

Determination of heat fluxes and surface temperatures during magnetron sputtering with a cold and hot target

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Abstract. The method of calculation of heat fluxes and surface temperatures during magnetron sputtering of cold and hot targets developed from using the algebraic method for calculating radiant fluxes is presented, which allows to predict the required power characteristics for obtaining the desired temperature on the target and the substrate. Comparison of the experimental data and the demonstrated results of the calculations testify to the possibility of applying this technique. The temperature on the substrate can be controlled by changing the distance between the substrate and the target within certain limits, and the value of the distance can be estimated using the suggested calculation model.

The processes of obtaining films by the method of magnetron sputtering are accompanied by heating of the substrate [1–3]. When forced heating is used, the actual substrate temperature can be significantly higher than the assumed value due to the thermal processes during sputtering [4, 5]. The determination of the substrate temperature is essential for various processes [6, 7]. To solve it calculation of the heat fluxes in the process under consideration is required. Such calculation makes it possible to compare the thermal effect of the process with the geometric parameters of the system of bodies under consideration for the magnetron sputtering flowsheet specified, as well as with the target size and mass, making it possible to estimate the temperature and time of substrate heating depending upon the shape, size and material of the elements in the working chamber of the process unit. This approach allows calculations for processes with both cold and hot targets. The thermal scheme of the process in hand is shown in figure 1.

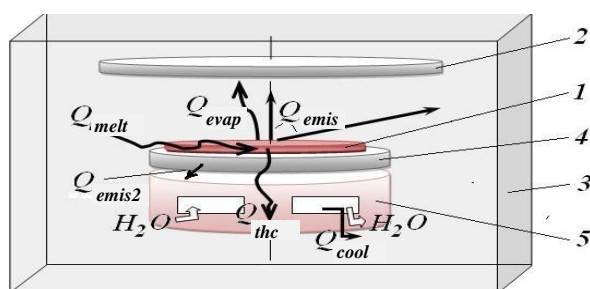


Figure 1. The thermal scheme of the process in hand:

1 – target, 2 – substrate, 3 – working chamber, 4 – crucible, 5 – magnetron.



The thermal flow P is the power released in a magnetron sputtering unit which generates a stream of ions bombarding the target 1. The part of the full power which provides heating and melting the target to the liquid state, when needed, will be referred to as the net power P_{net} within the framework of the task. After warming up the target to the preset temperature the net power is spent on the compensating of heat loss fluxes, of which the following will be considered significant: the heat flow Q_{emis} of the heated target emission onto the substrate 2 and the walls of the working chamber 3; the heat flow Q_{thc} of the thermal conductivity from the target to the magnetron 5 through the crucible (target holder) 4 or the heat flux Q_{emis2} of crucible emission onto the surface of the water-cooled magnetron; the heat flux Q_{evap} transported onto the substrate and the walls of the working chamber by the target material evaporated from the target; the heat flux Q_{melt} spent on the target melting.

The heat loss power P_{loss} is a part of the full power spent on heating the magnetron itself, which equals the value of the heat flux Q_{cool} given to the cooling liquid in case of magnetron cooling. It should be borne in mind that the full value of the heat flux taken from the inner surface of the magnetron during its liquid cooling equals the sum $Q_{cool} + Q_{thc}$ or $Q_{cool} + Q_{emis2}$.

Let's compose the heat balance equation on the assumption that the system goes to steady-state condition during the process under consideration. In this case, the released thermal energy has a useful component, distributed in accordance with the above mechanisms, and the heat loss power

$$P = P_{net} + P_{loss},$$

$$P = Q_{emis} + Q_{thc}(\text{or } Q_{emis2}) + Q_{evap} + Q_{melt} + Q_{cool}.$$

The heat flux during the target material melting Q_{melt} , W, in a time τ , sec

$$Q_{melt} = \frac{Q_{\tau_{melt}}}{\tau}.$$

Where the heat of the target material melting $Q_{\tau_{melt}}$

$$Q_{\tau_{melt}} = c_{melt}m.$$

The heat flux Q_{evap} of the evaporated target material, W

$$Q_{evap} = 5,83 \cdot 10^{-5} \cdot k N_A p_{sat} \left(\frac{T_{evap}}{M} \right)^{\frac{3}{2}} F_{evap} \text{ [W]},$$

where T_{evap} – the evaporation temperature, K; k – Boltzmann constant, J/K; N_A – Avogadro constant, atom/mol; M – molar mass of the evaporant, kg/mol; p_{sat} – saturated vapour pressure of target material, Pa; F_{evap} – evaporation surface area, m².

In case of a gap, the heat flux from the target to the magnetron is defined by the value of the emission heat flux from the crucible to the magnetron

$$Q_{emis2} = \sigma_0 \frac{T_{cr}^4 - T_{mag}^4}{\frac{1}{\varepsilon_{cr}} + \frac{1}{\varepsilon_{mag}} - 1} F_{cr}.$$

The greatest difficulty is the calculation of the emission heat flux Q_{emis} from the target surface onto the substrate and the walls of the working chamber. The difficulty is that in this case it is the matter of the radiant interaction of several surfaces with different temperatures and emission coefficients. It is expedient to solve similar problems using the algebraic method. Let's use the computational scheme shown in figure 2.

The algebraic system of radiant heat transfer for the scheme under consideration is as follows:

$$\begin{aligned} Q_{res1} &= \varphi_{21}(E_{02}F_2 + R_2Q_{res2}) + \varphi_{31}(E_{03}F_3 + R_3Q_{res3}), \\ &\quad -(E_{01}F_1 + R_1Q_{res1}), \\ Q_{res2} &= \varphi_{12}(E_{01}F_1 + R_1Q_{res1}) + \varphi_{32}(E_{03}F_3 + R_3Q_{res3}), \\ &\quad -(E_{02}F_2 + R_2Q_{res2}), \end{aligned}$$

$$Q_{res3} = \varphi_{13}(E_{01}F_1 + R_1Q_{res1}) + \varphi_{23}(E_{02}F_2 + R_2Q_{res2}), \\ -(1 - \varphi_{33})(E_{03}F_3 + R_3Q_{res3}).$$

We'll make the calculations for the case that the substrate has a thermal decoupling with the walls of the working chamber. T_1 and T_3 are known, T_2 on the substrate holder is unknown, the heat equilibrium is ($Q_{res2}=0$). It is possible to determine the power emitted by the target using the condition $Q_{emis}=Q_{res}=Q_{res1}=Q_{res3}$, as the equation

$$Q_{res1} + Q_{res2} + Q_{res3} = 0$$

is valid for the entire system in the steady-state condition.

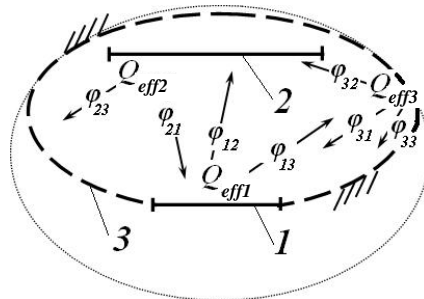


Figure 2. The computational scheme for determining the emission heat flux from the substrate surface: 1 – target, 2 – substrate, 3 – walls.

After calculating the corresponding determinants, taking into account the values of the angle coefficients φ_{ij} , the emission coefficients ε_i or the fractional reflectivities R_i , the known temperatures and areas T_1 , T_3 , F_1 , F_2 , F_3 , we determine the unknown values of the resultant flux Q_{res} and the intrinsic emission of the surface 2 as an absolute black body

$$Q_{res} = \frac{\Delta Q_{res}}{\Delta}, \\ E_{02} = \frac{\Delta E_{02}}{\Delta} \frac{1}{F_2}.$$

When determining the heat loss flux of the magnetron sputtering system, namely, the heat flux vented by the cooling liquid, it is problematic to distinguish the component Q_{cool} , which is determined by the heat liberation in the magnetron itself. It is more correct to talk about the heat dissipation of the total heat flux $Q_{cool} + Q_{thc}$ or $Q_{cool} + Q_{emis2}$. This value can be most easily determined for any time point during the system operation by registering the coolant temperature upstream of the cooling system t_{cool_in} and downstream of it t_{cool_out} , as well as the flow rate W_{cool} of the coolant with the heating capacity c_{cool} by the formula

$$Q_{cool} + Q_{thc} \text{ (or } Q_{cool} + Q_{emis2}) = c_{cool}W_{cool}(t_{cool_out} - t_{cool_in}).$$

In the absence of such data, the power Q_{cool} , released as heat during the interaction between the electromagnetic field and the magnetron, can be estimated as a fraction of the total power

$$Q_{cool} = \eta P.$$

According to the available estimates, the coefficient value is $\eta = 0,6 \dots 0,8$. Using this approach, it is possible to determine the values of all the components of the heat fluxes when the desired temperature on the target is reached. Having made a similar calculation for various intermediate temperature values in the range of room temperature to the required maximum, one can obtain the temperature dependences

$$P(T) = Q_{emis}(T) + Q_{thc}(T) \text{ [or } Q_{emis2}(T)] + Q_{evap}(T) + Q_{melt}(T) + Q_{cool}(T).$$

If the supplied power is fixed at the level $P_{roundup}(T_{max})$ which is somewhat larger than the total loss power generated when the required maximum temperature on the product T_{max} is reached, assuming that the magnetron is almost immediately output to this power upon power-up, it is possible

to determine the power Q_{heat} , spent on heating the target and the heat-insulated substrate during a temperature change in time as a function of $Q_{heat}(\Delta T)$

$$Q_{heat}(\Delta T) = P_{roundup}(T_{max}) - P(\Delta T),$$

$$Q_{heat}(\Delta T) = P_{roundup}(T_{max}) - [Q_{emis}(\Delta T) + Q_{thc}(\Delta T)[\text{or } Q_{emis2}(\Delta T)] + Q_{evap}(\Delta T) + Q_{melt}(\Delta T) + Q_{cool}(\Delta T)].$$

where ΔT is the temperature excess between the current temperature of the target and its initial temperature equal to the ambient temperature.

Let's depict the obtained dependence $Q_{heat}(\Delta T)$ graphically and form the corresponding trend line, for example, in the form of a polynomial. Assuming the heat accumulated by the substrate is insignificant, it is possible to calculate the target temperature history from the following fundamental equation

$$Q_{heat}(\Delta T)d\tau = c_v m d(\Delta T),$$

where $d\tau$ is the time interval during which the body of mass m with the specific mass heat capacity c_v is heated by the value $dT = d(\Delta T)$ at a temperature T at a power $Q_{heat}(\Delta T)$, spent on heating. Let's transform the formula

$$d\tau = \frac{c_v m}{Q_{heat}(\Delta T)} d(\Delta T).$$

Taking $c_v = \text{const}$, we can integrate and determine the minimum time of the target heating to a given temperature

$$\tau = \int_0^{\tau_{heat}} d\tau = \int_{T_0}^{T_{end}} \frac{c_v m}{Q_{heat}(\Delta T)} d(\Delta T).$$

The time of heating the target to the maximum temperature is much less than the time of heating the substrate to the maximum temperature. To calculate the substrate heating time, let's use the same approach as for calculating the target heating time, using the dependence of the power $Q_{heat,s}(\Delta T)$ spent on the substrate heating during the magnetron sputtering process at the maximum target temperature instead of $Q_{heat}(\Delta T)$.

Let us consider the results of the calculations performed for some experimentally studied processes [8]. The experiments on sputtering copper and titanium targets were carried out by the authors in a vacuum chamber with a volume of $7.8 \cdot 10^{-2} \text{ m}^3$, equipped with a flat magnetron with a diameter of 160 mm, operating on a direct current. A target of 1 mm thickness was bolted to a copper water-cooled card with a 1 mm gap. The residual pressure did not exceed 10^{-2} mT . The sputtering was carried out in an argon medium under a pressure of $p = 5\text{--}10 \text{ mT}$ and at a current density of $j = (5.5\text{--}14.4) \text{ mA/cm}^2$. A thermocouple sensor was used to study the thermal processes on the substrates, its sensitive element being a copper plate $10 \times 10 \text{ mm}^2$ with a thickness of 1 mm, on which a junction of the thermocouple was fixed. In each experiment, the sensitive element temperature change was measured for a given value of p and j during the magnetron operation.

According to the computational model, to heat a copper target in the solid state to a temperature close to the melting point of 1084°C , the required useful power of the magnetron should be in the range of 465–560 W. At the same time, when the distance between the target and the substrate varies from 40 to 160 mm with the above dimensions of the interacting surfaces, the maximum substrate heating temperature falls from 511 to 203°C (figure 3, curve 1). For a titanium target in the solid state around the melting point of 1668°C , the estimated required useful power of the magnetron is in the range of 1220–1500 W, and the maximum substrate heating temperature falls from 712 to 314°C with a change in the distance from the target in the same range (figure 3, curve 2).

The calculations of the substrate heating time as a function of the target heating temperature and the distance from the target to the substrate were carried out for the distance between the substrate and the target of 120 mm. In this case, for a given system configuration, the substrate heating time for a copper target with a maximum temperature of 800 and 1000°C is shown in figure 4, for a titanium target – in figure 5.

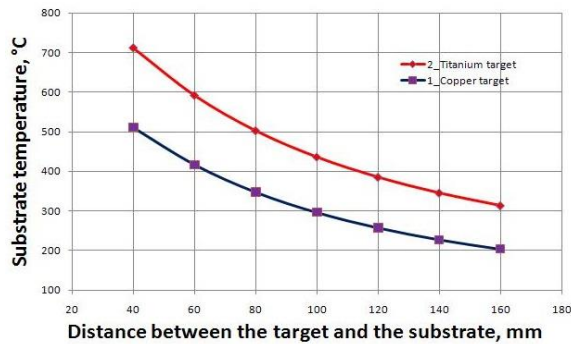


Figure 3. The substrate temperature, °C, change as a function of the change of the distance between the target and the substrate, mm, at the solid target temperature: 1 – copper at 1084 °C, 2 – titanium at 1668 °C.

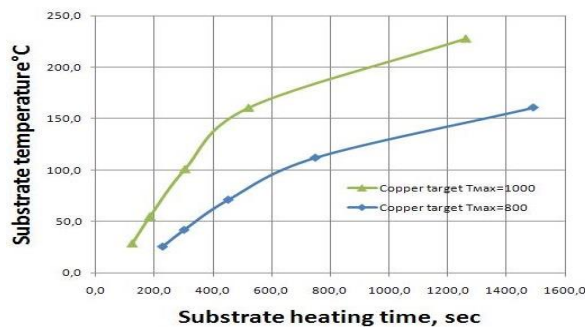


Figure 4. Temperature and time of the substrate heating in the system with a copper target with the maximum temperature of 800 and 1000 °C.

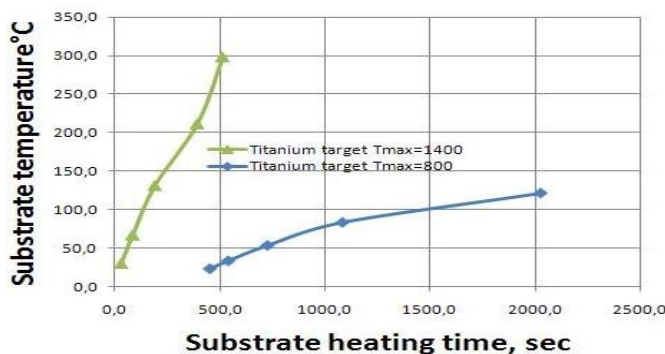


Figure 5. Temperature and time of the substrate heating in the system with a titanium target with the maximum temperature of 800 and 1400 °C.

Hence, a comparison of the experimental data and the presented calculations indicate the possibility of using the presented technique for calculating the heat fluxes and surface temperatures during magnetron sputtering of cold and hot targets, allowing to predict the required power characteristics to obtain the required temperature on the target. The temperature on the substrate can be controlled within certain limits by changing the distance between the substrate and target the value of which can also be estimated through the proposed computational model.

The computational task complexity was associated primarily with the lack of all the necessary data in the source used, for example, concerning the size and relative position of the target and the substrate. Therefore, the values of some important system parameters, which can significantly differ from the real ones, were used in the calculations, what is probably one of the main reasons for the deviation of the calculated results from the experimental ones. The refinement of the system characteristics will allow estimating the accuracy of the model more qualitatively.

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