Acta Universitatis Sapientiae
Electrical and Mechanical Engineering, 3 (2011) 82-92

Theoretical Study of the Gradient Method to Find the Optimal Control for the Reactive Sputtering Process

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Manuscript received September 15, 2011; revised December 15, 2011.

Abstract: One of the main tasks in the optimal control theory is to find a controller that provides the best possible performance with respect to some given measure of performance (optimality criterion). For linear plant dynamics and quadratic performance criteria it is possible to obtain the optimal control law by numerically integrating a Riccati type matrix differential equation. In general, for nonlinear plants the variational approach leads to a nonlinear two-point boundary value problem, which can be solved by iterative numerical methods, for example by the steepest descent (gradient) method.

A model of the reactive sputtering process can be determined from the dynamic equilibrium between the quantity of reactive gas inside the chamber and the quantity of 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 with nonlinear differential equations which can result in a hysteresis-type input/output nonlinearity. The present paper proposes a theoretical study of the steepest descent gradient method to obtain the optimal control signal and trajectory for this nonlinear reactive magnetron sputtering process.

Keywords: Optimal control, nonlinear systems, Hamilton-Iacobi equations, reactive sputtering process, gradient method**,** hysteresis loop, cost function, boundary conditions.

1. Introduction

Mathematical models may be developed along two methods. One method is the analytical modeling, which does not necessarily involve any experimentation on the actual system. The other method is known as system

identification and this is directly based on experimentation. The analytically obtained dynamical model generally is a system with nonlinear differential equations. In general optimal control theory the objective is to find a controller that provides the best possible performance with respect to some given measure of an optimality criterion (cost function). If the plant dynamics is linear and the cost function is a quadratic performance criterion than it is possible to obtain the optimal control law by numerically integrating a Riccati type matrix differential equation. 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. After linearization we obtain a linearized model, which is valid just in a small region around the selected operating point. In general for nonlinear plants the variational approach leads to a nonlinear two-point boundary value problem, which can be solved by iterative numerical methods, for example by the steepest descent (gradient) method.

The reactive sputtering processes frequently exhibit stability problems. The analytically obtained dynamical model is a system with nonlinear differential equations. The present paper proposes a theoretical study of the steepest descent gradient method to obtain the optimal control signal and trajectory for this nonlinear reactive magnetron sputtering process.

2. Analytical modeling and numerical simulation of the reactive sputtering process

A. Analytical modeling

A very sensitive aspect of the reactive sputtering process is the dynamic equilibrium between the reactive gas inside the chamber and the sputtered 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 of the metal and gettering of the reactive gas atoms. 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 by simulation using the mathematical model), and from practical measurements.

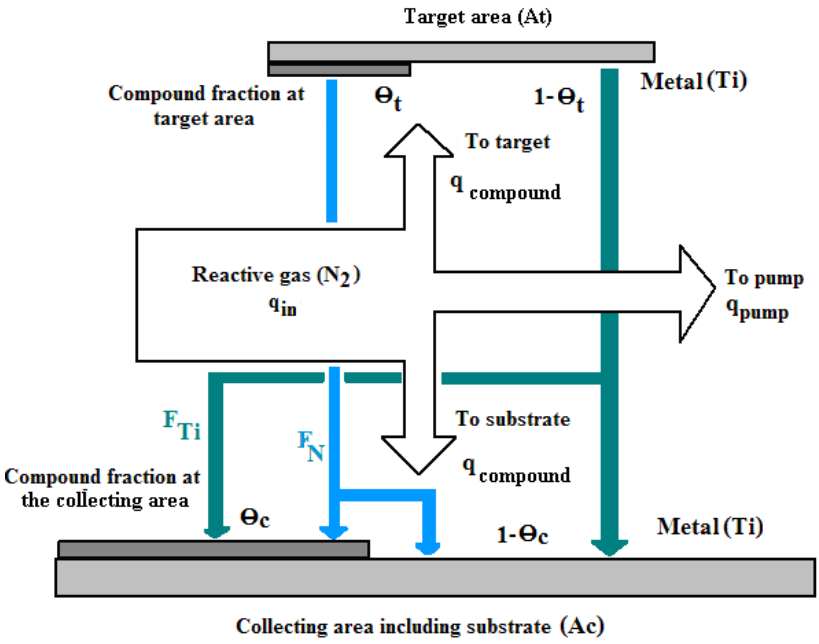


Figure 1: Schematic representation of the reactive gas balance and of the main particle fluxes on the target and substrate surfaces.

The mathematical model developed is based on the hypotheses and formulation used by S. Berg [1] [2] 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 [3][4]. 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 [5].

The dynamic model of the reactive magnetron sputtering process is defined by the system of equations (1):

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

In this mathematical model the following notation has been used:

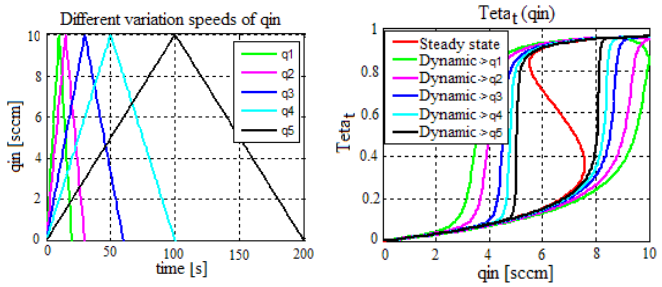
p_N- the partial pressure of reactive gas (nitrogen) in the sputtering chamber;
θ_t, θ_c - the surface fraction of the target and of the condensation area covered by compound molecules;
F_N- the flux of reactive gas molecules (N_2) on the target or on the substrate;
q_{in}, q_p- the input reactive gas flow and the gas flow evacuated by the vacuum pump;
A_t, A_c- the target area and the condensation (substrate and chamber) area;
m_N, m_{Ti} - mass of the reactive gas molecule (m_N=28 a.u.) and of the metal (m_{Ti}=47.9 a.u.);
η_M, η_N - sputtering yield of the elemental metal (titanium) and 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 Ti atoms on the surface of the metallic target;
J- the particle density of argon ions on the surface of the target, which is proportional to the discharge current intensity (I_d);
k_1- coefficient, calculated in function of temperature and chamber volume.

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 we can choose the surface fraction of the target covered by compound molecules (θ_t) or the sputtering rate (R_p) as the output signal.

B. Numerical simulation

The reactive sputtering process was simulated employing a Runge-Kutta algorithm, where the sampling time was set to 0.01 sec. The parameters used for simulation are: η_M=1.5, η_N=0.3, N_{Ti} =140e-12 m^{-2}, A_t=0.0084 m^2, A_c=0.22 m^2 and α_{tM}=α_{cM}=1, k_1=1.18e6 $J/(kg.m^3)$.The steady-state analysis of the process yields very nonlinear characteristics defining the steady-state relationship 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 simulations and experiments are presented in *Fig. 2. a*. The fractional coverage of the target (Θ_t) in function of the input quantity (q_{in}) is shown in *Fig. 2. b.*, where the particle density of argon ions (J) is calculated for a constant discharge current value (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} for different variation speeds of the input reactive gas flow in accordance with *Fig. 2.a.*



a) *b*

Figure 2: Variation in time of the reactive gas flow for different variation speeds (a), the steady-state and dynamic relationship between the fractional surface coverage of the target and the input reactive gas flow (b).

3. Application of the gradient method to find the optimal control

The nonlinear plant model in general state space representation is defined by the following equation:

$$\frac{\mathrm{d}}{\mathrm{dt}}\underline{x}(t) = \underline{f}(\underline{x}(t), \underline{u}(t), t) \tag{2}$$

where $\underline{x}(t)$ is the state vector and $\underline{u}(t)$ is the input vector.

The cost function is defined as:

$$J(\underline{u}) = \lambda(\underline{x}(t_f)) + \int_{to}^{tf} L(\underline{x}(t), \underline{u}(t), t)dt \tag{3}$$

where t_0 and t_f are the initial and the final time, $\lambda()$ and $L()$ are scalar functions.

For the system defined by the relation (2) we search the optimal control law that minimizes the cost function (3). To solve this problem we define the Hamilton function as:

$$H(\underline{x}(t), \underline{u}(t), \underline{p}(t), t) = L(\underline{x}(t), \underline{u}(t), t) + \underline{p}^T(t) \cdot \underline{f}(\underline{x}(t), \underline{u}(t), t), \tag{4}$$

where $\underline{p}(t)$ is the costate vector. The required conditions for optimality are:

$$\frac{d}{dt}\underline{x}(t)=\frac{\partial H}{\partial \underline{p}}\left(\underline{x}(t),\underline{u}(t),\underline{p}(t),t\right) \tag{5}$$

$$\frac{d}{dt}\underline{p}(t)=-\frac{\partial H}{\partial \underline{x}}\left(\underline{x}(t),\underline{u}(t),\underline{p}(t),t\right) \tag{6}$$

$$\frac{\partial H}{\partial \underline{u}}\left(\underline{x}(t),\underline{u}(t),\underline{p}(t),t\right)=0 \tag{7}$$

and the boundary conditions are:

$$\underline{x}(t_0)=\underline{x}_0;\quad \underline{p}(t_f)=\frac{\partial \lambda\left[\underline{x}(t_f)\right]}{\partial \underline{x}} \tag{8}$$

The resulting nonlinear two-point boundary-value problem cannot be solved analytically, so we will use an iterative numerical technique, the steepest descent gradient method, to determine the optimal control.

The formal algorithm of this method is [6], [7]:

0. Select a discrete approximation to the control signal $\underline{u}(t)^{<0>}$, $t\in[\,t_0, t_f]$, and fix the iteration index k at 0.

1. Using this control signal $\underline{u}(t)^{<k>}$ integrate the state equation (5) from t_0 to t_f with initial conditions $\underline{x}(t_0)$.

2. Integrate the costate equation (6) from t_f to t_0 with „initial condition" $\underline{p}(t_f)$.

3. Evaluate the $\frac{\partial H}{\partial \underline{u}}$ expression. We can calculate its norm as follows:

$$\left\|\frac{\partial H}{\partial \underline{u}}\right\|=\int_{to}^{tf}\left[\frac{\partial H}{\partial \underline{u}}\right]^T\cdot\left[\frac{\partial H}{\partial \underline{u}}\right]dt\,. \tag{9}$$

Terminate the iterative procedure (the outputs of the algorithm are the external state vector $\underline{x}(t)^{<k>}$ and the control signal $\underline{u}(t)^{<k>}$), if

$$\left\|\frac{\partial H}{\partial \underline{u}}\right\|\le\varepsilon \tag{10}$$

where the ε is a preselected small positive constant. If the stopping criterion (10) is not satisfied we generate a new control function given by (11) and return to step 1

$$\underline{u}(t)^{<k+1>}=\underline{u}(t)^{<k>}-\gamma\cdot\frac{\partial H}{\partial \underline{u}}\,. \tag{11}$$

In (11), γ is the constant step size for the gradient method.

4. Numerical simulation of the gradient algorithm for the optimal control of the reactive sputtering process

A. Determination of the Hamilton-Iacobi equations

The nonlinear mathematical model (1) for the reactive sputtering process can be written in the general state space form (2), where the state vector is $\underline{x}(t)=[x_1(t)\ x_2(t)\ x_3(t)]^T=[p_N(t)\ \theta_t(t)\ \theta_c(t)]^T$, and the control input vector is $\underline{u}(t)=[u_1(t)\ u_2(t)]^T=[q_{in}(t)\ I_d(t)]^T$. We select a linear quadratic cost function

$$J(\underline{u})=\frac{1}{2}\underline{x}_e(t_f)^T\cdot F\cdot\underline{x}_e(t_f)+\frac{1}{2}\int_{to}^{tf}\left(\underline{x}_e(t)^T\cdot Q\cdot\underline{x}_e(t)+\underline{u}_e(t)^T\cdot R\cdot\underline{u}_e(t)\right)dt \qquad (12)$$

where R, Q, F are positive defined diagonal matrices, $\underline{x}_e(t)=\underline{x}(t)-\underline{x}_p(t)$ and $\underline{u}_e(t)=\underline{u}(t)-\underline{u}_p(t)$, where the $\underline{x}_p(t)$ is the prescribed state vector and $\underline{u}_p(t)$ is the value of control input which is necessary to keep the states at their prescribed stationary values. The required conditions for optimality are characterized by the following differential equations for states:

$$\frac{\partial H}{\partial p_i}=\dot{x}_i(t)=f_i(\underline{x}(t),\underline{u}(t))\quad i=1,2,3 \qquad (13)$$

and the following differential equations for costates:

$$\frac{\partial H}{\partial x_i}=-\dot{p}_i(t)=Q_i\cdot(x_i(t)-x_{p_i}(t))+p_1(t)\cdot\frac{\partial f_1}{\partial x_i}+p_2(t)\cdot\frac{\partial f_2}{\partial x_i}+p_3(t)\cdot\frac{\partial f_3}{\partial x_i}\quad i=1,2,3 \qquad (14)$$

The expressions of the derivate of the Hamilton function versus the control signals are:

$$\frac{\partial H}{\partial u_i}=R_i\cdot(u_i(t)-u_{p_i}(t))+p_1(t)\cdot\frac{\partial f_1}{\partial u_i}+p_2(t)\cdot\frac{\partial f_2}{\partial u_i}+p_3(t)\cdot\frac{\partial f_3}{\partial u_i}\quad i=1,2 \qquad (15)$$

For updating the control signal we can use the relationship:

$$u_i(t)^{<k+1>}=u_i(t)^{<k>}-\gamma_i\cdot\frac{\partial H(t)}{\partial u_i(t)}\quad i=1,2 \qquad (16)$$

Using these relations the algorithm has been implemented in Matlab environment in order to obtain the optimal control for the reactive sputtering process.

B. Results of the numerical simulation

For numerical integration of the differential equations (13) and (14) there was used a Runge-Kutta method [8], [9]. The initial points and the prescribed

points were selected from the steady state simulation of the reactive sputtering process. There were simulated the following control versions:

V1: control with input reactive gas flow (q_{in});

V2: control by means of the discharge current intensity (I_d);

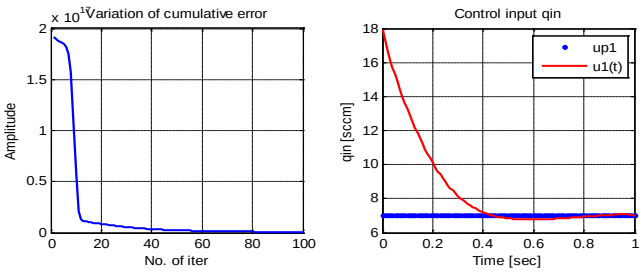
V3: control with both input signals (q_{in} and I_d).

The results of simulation are influenced by the step sizes (γ_1 and γ_2) of the gradient methods, the selected initial control trajectory ($u_1(t)^{<0>}$ and $u_2(t)^{<0>}$), the maximum number of iterations (N_{max}), the values of weighting matrices (R_1, R_2 respectively Q_1, Q_2 and Q_3) and the position of prescribed state vector in comparison with the initial state vector. The simulation time interval and the sampling time are fixed for each version: $t \in [0, 1]$ sec and T_s=0.01 sec. The other simulation parameters are presented in Table 1.

Table 1: Simulation parameters for the three types of control

Control type	γ_1	γ_2	R_1	R_2	Q	N_{max}
V1	10^{-16}	0	10^{-4}	0	10 I_3	100
V2	0	0.1	0	10^{-5}	10 I_3	100
V3	10^{-17}	0.01	10^{-3}	10^{-3}	10 I_3	800

Diagrams from *Fig.3* to *Fig.8* are presented for the visualization of some simulation results of this control algorithm. At first we considered that the system is controlled just by the input reactive gas flow (q_{in}). In *Fig. 3.a* there is presented the cumulative error (corresponding to relation (9)), and in *Fig. 3.b* there is presented the evolution in time of the control signal. The controlled quantities are presented in *Fig.4*, along with the prescribed constant state values. Similarly, when we considered as control input signal the discharge current (I_d), the corresponding simulation results are presented in *Fig.5* and *Fig. 6.*



a) *b)*

Figure 3: Variation of the cumulative error (a) and variation in time of the control signal input (b) – version V_1.

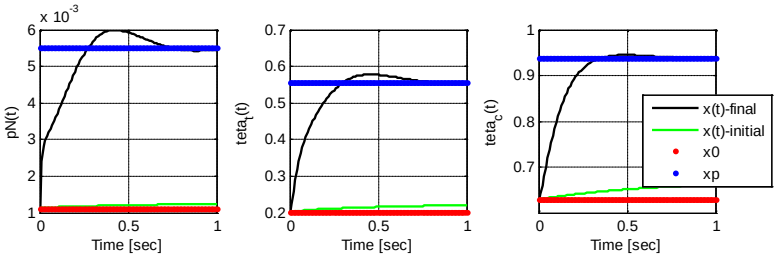
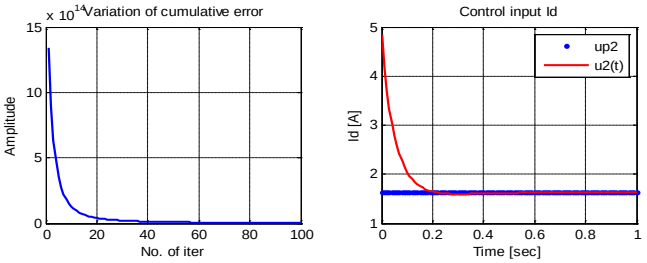


Figure 4: Variation in time of the controlled states obtained for the initial and the final control signals – version V_1.



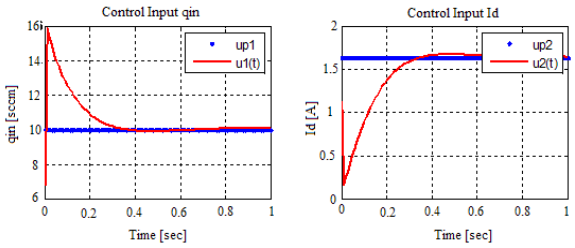
a) *b)*

Figure 5: Variation of the cumulative error (a) and variation in time of the control signal input (b) – version V_2.

Finally we realize simulation for the case when the plant is controlled simultaneously by both inputs (q_{in} and I_d). The results are shown in *Fig. 6* and *Fig. 7*. We present the evolution in time of the control signals: the input reactive gas flow (*Fig. 6.a*) and the discharge current variation (*Fig. 6.b*). On the other hand there are presented in *Fig. 7* the controlled quantities (the partial pressure of the reactive gas (p_N), the fractional surface coverage of the target (θ_t) and the fractional surface coverage of condensation area (θ_c)) versus the input reactive gas flow (q_{in}). The dashed curves represent the characteristics obtained using the steady state model. These put in evidence the initial values and the prescribed final values of the states.

The prescribed final operating point is situated on the negative slope of the steady state characteristic. This is an unstable operating point for the plant. From the simulation it results that first the control by means of the reactive gas flow has a bigger emphasis than the control by means of the discharge current. When the reactive gas flow is close to its value corresponding to the prescribed states (u_{p1}) than the second control quantity (I_d) is gaining more importance. The efficiency of the algorithm is determined by the initial conditions and the maximum number of iterations because the determination of the control signals

needs time. In this algorithm the restrictions of the control signals can be realized just by the proper choice of the weight matrices (*R* and *Q*).



a) *b)*

Figure 6: Evolution in time of the control signals: input reactive gas flow (a) and discharge current intensity (b)–version V_3..

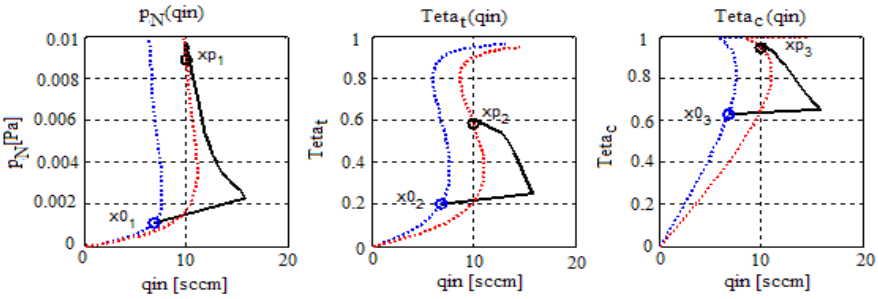


Figure 7: Variation of the three controlled quantities (p_N , θ_t and θ_t) versus the input reactive gas flow (qin) - version V_3..

3. Conclusion

The present investigation shows that the dynamical modeling of the reactive sputtering process is characterized by nonlinear differential equations and the optimal control of this plant is a very complex problem. In case of most of the modern control theories it is needed to know the linear model of the controlled process. In this paper there was presented a theoretical study about the application of the optimal control algorithm, where the results are obtained by numerical iterative techniques. The nonlinear optimal control problem is solved using the gradient method applied directly to the highly nonlinear model and was simulated for the nonlinear reactive sputtering process. Both the input reactive gas flow and the discharge current have been considered as control variables and the results of simulation have shown that this method is can be

used only if we have some proper preliminary information for the algorithm: initial input sequences of the control inputs, values of weight matrices, etc.

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