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Optimization of a vacuum thermal evaporation process through Model-based Predictive Control of the source temperature

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Abstract: The Vacuum Thermal Evaporation (VTE) process is a technique for the production and deposition of thin films, which are used in various industrial applications. Here, the coating process is performed by evaporating a raw material in a high vacuum (HV) environment. The major goal is to produce a thin layer through a well-defined deposition rate. Due to high demands on the layer thickness, the tolerance for the temperature within the vacuum chamber is less than 0.2 K. This requieres the design of very well tuned controllers. In this paper, a Model-based Predictive Control (MPC) approach is presented for controlling the temperatures in the VTE process that explicitly takes into account the limitations arising from the requirements. First, the heat transfers within the heater and the source are investigated and described by physically motivated equations. As the heat transfer in the HV is dominated by radiation, this approach leads to a nonlinear system. Reliable measurement data are used to parameterize the previously derived dynamic model of the temperature behavior. An advantage of this physically motivated model is, in contrast to a linear operating point model, to allow an extrapolation and therefore to adequately depict the system behavior in a large operating range. Based on this approach, a MPC is developed and implemented on a pilot plant. It is shown that the high requirement on the temperature accuracy is met by the use of the proposed MPC. Experimental results show the potential of the introduced control scheme.

Keywords: Model-based control, physical model, predictive control, process parameter estimation, production systems, temperature control

1. INTRODUCTION

Thin films of a wide range of metallic, dielectric or semiconducting materials are used nowadays in many industries. Their applications range from surface finishing of architectural and automotive glass on applications in optics to highly technological applications in electrical engineering. Depending on the application, the layer thickness can range from a few nanometers to a few micrometers. Due to the varying requirements of the layer thickness, various manufacturing processes exist. One possibility for the production and deposition of thin films is the vacuum thermal evaporation process (VTE). In this coating technique the entire material of the film is heated by several heaters to temperatures near the boiling point. The evaporated material rises to the substrate on which it precipitates, condenses and forms a thin layer. As shown in (Steinberger et al., 2013a), a change in the temperature inside the source has a direct effect on the evaporation rate. Thus, the process can be significantly influenced and thereby later controlled by the temperature dependence of the evaporation source. Due to high requirements for the layer thickness in the investigated process, the admissible tolerance for the temperature inside the vacuum chamber has to be less than 0.2 K.

Depending on the material and its evaporation behaviour, different control schemes can be utilized. Regarding the deposition of metallic materials, PID-controllers are suggested in (Klokov and Galkina, 1991). For the deposition of organic semiconducting materials (Steinberger et al., 2013a) introduce a differential flatness-based control approach. A common feature of these control strategies is that the deposition rate is controlled directly, which imposes additional problems with the evaporation rate sensor in the investigated process which are not investigated here.

In this contribution a new control approach based on a cascade structure is presented. In case of a well tuned secondary loop (low-level) temperature controller, the primary loop (high-level) rate controller can have a much simpler structure. In this case the presented temperature control approach is formulated as a multiple-input multiple-output trajectory following problem. As the temperature trajectory, provided by a trajectory planner, is considered to be given over a finite time horizon and physical constraints such as the electric power limit shall be taken into account, a Model-based Predictive Control (MPC) scheme, as described in (Maciejowski, 2001), is utilized.

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A linear time-varying MPC (LTV-MPC) scheme has been chosen to cover model nonlinearities while being able to apply the controller in real-time during experimental tests.

This paper is organized as follows: Within section 2 the basic structure of a thermal evaporation plant is shortly introduced. Afterwards a physically based modeling approach which describes the thermal behavior of this process is presented. Subsequently, in section 3 the control scheme is outlined. Finally, experimental results are discussed in section 4. Conclusions will be drawn in section 5.

2. THE VACUUM THERMAL EVAPORATION PROCESS

2.1 System Description

As mentioned in the previous section, the VTE process is a proven method of thin film deposition. The entire structure of this process is located, as shown schematically in figure 1, in a vacuum chamber, surrounded by an actively cooled coat with temperature T_{Coat}. The material to be evaporated is poured into a crucible (Q) with temperature T_Q. The crucible is enclosed by a group of electric resistance heaters ($H_1, ..., H_n$) that transfer heat to the evaporating material (M), either directly via conduction or indirectly via thermal radiation, until the material reaches temperatures near the boiling point. The temperatures of the heating elements ($T_{S,1}, ..., T_{S,n}$) can be measured by temperature sensors on the inside of the crucible.

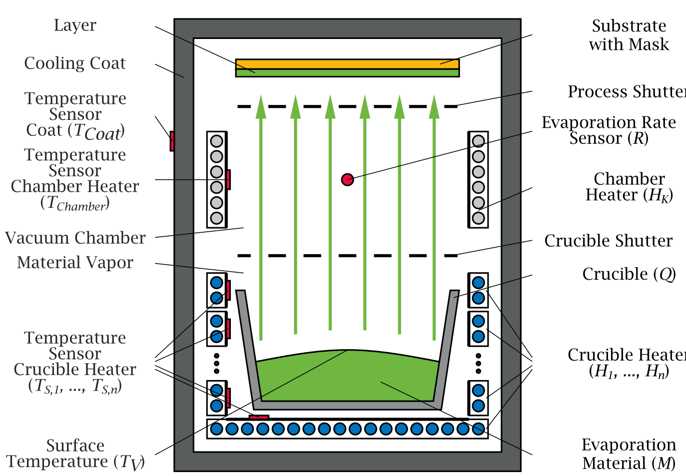

Fig. 1. Scheme of the VTE process with multiple heaters

However, direct measurement of the surface temperature (T_V) is not possible in the shown structure. To avoid oxidation and contamination of the coating by foreign atoms, the evaporation process takes place in a high vacuum (HV), causing the evaporation material to sublimate from solid to gaseous state. The evaporated particles spread almost perpendicular to the material surface. The material vapor leaves the crucible and passes through the open crucible shutter into the process chamber where the deposition rate can be measured. For this purpose, a sensor is positioned in front of the substrate in the presented system. The temperature in this section of the vacuum chamber can be influenced by an additional heater (H_K).

If the deposition rate is sufficiently high, the process aperture is opened and the material vapor reaches the substrate. Because the temperature of the substrate is lower than the material vapor, the vapor condenses and forms a thin layer. According to (Bunshah, 1994) the magnitude of the layer growth per time ranges from 100 to 250,000 Å/min. Therefore the layer growth is directly influenced by the deposition rate of the evaporation which results from the surface temperature. This can be set with the supplied heating power.

2.2 System Modeling

To create a simulation model of the evaporation process, as described in (Zöller et al., 2014), physical links need to be identified in the evaporation of the material in the crucible. The description of the surface temperature T_V is of particular importance, as this is crucial for the evaporation rate and, consequently, for the resulting layer thickness. If during the thermal evaporation a homogeneous density of the material to be evaporated and a uniform growth of the layer can be assumed, the stationary evaporation rate R_{stat} is, according to the kinetic theory of gases (Steinberger et al., 2013b), a function of T_V:

$$R_{stat} = c_1 \cdot \frac{e^{-\frac{c_2}{T_V}}}{\sqrt{T_V}} \quad (1)$$

with the material parameters c_1 and c_2 respectively.
By stating the heat balance of the components of the vaporization system, the relationship between the heating and the surface temperature can be modeled. To construct a process model of the evaporation system, it is necessary to study the heat transfer within the vacuum chamber. The basic procedure for modeling the present evaporation plant will be considered briefly below.

From the fundamental equation of thermodynamics:

$$\Delta Q = m \cdot c_p \cdot \Delta T \quad (2)$$

the relationship between a change in temperature ΔT of a body and the recorded output heat ΔQ can be obtained as a function of its mass m and its specific heat capacity c_p. To maintain an expression for the temperature change of a body over time due to the net heat flow $\Delta\dot{Q}$, it is necessary to differentiate with respect to time:

$$\Delta\dot{Q} = m \cdot c_p \cdot \frac{dT}{dt} \quad (3)$$

Accordingly, the temperature change of a body can be modeled based on a heat balance which arises from the difference of the supplied ($\dot{Q}_s$) and the dissipated ($\dot{Q}_d$) heat flows:

$$\Delta\dot{Q} = \dot{Q}_s - \dot{Q}_d \quad (4)$$

For modeling the presented evaporation system it is assumed that the dominant heat flows are based on thermal radiation and heat conduction.
The dependence of the heat flow $\dot{Q}_C$ due to thermal conduction between any two bodies, such as body A and body B in figure 2 is given by:

$$\dot{Q}_{C,A\to B} = -K_{C,AB} \cdot (T_A - T_B) = -\dot{Q}_{C,B\to A} \quad (5)$$

with $K_{C,AB} = (\lambda_{A,B} \cdot A_{A,B})/d_{A,B}$ describing the dependence of the heat flow on the thermal conductivity λ_{AB}, the thickness $d_{A,B}$ and the surface area $A_{A,B}$. The direction of the thermal conduction is taken into account