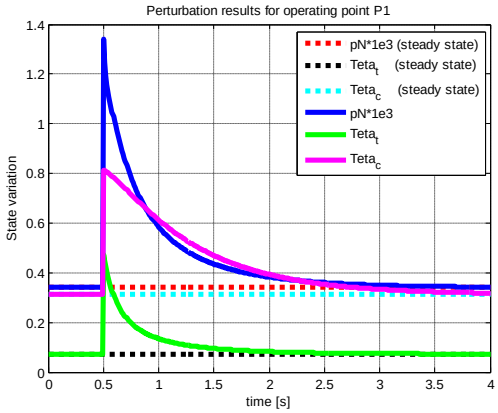

Fig. 5 – Perturbation results for operating point P_1

After simulation we can draw the conclusion that the operating points P1 and P3 are stable operating points, but the P2 is an unstable operating point. Using these selected operating points we can calculate the linearized discrete time Φ matrices (fundamental matrices). For stability analysis we determine the eigenvalues for these operating points:

$$P_1: \quad |\lambda_1| = 0.7744 \quad |\lambda_2| = 0.9986 \quad |\lambda_3| = 0.9915$$
$$P_2: \quad |\lambda_1| = 1.0014 \quad |\lambda_2| = 0.9654 \quad |\lambda_3| = 0.9769$$
$$P_3: \quad |\lambda_1| = 0.9988 \quad |\lambda_2| = 0.8690 \quad |\lambda_3| = 0.8690$$

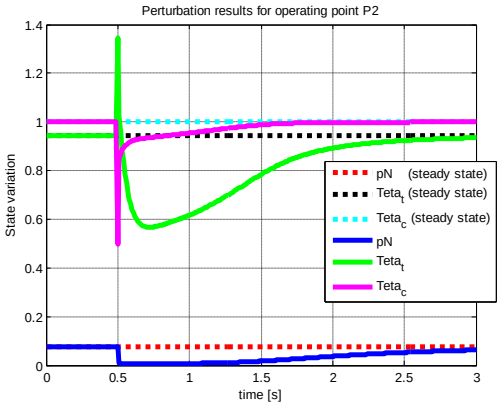

Fig. 6 – Perturbation results for operating point P_3

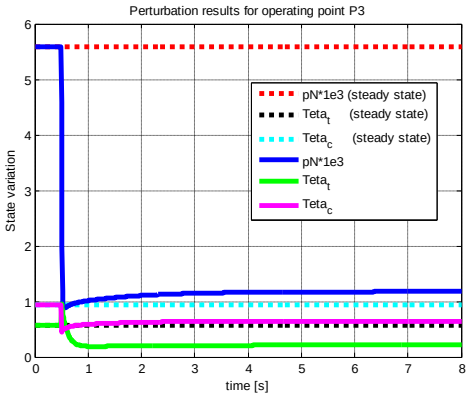

Fig. 7 – Perturbation results for operating point P_2

It can be observed the existence of a single unstable pole in case of the operating point situated on the negative slope of the characteristic (P_2). For this unstable operating point the root locus method can be used to test the controllability [6].

Two control methods have been analyzed: by means of the reactive gas flow (q_{in}) only (fig.8) and by means of the discharge current (I_d) (fig.9).

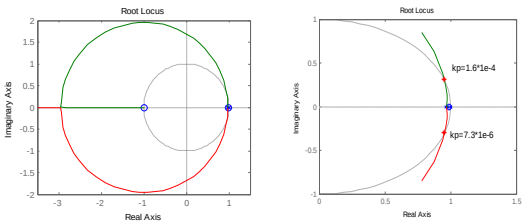

Fig. 8 – Root locus for the reactive gas flow controlled system (operating point P_2). The right side figure shows details of the root locus.

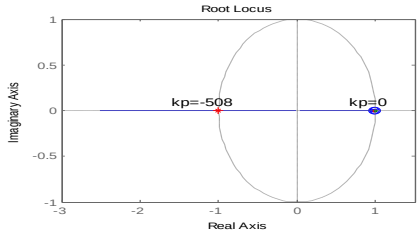

Fig. 9 – Root locus for the discharge current controlled system (operating point P_3)

Analyzing the root locus, the following conclusions can be drawn: if the process works in this unstable operating point P_2, the system is controllable using a proportional controller in case of both types of control input. When the control signal is the reactive gas flow then the controller gain may be varied only in a small range ($k \in (7.3 \div 160) \cdot 10^{-6}$). In this case the discharge current is fixed (I_d=1.125A). In the other case, when the control signal is the discharge current the controller gain can be in the range $k \in (-508 \div 0)$. In this case the input reactive gas flow is q_{in}=6.23 sccm. In conclusion we can say that for this unstable operating point the controller parameter tuning is much easier in case of control by means of the discharge current than in case of control by means of the reactive gas flow. The simulation results obtained in case of the two different control inputs are presented in fig. 10 and fig. 11.

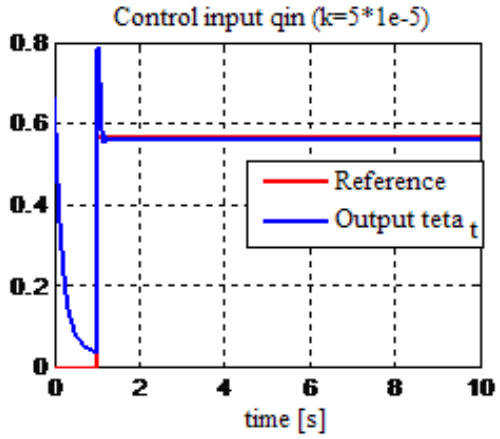

Fig. 10 – Results of simulation for gain controlled system, when the control signal is q_{in}

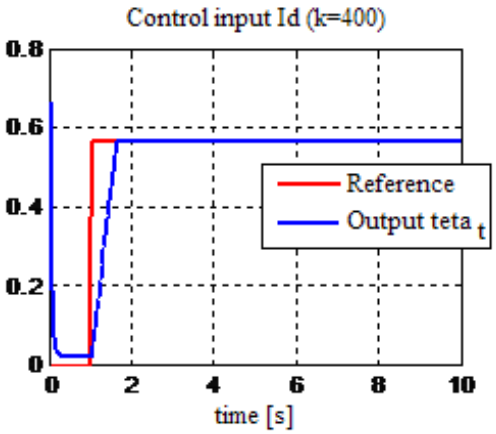

Fig. 11 – Results of simulation for gain controlled system, when the control signal is I_d

6. Conclusions

The present investigation shows that the dynamical modeling of the reactive sputtering process is characterized by nonlinear differential equations. The majority of design methods on the classical control theory require the knowledge of a linear model of the controlled process. The first approach usually is the linearization of the nonlinear model. In this paper there was presented a simple linearization method based on the analytical model of the reactive sputtering process, which is valid only in a small region around the selected operating point. The linearization approach presented in this section is based on the small signal linearization method, using the Taylor series approach. The linearization method has been performed for three operating points selected on the steady state characteristics, There have been analyzed the stability and the degree of controllability of the system in these points. The existence of a single unstable pole has been proven in case of the operating points situated on the negative slope of the steady state characteristic.

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