Fundamentals of Feedback Control for Reactive Sputtering

M.A. George and E.A. Craves, Deposition Sciences Incorporated, Santa Rosa, CA; and
R. Shehab and K. Knox, Ametek Incorporated, Pittsburgh, PA

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ABSTRACT

The reactive sputtering process is characterized by a hysteresis of reactive gas concentration and reactive gas flow [1,2]. The precise control of the reactive sputtering process requires operating at points on the hysteresis that ensures the desired high sputter flux and deposited thin film stoichiometry. The hysteresis is highly nonlinear in these preferred operating regimes. The practical challenge of meeting this in a batch coating system requires a control system that can compensate for changes in reaction rate for various sputtered metals, system pumping speed changing with thermal variations, and dynamic compensation of detrimental periodic cathode arcs. Closed loop control algorithms that rapidly bring the reactive sputtering system to the desired hysteresis steady state operating point are desired for multilayer applications such as thin film interference filters that require many target starts (and stops). Conventional methods of starting the reactive sputtering process such as temporal ramping of target power, voltage, or current and target shutters, are undesirable for precision thin film interference filters. We will discuss control system hardware and closed loop control algorithms that permit the achievement of steady state operating points in less than 500 milliseconds on a reactive sputtering drum coater. We will present an interactive model of the reactive sputtering system that will demonstrate in real time the effect of various elements of control algorithms on system performance.

INTRODUCTION

The reactive sputtering process is used for applying thin films of oxides, nitrides or carbides to substrates in a variety of industrial applications. The reactive sputtering process has been characterized by a number of researchers as being highly nonlinear and exhibiting a hysteresis behavior. Berg et al. [3] have developed a closed form reactive sputtering model that captures the relationship of the relevant parameters of the reactive sputtering process. In further work, Berg et al. combined a feedback controller to their experimental reactive sputtering system to control the process in such a way as to explore the process space "inside" the hysteresis region predicted by their model [4]. In that work Berg did not explore the question of the limits of the applicability of a feedback control system. The Berg model teaches that the strongest determinant of the hysteresis behavior is the relative speed of the physical pump and the thin film pump. In a separate paper Berg et al. explored the question of instabilities of this reactive sputtering model and could predict if that system would exhibit a hysteresis. Those systems with relatively large physical pumping compared to their thin film pump exhibit no or minimal hysteresis. In some systems it is possible to create a situation where the physical pumping speed dominates the "consumption" of the reactive gas; however, in industrial reactive sputtering coaters this condition is generally not realized. Here we explore the application of feedback and feedforward control algorithms to a reactive sputtering process that exhibits hysteresis and brings that system to the desired operating point within one second.

MATHEMATICAL MODEL OF THE REACTIVE SPUTTERING COATER

Mass Balance

For the system of interest in this paper we will consider a reactive sputtering coater used to form metal oxide from a metal target in a working gas of argon and a reactive gas of oxygen. A mass balance is utilized to account for the moles of oxygen in the chamber at any instance of time by adding oxygen introduced into the chamber, subtracting the moles of oxygen consumed by the reactive sputtering process and subtracting the amount of oxygen exhausted through the pump. This mass balance is shown mathematically in Equation 1.

$$M_{In} - \frac{S \cdot P_{total} \cdot y}{RT} - C_{Consumed} = \frac{V \cdot P_{total}}{RT} \cdot \frac{dy}{dt}$$

Equation 1

The first term is the molar flow rate of oxygen delivered to the chamber, M_{In}, via a gas flow control device. The second term is the molar flow of oxygen swept out of the chamber by the pump. This is calculated by the known system vacuum speed, S, the total pressure in the chamber P_{total} and the fraction of that total which is comprised of oxygen, introduced here as the mole fraction, y. The third term is the moles of oxygen consumed by the reactive sputtering process, $C_{consumed}$. The consumption of oxygen is that oxygen consumed by both the targets and the thin film deposited on the drum and shields

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described by Berg. The difference in the moles of oxygen flowing into the chamber and the sum of the oxygen pumped and that consumed by the sputter action is equal to the time rate of change of number of moles of oxygen in the chamber or the "accumulation" of oxygen in the reactive sputtering coater. At steady state this rate of change is nearly zero so that the mole fraction, y, is constant.

The choice of the mole fraction as a controlled variable for our reactive sputtering model was motivated by the work of Schiller et al. [5]. They introduced the ratio of the partial pressure of the reactive gas to total pressure to determine operating points on the hysteresis of reactive sputtering deposited TiO_2 thin films in atmospheres of oxygen and argon.

In practice, a sensor is used to measure a physical response that is directly proportional to the mole fraction of oxygen at some location in the coater. The sensor's measurement is incorporated into a feedback loop, which controls the molar flow rate of oxygen into the chamber M_{In}, to keep the reactive sputtering coater at steady state and acts to keep the accumulation of oxygen to a minimum. It is the measurement of the oxygen not consumed by the sputtering action that is used for purposes of control.

The block diagram of a Proportional (P), Integral (I) and Derivative (D) controller incorporated for a reactive sputtering process is shown in Figure 1. The development of this block diagram is beyond the scope of this paper, but is reviewed by the authors in a separate publication [6]. The desired operating point at mole fraction y_{SP} is subtracted from that measured by the sensor at the comparator. This difference or "error" is used by the PID controller algorithm to calculate the required flow rate of oxygen to keep the rate of change of the mole fraction or "accumulation" at a minimum.

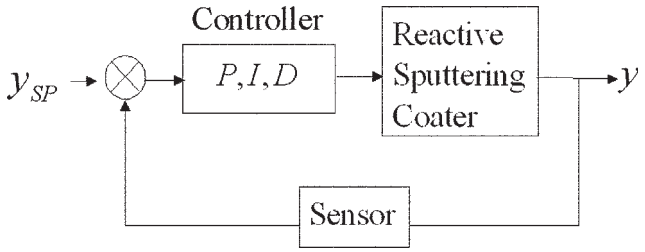

Figure 1: Block diagram representation of a Reactive Sputtering Coater with a PID controller.

REACTIVE GAS SENSOR

The mole fraction of reactive gas fed back into the system's controller must be stable, repeatable and updated frequently enough so as not to compromise the controller's response. Many PID controllers such as those that are implemented in Programmable Logic Controllers and PC's are discrete. The discretization of the controller algorithms places a premium on the temporal accuracy of the mole fraction sample signal sent back from the process to the controller.

In the development of the controller for a reactive sputtering system with feedback, we turned to a quadrupole mass spectrometer to sense the composition of the reactive sputtering system's effluent. Mass spectrometers have been employed on other reactive sputtering systems for use as sensors integrated into feedback control loops [7,8].

The stability of the partial pressure signal for both argon (40 m/z) and oxygen (32 m/z) on a representative deposition chamber measured over a period of several days drifted with relative standard deviation of ~12% for both signals. The signals for both the gases tend to deviate in the same direction due to thermal variations inside the quadrupole mass spectrometer. This rather large relative standard deviation is unacceptable for manufacturing processes. The partial pressure signals are normalized by defining a mole fraction (y), consistent with our mathematical model, as a combination of these two signals for our binary mixture.

$$y = \frac{S_{O2}}{S_{O2} + S_{Ar} \cdot f}$$

Equation 2

Where:
S_{O2} = Signal for O_2 (32 amu)
S_{Ar} = Signal for Ar (40 amu)
f = sensitivity factor for O_2 relative to Ar

The relative standard deviation of the mole fraction signal for oxygen in argon calculated in this manner for the same partial pressure data set is 2.3%. This level of noise in the mole fraction is satisfactory for manufacturing requirements.

The method by which this signal is acquired from the mass spectrometer can be a limiting factor in its usefulness in a feedback loop. For the mass spectrometers developed for this work the acquisition of the mole fraction signal required communication between a software module running on a PC and the mass spectrometer's controller. If calculation of the mole fraction takes place in a software module running on the PC it is paced by the serial communication queuing system of the PC's operating system. We have observed that the servicing of the queue by the PC's operating system can delay the arrival of an updated mole fraction signal to the feedback loop by several seconds. A delay of this magnitude is detrimental to the feedback controller operating at loop times of the order of 100 to 200 milliseconds. In order to achieve

better time resolution of the mole fraction signal, a program module is transferred to the mass spectrometer's controller that performs the calculation of Equation 2 and delivers the result to a digital-to-analog converter on the mass spectrometers controller. The analog signal representing the mole fraction is then delivered to the input of the feedback controller, via the analog signal, circumventing the bottleneck of the serial communication queue of the PC. The temporal response of the quadrupole mass spectrometer sensor is now limited only by the chosen signal averaging method in the mass spectrometer and the gas sampling and pumping apparatus. By selection of an appropriate signal averaging method and gas sampling approach, the sensor delay has been decreased to an acceptable several hundred milliseconds.

APPLICATION OF THE CONTROLLER

Reactive Sputtering Drum Coater

The industrial reactive sputtering system examined for this work has a chamber volume of 700 liters with an effective pumping speed for Ar of 1100 liters/sec. The reactor turnover time, for this system is ~600 milliseconds. To prevent signal aliasing, the mole fraction should be sampled at least two times the rate dictated by this fundamental time constant of the reactive sputtering system with three to five times this rate preferred.

The industrial reactive sputtering batch drum coater is an octagon with a 50" maximum diameter. The system is equipped with a 47" diameter drum 20" in height, supported with spokes connected to a hub that engages a rotary vacuum feedthrough. The drum is rotated at one revolution per second. The system is equipped with two AC pairs of 5x15" rectangular magnetrons mounted on opposing facets of the octagon. Two other opposing facets of the octagon are equipped with two 5x15" planar microwave plasma wave guides. The differentially pumped mass spectrometer is mounted in the plenum of a 2000 liter/sec. turbo pump mounted at the bottom of the chamber on a 10" port inside the perimeter of the drum. One cathode pair is equipped with silicon targets and the other cathode pair is equipped with tantalum. Layers of each material are deposited by sequential passes of the substrate in front of a pair of the sputtering cathodes. The hysteresis behavior for each material is recorded with a fixed flow of 100 sccm of argon at the active cathode pair, 35 sccm of argon at each microwave plasma guide and oxygen flow, controlled by the feedback controller, is equally distributed between the two microwave plasma guides. The oxygen flow is controlled by two 0-200 sccm wave guide. Plasmas at each of the microwave plasma wave guides are driven at 2.45 GHz and 3 kW of forward power. The microwave plasmas activate and dissociate the molecular oxygen to monatomic oxygen radicals to improve the oxidation efficiency of the oxygen . A 40 KHz AC power supply operating at 8 kW drives the power on the AC cathode pairs.

PID Controller Effectiveness

In order to demonstrate the effect of the integral and derivative terms on the sputter coater response to a target start, a comparison of the temporal response with integral action and integral plus derivative action is presented. In this experiment a target is started instantaneously (within 35 milliseconds) and the response of the mole fraction and the manipulation of the oxygen flow by the controller is recorded. For this system the desired oxygen mole fraction set point is 7%.

In Figure 2 the response of a PI controller (derivative term set to 0) is recorded. The proportional and integral terms for this controller were 4 sccm/sec/% mole fraction and 1.5 sec., respectively. There are several features in the coater's response that are worth noting. The flow rate of oxygen at 0 seconds is that needed to keep the chamber at 7% mole fraction without the target energized. The difference between this and the final steady state at 10 seconds is the oxygen consumption by the reactive sputtering process. In this case the consumption is approximately 50 sccms of oxygen.

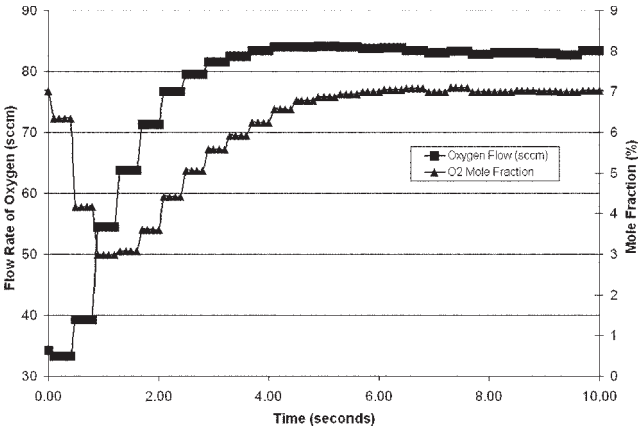

Figure 2: Coater response to a target start with P and I control.

In tuning the controller, the process engineer is careful not to introduce control settings that tend to overshoot the desired mole fraction set point. If the drum coater were to overshoot the desired mole fraction set point, there is a possibility that the target could poison. The process limitation of avoiding overshoot requires the process engineer to use conservative PI settings that tend to provide a somewhat sluggish response.

The sluggish response of the controller results in an oxygen deficient condition for approximately seven seconds. During this time the thin film deposited on the drum surface is not fully oxidized. To combat this problem, several methods have been employed to mitigate this effect. Slowly ramping the target power to permit the controller to keep up with the increasing oxygen consumption minimizes the poorly oxidized material but results in an ambiguity of the deposition

rate until the target stabilizes. In general, optical thin film designs do not have the same thickness for each layer so that the proportion of each layer represented by the target ramps is different resulting in poorer performing optical designs.

Another alternative is the use of target shutters to stabilize the targets before exposing the drum surface to the sputter flux. As the shutters are withdrawn and the drum surface is exposed, a perturbation is introduced in the consumed oxygen causing a similar disruption in oxygen mole fraction. The duration of this perturbation is dependent on the retraction time of the shutters. In practice, full shutter movement is approximately two to five seconds.

Derivative action is sometimes used to improve the controller's temporal response. In Figure 3, the effect of 0.5 seconds of derivative action is shown. Only a modest improvement in the temporal response is demonstrated by the derivative action reducing the stabilization time by about one second.

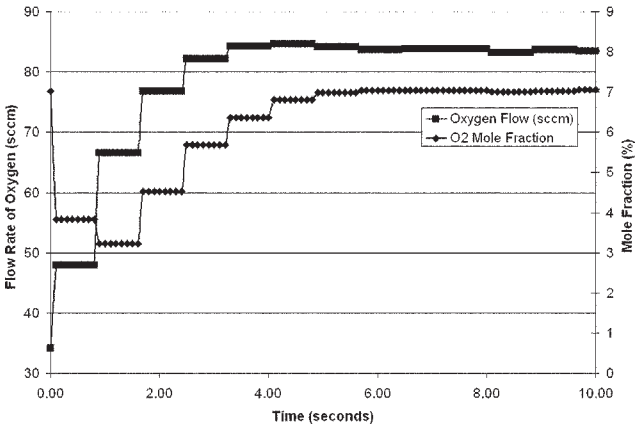

Figure 3: Coater response to a target start with P, I and D control.

IMPROVED CONTROLLER

It is obvious that an improvement in controller response to the perturbation introduced by the target start is desirable. The delay in the oxygen mole fraction response is attributed to several mechanisms. There is a lag of the MFC response, a transportation lag for the oxygen to flow from the MFC through the manifold, the inertia of the chamber and the lag associated with the gas sample arriving at the RGA. It is possible to anticipate the oxygen required by the sputtering process and provide a means for compensating for all of these delays.

Here we employ a feedforward controller that will provide an open loop addition to the output of the feedback controller. The feedforward controller's settings are the feedforward gain, K_F, and the feedforward lead, τ_F. The block diagram for this controller is shown in Figure 4.

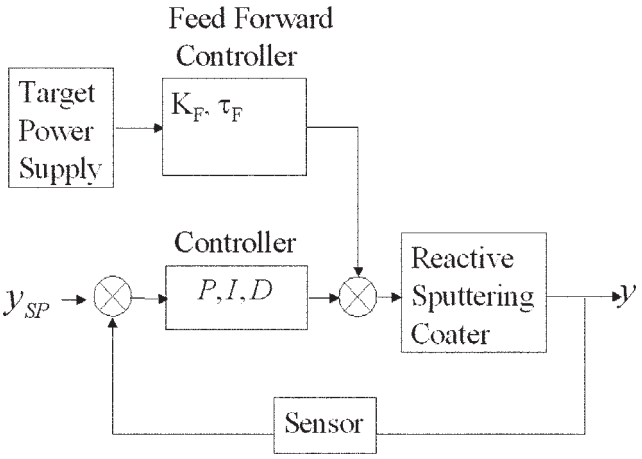

Figure 4: Control loop for feedforward controller with feedback trimming.

The effect of the feedforward gain is to provide a fixed flow of oxygen directly proportional to the power supplied via the target or targets energized. By referring to Figures 2 or 3, one can see the delay in the system response of the mole fraction with oxygen flow. It is important that the feedforward output be less than the total oxygen flow required at steady state so that the PID feedback controller can trim to the required flow. We have found for our drum coater that the feedforward output contribution should be approximately 70% to 80% of the total consumed oxygen flow required at steady state.

An example of the PID feedback controller with feedforward gain alone is shown in Figure 5. In this example the same PID gain set is used with the addition of a feedforward gain of 4.5 sccm/kW resulting in 36 sccm of oxygen flow from the feedforward controller. The response of the system is fairly dramatic. The addition of the feedforward action causes the mole fraction of oxygen to overshoot the desired 7% setpoint. However, there is still a slightly oxygen deficient condition, that while delayed by 1.75 seconds, does not stabilize for three seconds.

The delay in the oxygen flow stabilization can be further improved by addition of lead, τ_F, that anticipates the required oxygen flow at steady state and reacts before the disturbance is detected by the RGA sensor. The effect of 0.5 seconds of lead to the controller is shown in Figure 6.

The effect of the feedforward lead is to deliver more gas than is necessary at steady state for a short duration to compensate for the lags associated with the systems related to oxygen delivery and oxygen sensing, as described above. At the target start, the feedforward controller initially delivers 85 sccm for a duration of 500 milliseconds and then reduces this to minimize the overshoot of the oxygen mole fraction within the next 500 milliseconds. The oxygen depletion is further improved with the addition of this feedforward lead action.

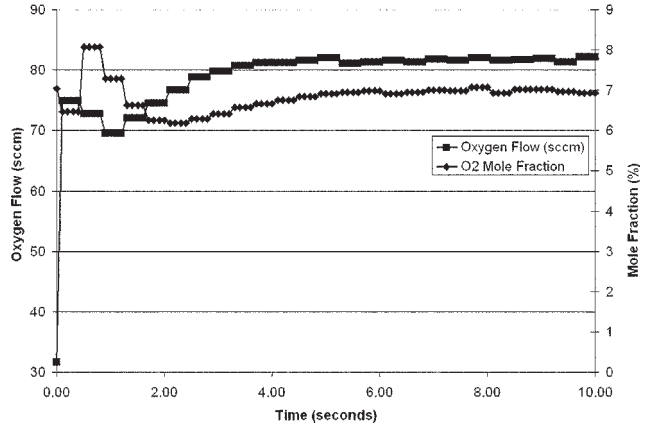

Figure 5: Coater response to a target start with feedforward gain and PID feedback trimming.

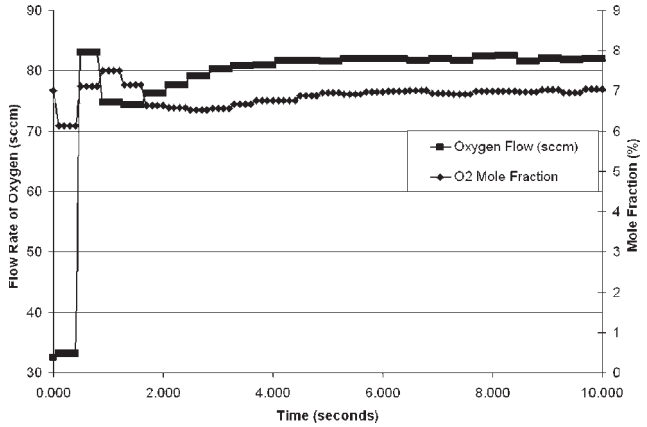

Figure 6: Coater response to a target start with feedforward gain and lead and PID feedback trimming.

CONCLUSION

The reactive sputtering batch coater requires a stabilization period after a target start. The disturbance represented by the sudden consumption of the reactive gas can lead to thin films with inhomogeneous stoichiometry. This inhomogeneity occurs at the interfaces that are often times the most sensitive portion in a thin film application. The commonly used PID controller while adequate for many applications is not capable of compensating for the target disturbance. More aggressive PID gain scheduling to improve response time will result in overshooting the desired mole fraction set point. An overshoot of the desired mole fraction set point can poison the target causing a loss of deposition rate stability. Our feedforward control loop operates by monitoring the power to the target or targets of the chamber and nearly eliminates the oxygen depletion condition.

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