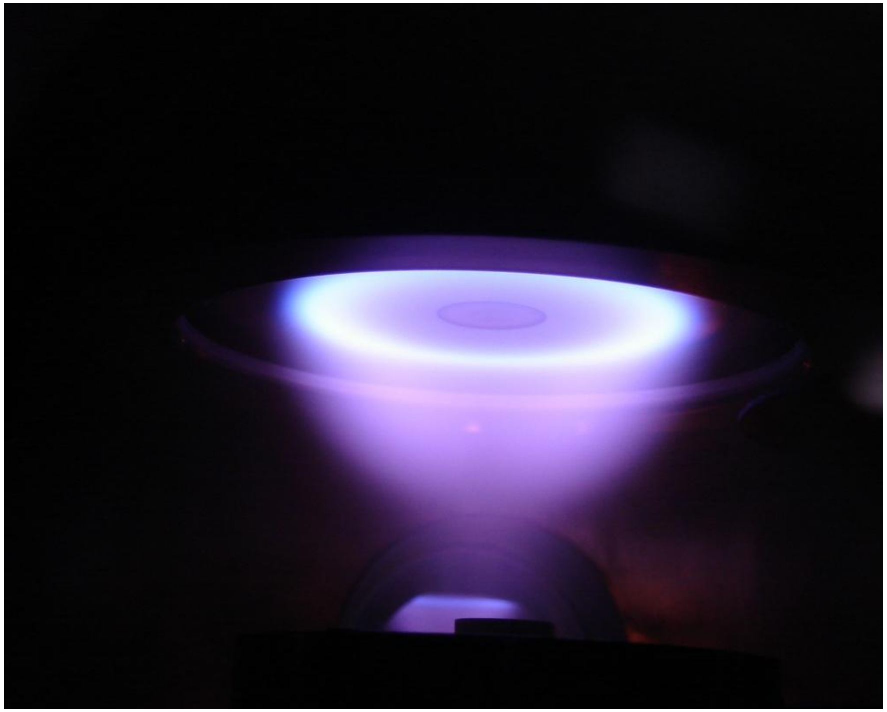
Modelagem de deposição reativa por sputtering usando o modelo de Berg

J. C. Sagás

Sumary

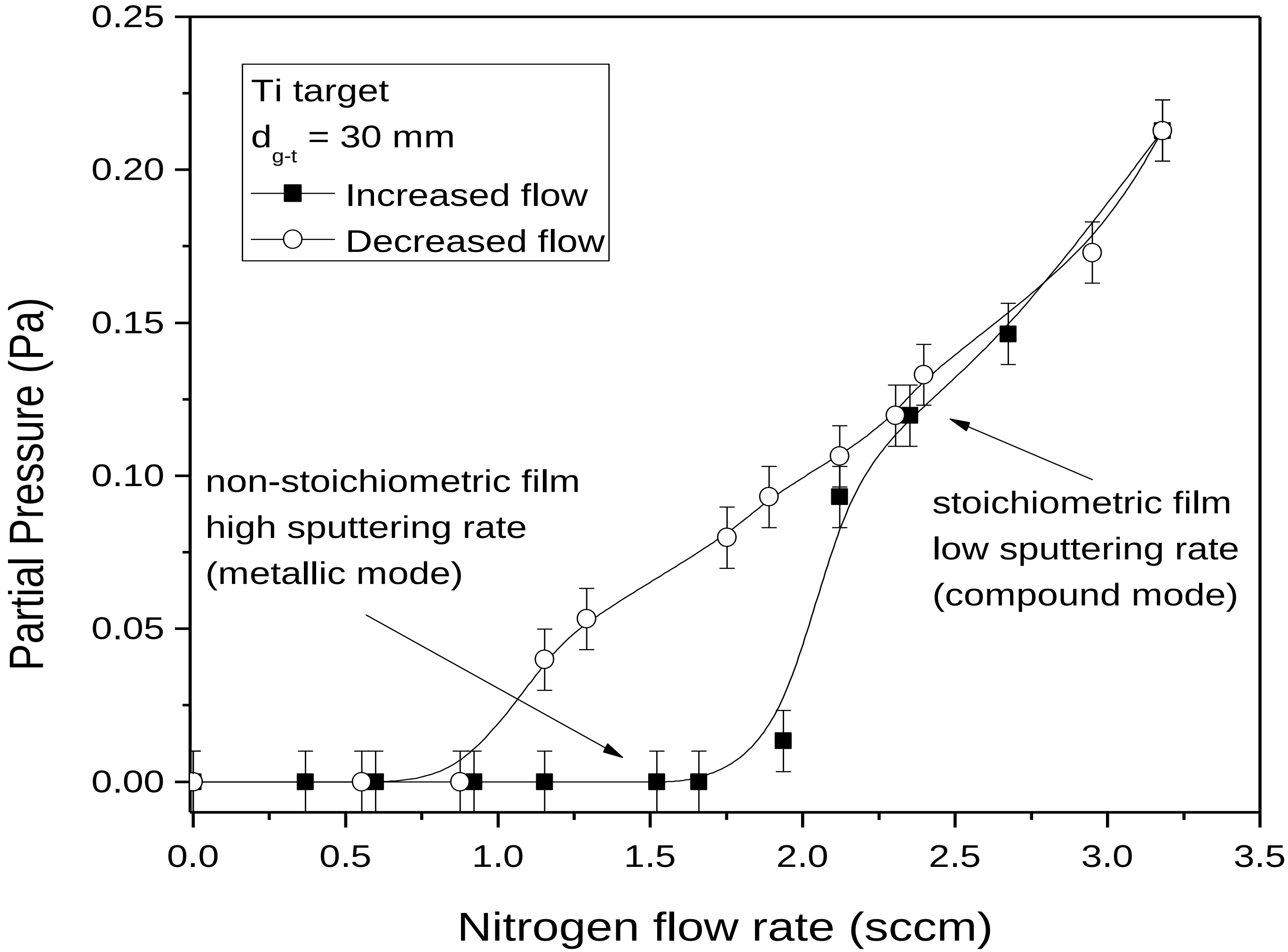
- Reactive sputter deposition: the hysteresis problem
- Berg's model: a qualitative way to understand the process
- TMS (GAMS)
- Model and experiments
- Results
- Conclusions

Reactive sputter deposition



- Efficient way to deposit compound films from metallic targets;
- Formation of compound both in the film and on the target surface;

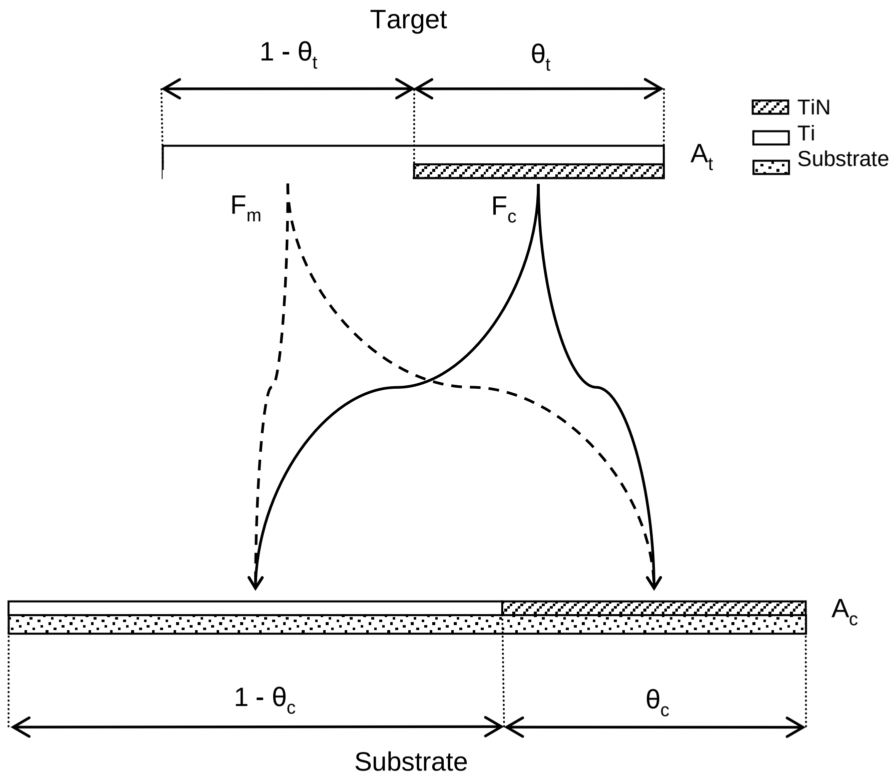
Hysteresis



Ti target
d g-t = 30 mm
Increased flow
Decreased flow
non-stoichiometric film
high sputtering rate
(metallic mode)
stoichiometric film
low sputtering rate
(compound mode)
Partial Pressure (Pa)
Nitrogen flow rate (sccm)
0.00
0.05
0.10
0.15
0.20
0.25
0.0
0.5
1.0
1.5
2.0
2.5
3.0
3.5

Berg's model

- A qualitative way to describe reactive sputter deposition



$$\frac{J}{q} Y_c \theta_t = 2\alpha F (1-\theta_t)$$

$$2Q_c + F_c(1-\theta_c) = F_m \theta_c$$

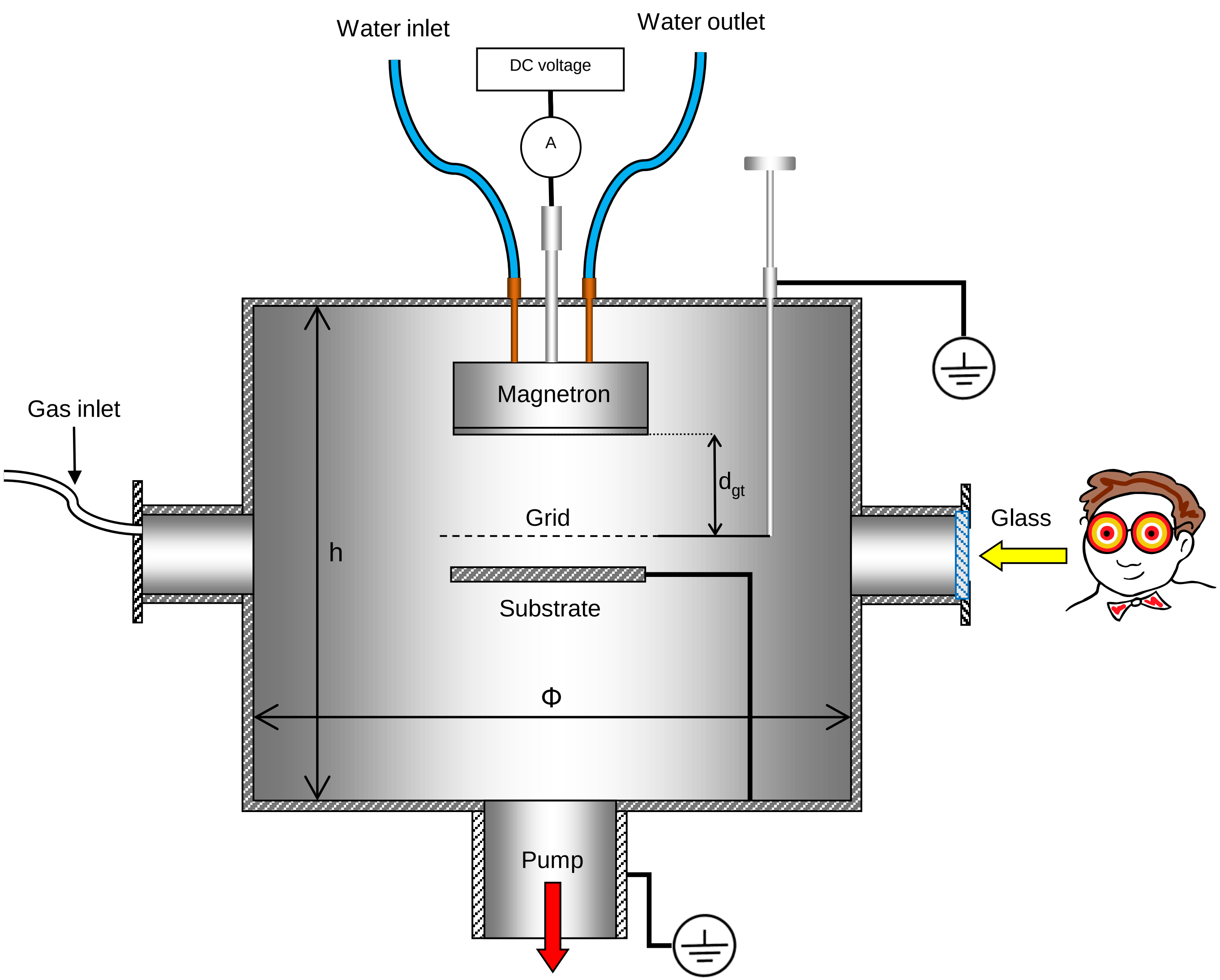
$$Q_{total} = Q_t + Q_c + Q_p$$

S. Berg, T. Nyberg, Thin Solid Films, 476 (2005) 215-30.

How to avoid hysteresis?

- Gas pulsing
- Small target
- High pumping speed
- And others
- And about geometry system?

TMS (GAMS - Grid Assisted Magnetron Sputtering)



L. C. Fontana, J. R. L. Muzart., Surf. Coat. Technol., 107 (1998) 24-30.

GAMS - Grid Assisted Magnetron Sputtering

- Reduction and, in some cases, elimination of the hysteresis. But what is the mechanism?

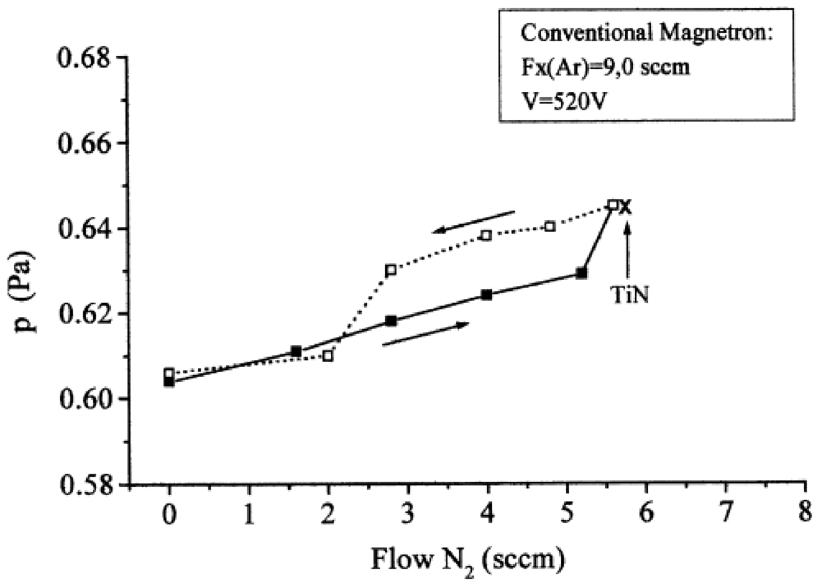


Fig. 4. Evolution of the total pressure as a function of N_2 flow in the conventional magnetron. The argon flow is fixed at 9.0 sccm.

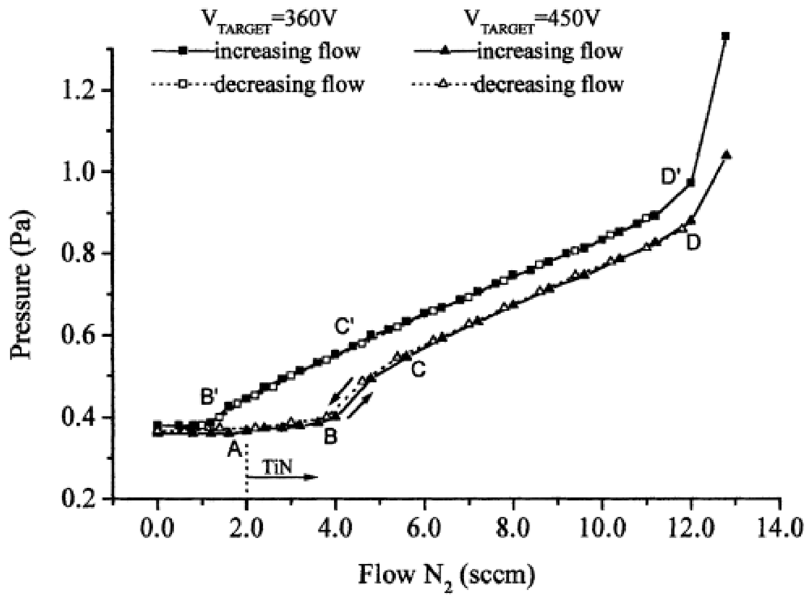


Fig. 5. Evolution of the total pressure as a function of N_2 flow in the triode configuration. The argon flow is fixed at 5.6 sccm.

L. C. Fontana, J. R. L. Muzart., Surf. Coat. Technol., 114 (1999) 7-12.

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Modeling reactive sputter deposition of titanium nitride in a triode magnetron sputtering system

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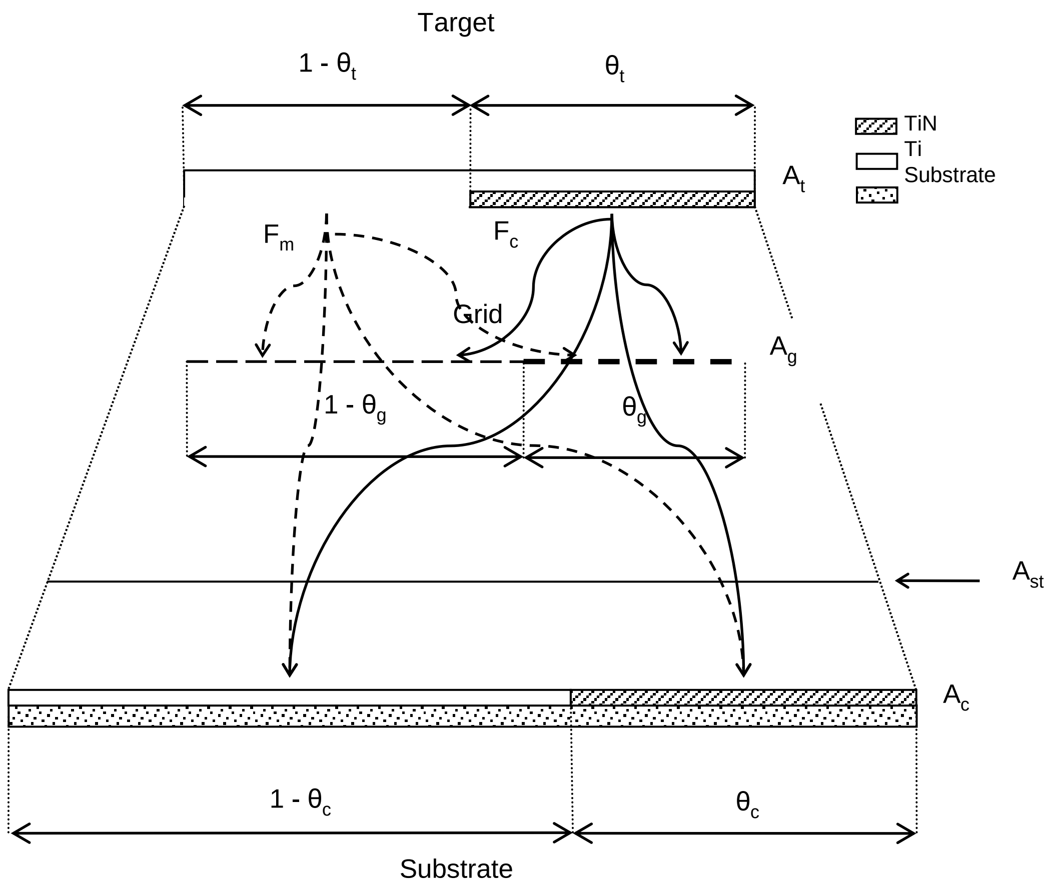
Titanium nitride

A B S T R A C T

In this paper, the so-called Berg's model was successfully employed in order to model the reactive sputter deposition of titanium nitride (TiN) by a triode magnetron sputtering (TMS) system. Such system consists of a grounded grid introduced between the target and the substrate. The grid acts as the anode, and the glow discharge is formed between the target and grid. The qualitative model was compared to experimental data. In addition, results from a conventional MS system were also compared to the ones from the modified TMS system. It was possible to observe that (a) the width of the hysteresis region is narrower for TMS for all modeled conditions; (b) the hysteresis width increases as a function of grid-to-target distance.

Berg's model applied to GAMS



$$\frac{J}{q} Y_c \theta_t = 2\alpha F(1-\theta_t)$$

$$2Q_g + F_c(1-\theta_g)\beta = F_m \theta_g \beta$$

$$2Q_c + F_c(1-\theta_c)(1-\beta) = F_m \theta_c (1-\beta)$$

$$Q_{total} = Q_t + Q_c + Q_g + Q_p$$

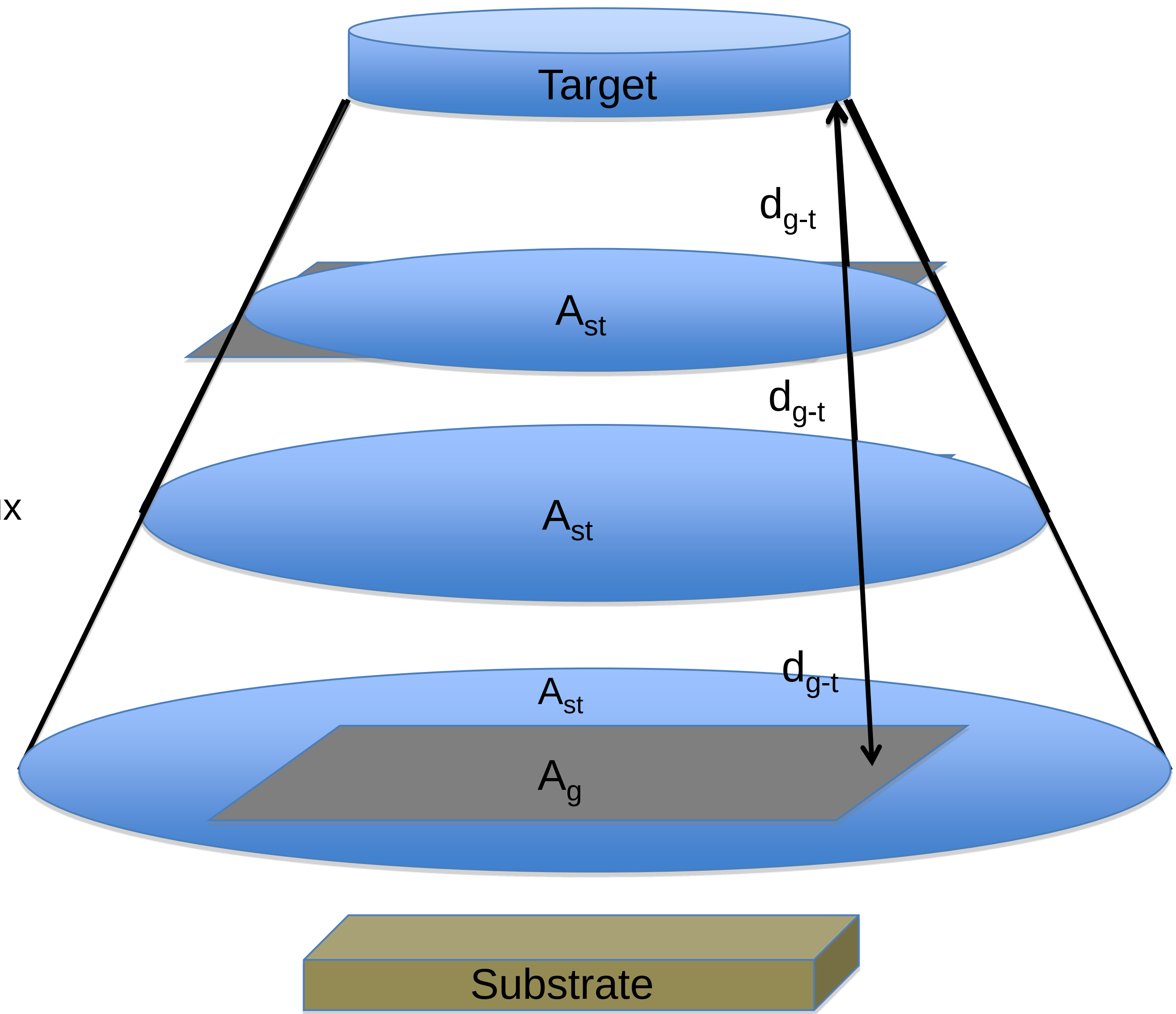
$$\beta = \frac{A_g}{A_{st}}$$

Berg's model applied to GAMS

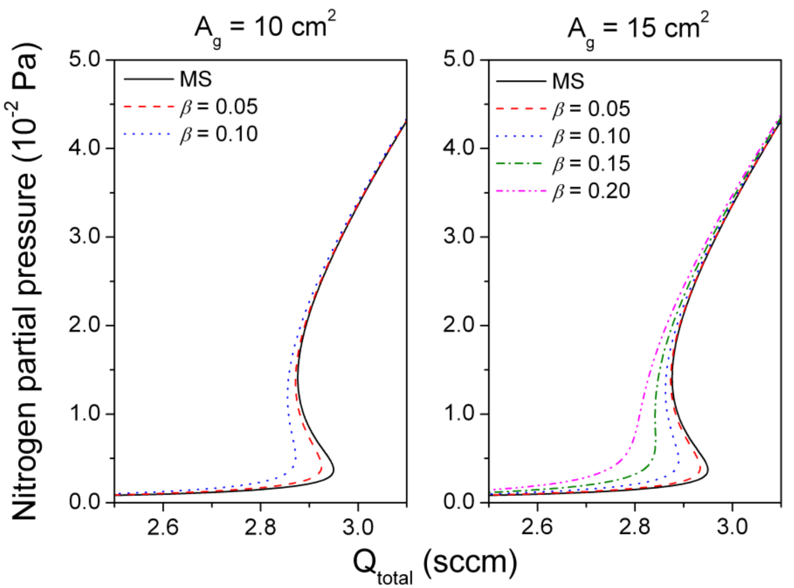
$$\beta = \frac{A_g}{A_{st}}$$

A_g – effective grid area

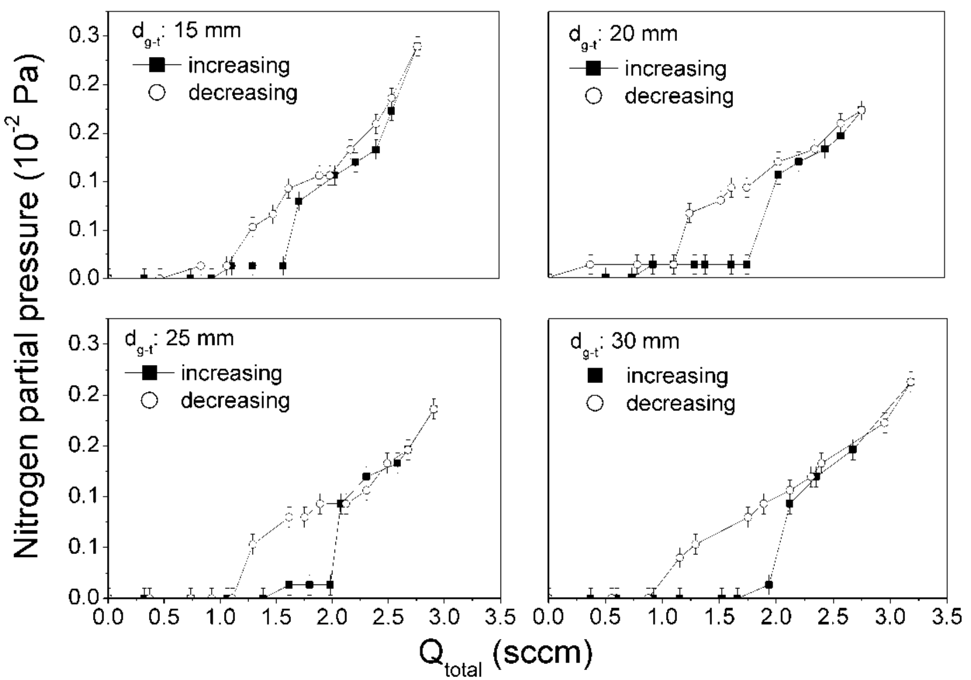
A_{st} - transversal area of the sputtered particles flux



Model and experiments

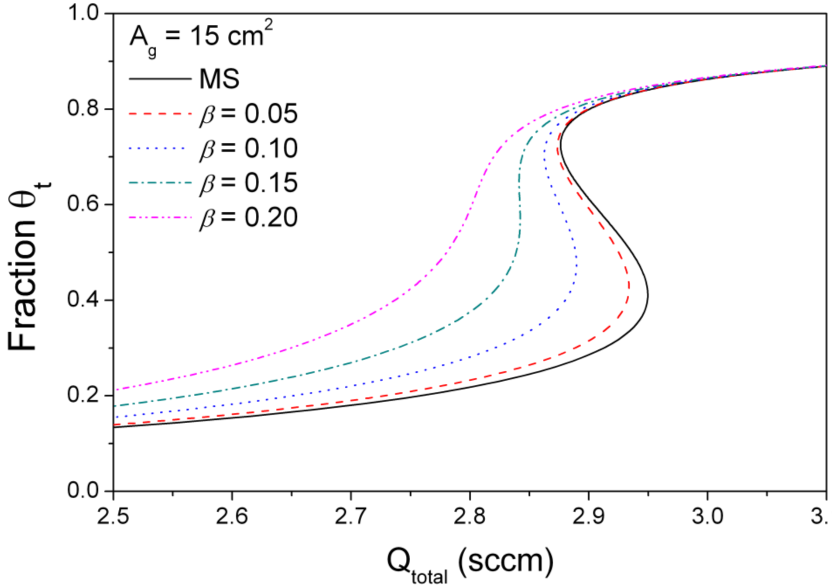


- Reduced hysteresis with increased β



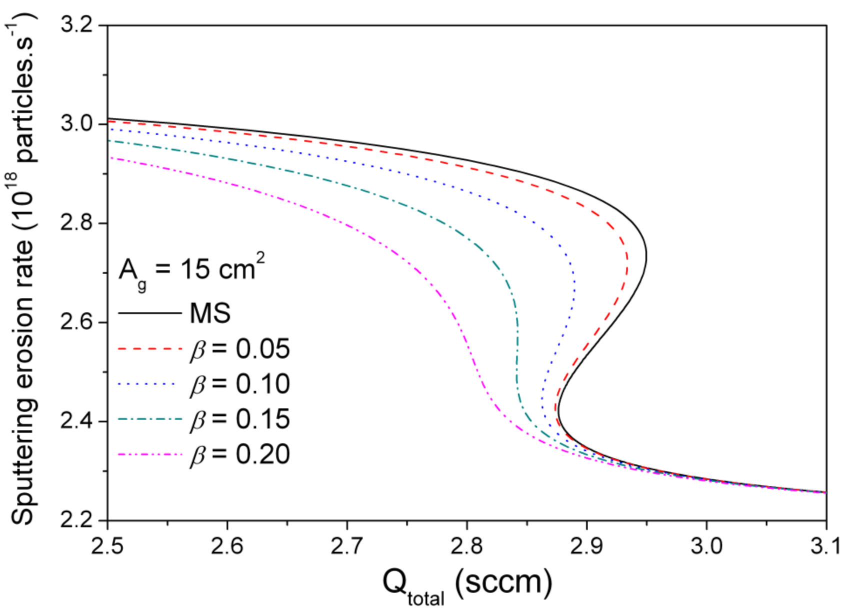
- Reduced hysteresis with decreased $d_{g\text{-}t}$

Sputter erosion rate

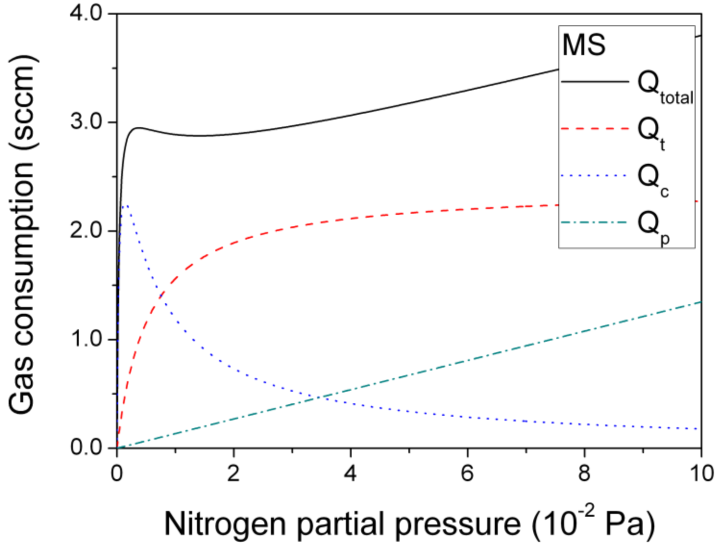


- Increasing β the target is poisoned faster

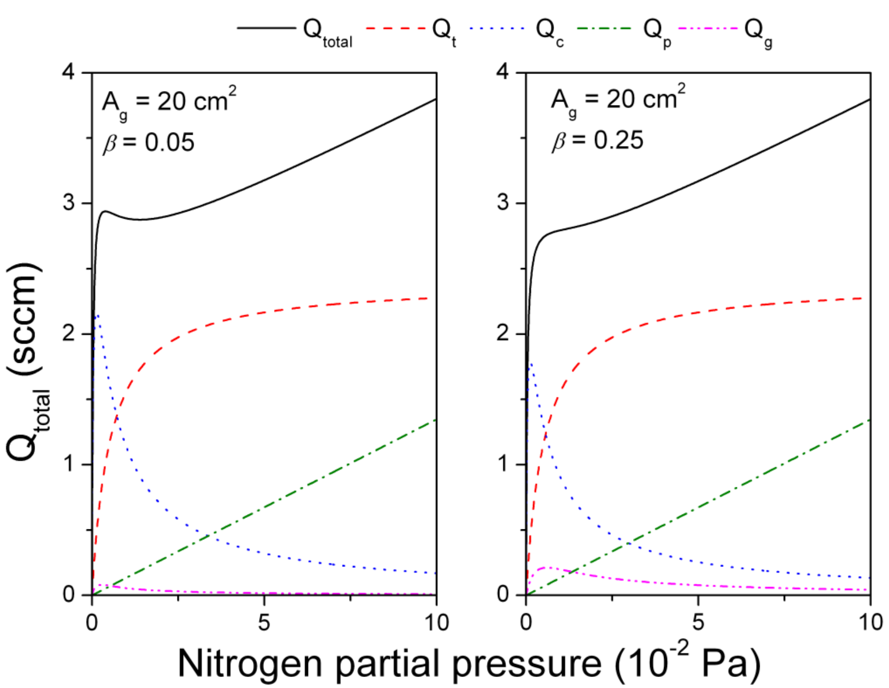
- This results in a lower sputtering rate



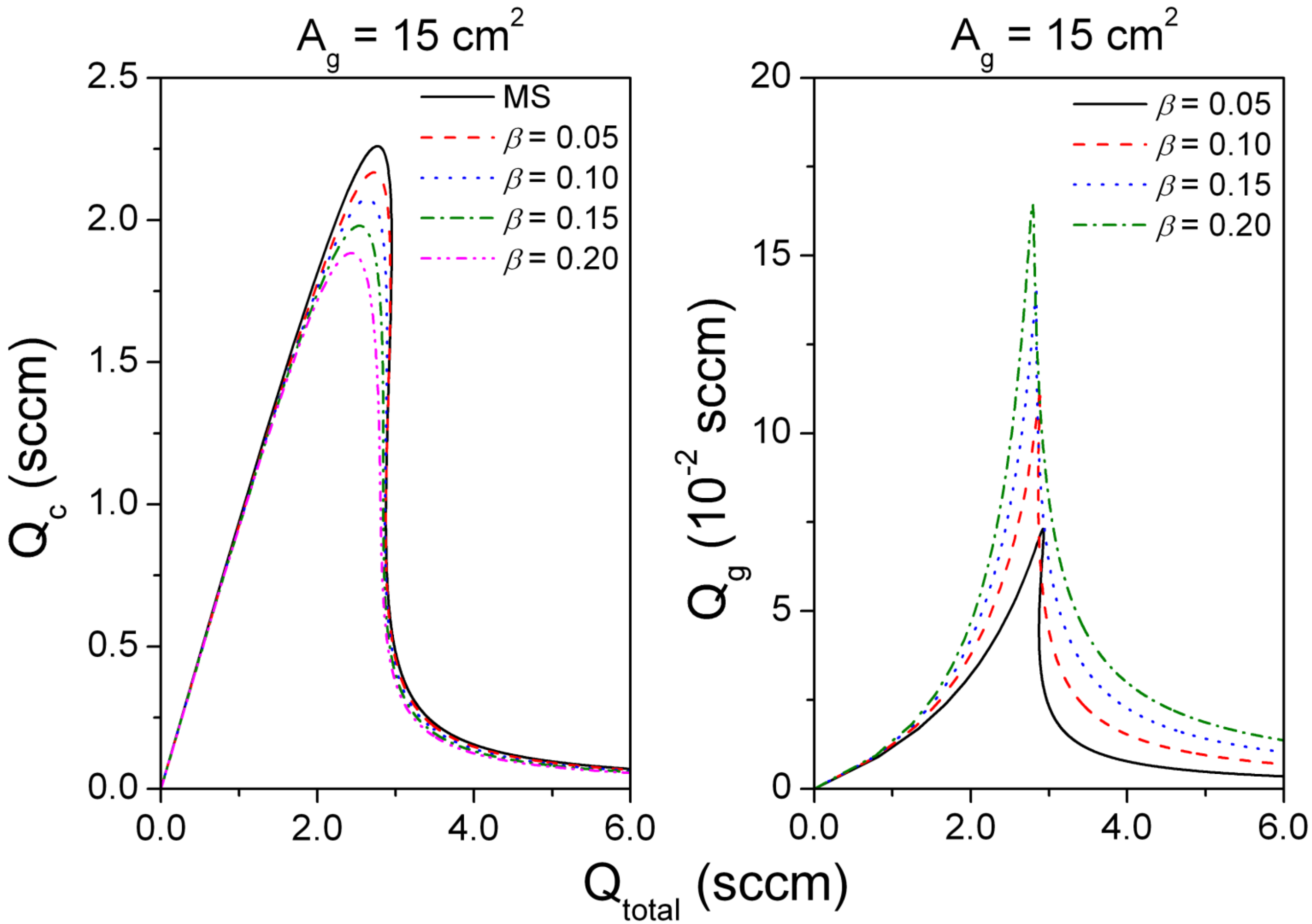
The effect of the grid



The introduction of the grid decreases the role of the collecting area



The effect of the grid



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Modeling the reactive sputter deposition of N-doped TiO_2 for application in dye-sensitized solar cells: Effect of the O_2 flow rate on the substitutional N concentration

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ABSTRACT

In this paper an original numerical model, based on the standard Berg model, was used to simulate the growth mechanism of N-doped TiO_2 deposited at different O_2 concentrations in the reactive gas mixture. For evaluation of the numerical model, films were deposited in the same conditions as those used in the numerical approach. Films were analyzed by profilometry, optical spectrophotometry, Rutherford back-scattering spectroscopy (RBS) and X-ray photoelectron spectroscopy (XPS). Results show that oxidation of TiN plays a fundamental role for incorporation of substitutional N in the TiO_2 lattice and the overall structure of the films, as well as, the chemical composition obtained from numerical model is in agreement to experimental data.

Deposição de TiO_xN_y

Table 1
Reactions employed in the numerical model.

i	Reaction	Equation
1	$Ti(s)+O_2(g) \rightarrow TiO_2(s)$	$Q_1^S = \alpha_{\theta_{6S}}^{O_2} F_{O_2}\theta_{6S}A_S$
2	$Ti(s)+O(g) \rightarrow TiO(s)$	$Q_2^S = \alpha_{\theta_{6S}}^{O} F_O\theta_{6S}A_S$
3	$TiO(s)+O(g) \rightarrow TiO_2(s)$	$Q_3^S = \alpha_{\theta_{4S}}^{O} F_O\theta_{4S}A_S$
4	$TiO(s)+N(g) \rightarrow O{-}Ti{-}N(s)$	$Q_4^S = \alpha_{\theta_{4S}}^{N} F_N\theta_{4S}A_S$
5	$2TiO(s)+N_2(g) \rightarrow 2O{-}Ti{-}N(s)$	$Q_5^S = \alpha_{\theta_{4S}}^{N_2} F_{N_2}\theta_{4S}A_S$
6	$2TiO(s)+O_2(g) \rightarrow 2TiO_2(s)$	$Q_6^S = \alpha_{\theta_{4S}}^{O_2} F_{O_2}\theta_{4S}A_S$
7	$2Ti(s)+N_2(g) \rightarrow 2TiN(s)$	$Q_7^S = \alpha_{\theta_{6S}}^{N_2} F_{N_2}\theta_{6S}A_S$
8	$Ti(s)+N(g) \rightarrow TiN(s)$	$Q_8^S = \alpha_{\theta_{6S}}^{N} F_N\theta_{6S}A_S$
9	$TiN(s)+O_2(g) \rightarrow TiO_2(s)+N(g)$	$Q_9^S = \alpha_{\theta_{3S}}^{O_2} F_{O_2}\theta_{3S}A_S$
10	$TiN(s)+O(g) \rightarrow TiO(s)+N(g)$	$Q_{10}^S = \alpha_{\theta_{3S}}^{O} F_O\theta_{3S}A_S$
11	$2TiO(s)+O(g) \rightarrow Ti_2O_3(s)$	$Q_{11}^S = \alpha_{\theta_{4S}}^{O} F_O\theta_{4S}A_S$
12	$Ti_2O_3(s)+O(g) \rightarrow 2TiO_2(s)$	$Q_{12}^S = \alpha_{\theta_{5S}}^{O} F_O\theta_{5S}A_S$
13	$2Ti_2O_3(s)+O_2(g) \rightarrow 4TiO_2(s)$	$Q_{13}^S = \alpha_{\theta_{5S}}^{O_2} F_{O_2}\theta_{5S}A_S$

Deposição de TiO_xN_y

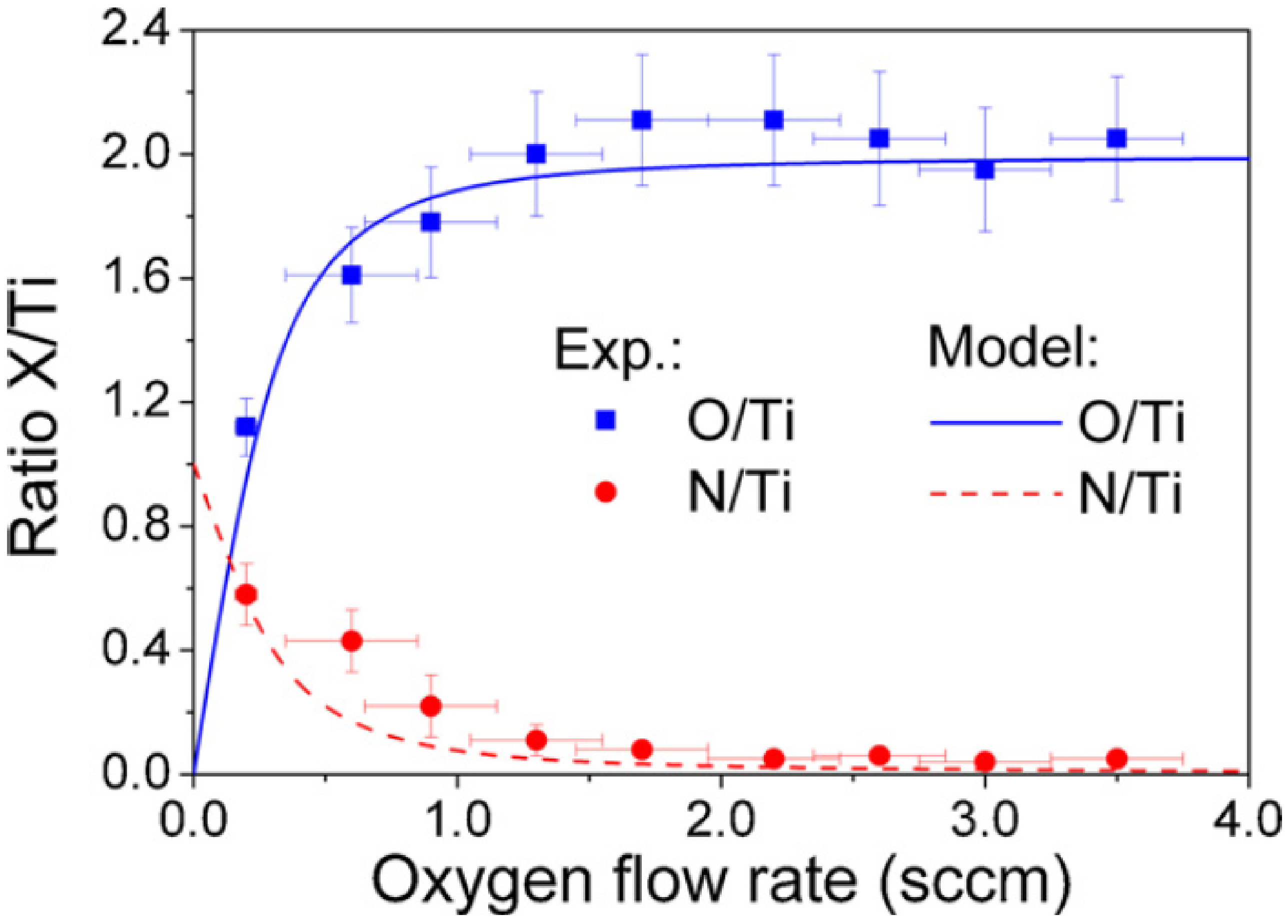


Fig. 3. Chemical composition at the collecting area obtained from Berg model and RBS as function of the O_2 flow rate.

Deposição de TiO_xN_y

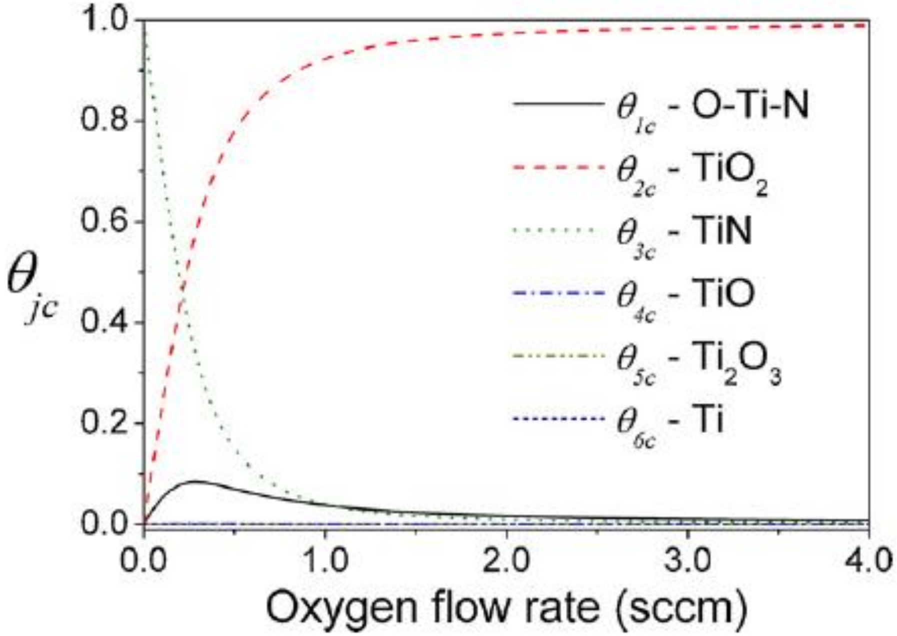
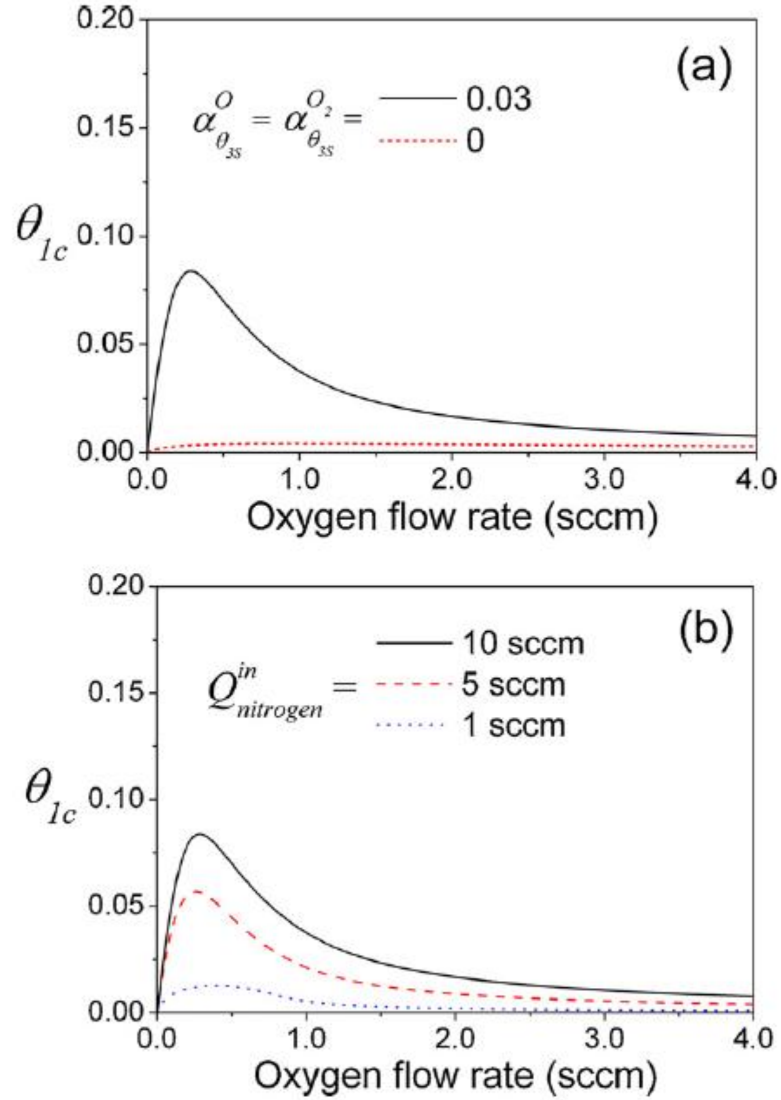
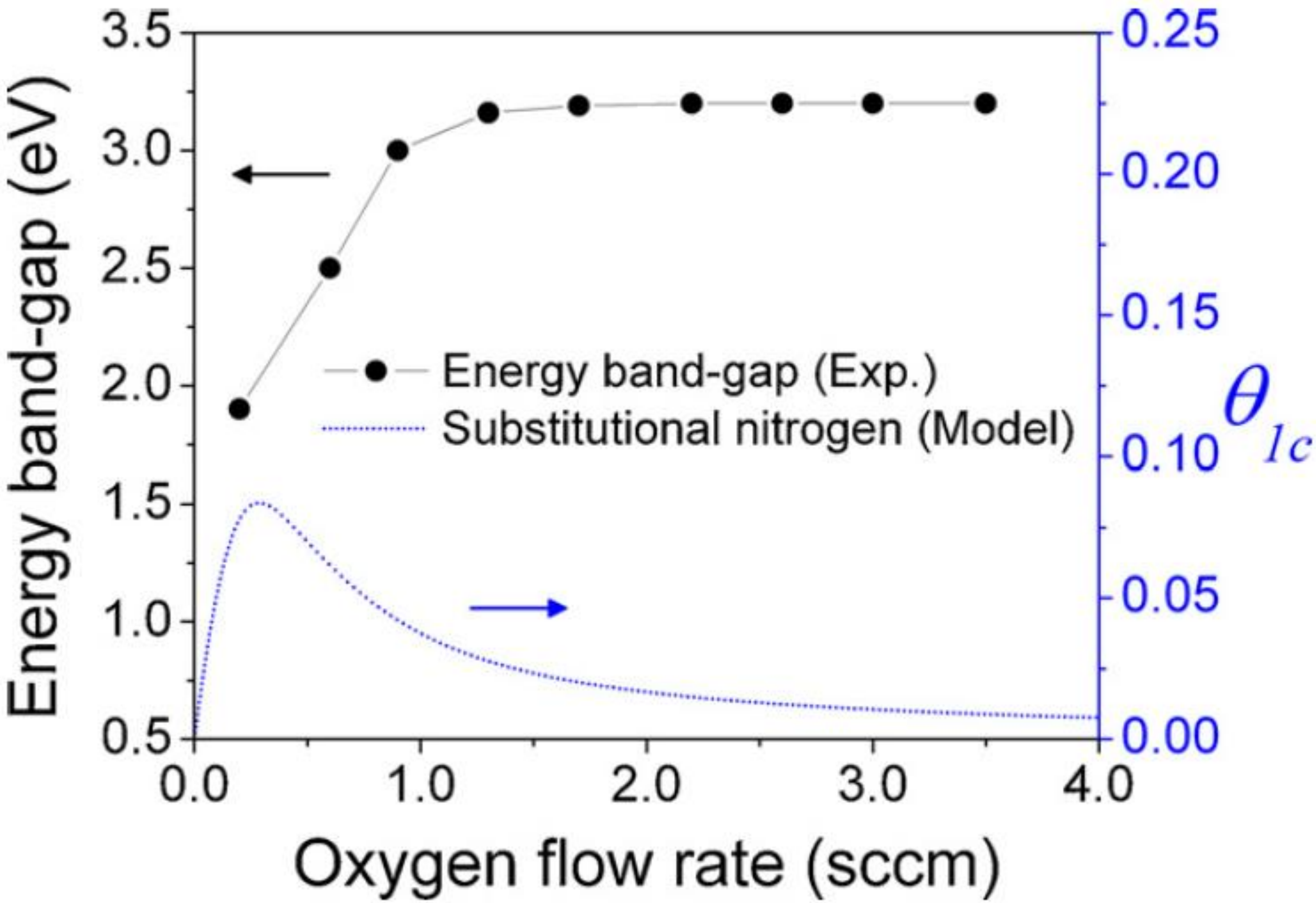


Fig. 2. Compound fractions at the collecting area as function of the O_2 flow rate.



Deposição de TiO_xN_y



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Hysteresis-free deposition of TiO_xN_y thin films: Effect of the reactive gas mixture and oxidation of the TiN layers on process control

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TiO_2

ABSTRACT

This paper investigates the effect of the reactive gas mixture ($N_2 + O_2 + Ar$) and oxidation of the nitride layers on the system stability during the reactive sputter deposition of TiO_xN_y thin films. The present research is an extension of previous investigations conducted by Severin et al. (Appl. Phys. Lett., 88 (2006) 161504) and Duarte et al. (Appl. Surf. Sci., 269 (2013) 55–59) in which the Berg's model was used to study reactive deposition of oxynitrides. The results show that the addition of N_2 to the process avoids the formation of a hysteresis loop and facilitates the deposition of films with fractions of TiO_2 at any value. These achievements are not possible without this procedure. In contrast, despite eliminating plasma instabilities, the addition of N_2 decreases the mass deposition rate due to the modifications in the sputtering yield. Other results show that the oxidation of TiN also plays a key role in the mass deposition rate and in the hysteresis loop.

Deposição de TiO_xN_y

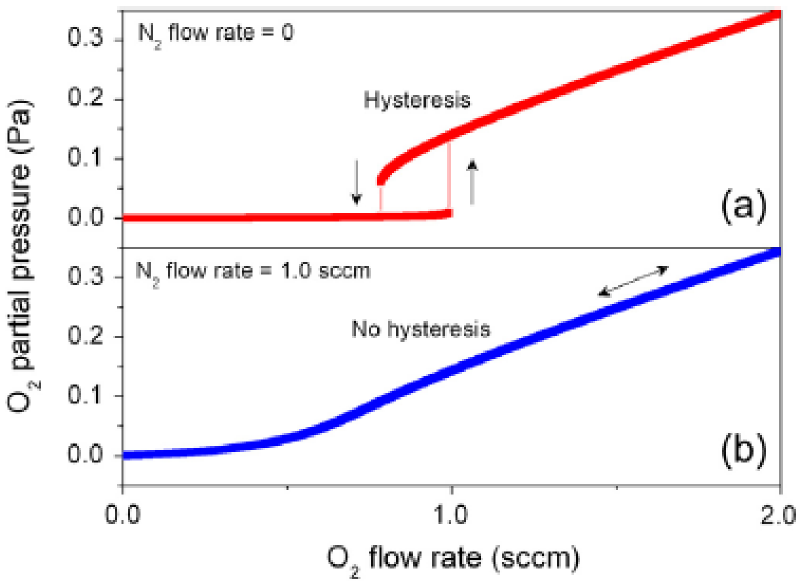


Fig. 2. O_2 partial pressure as a function of the O_2 flow rate at N_2 flow rates of (a) 0 and (b) 1.0 sccm. The double-headed arrow indicates that the curves overlap.

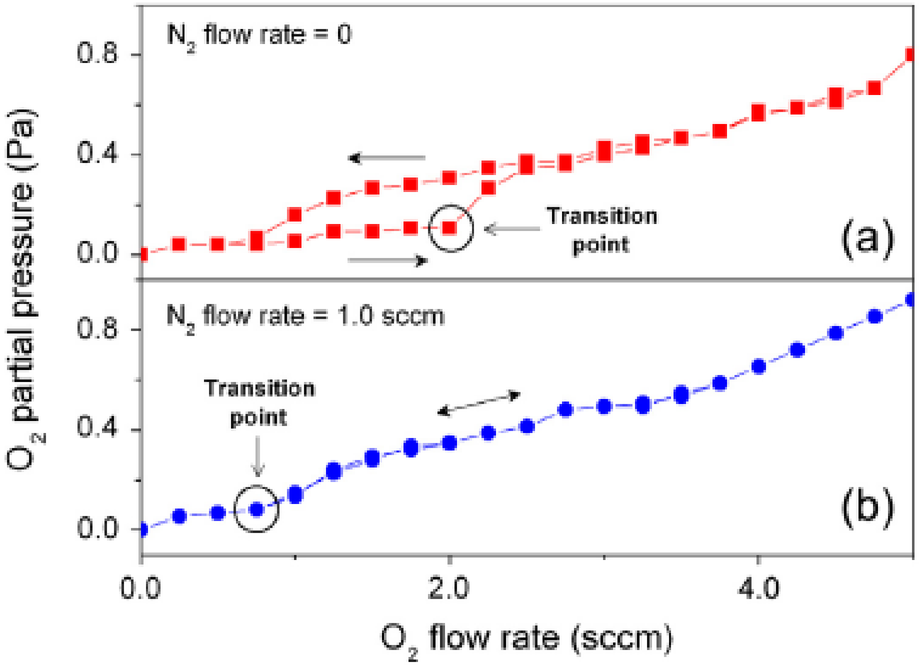


Fig. 3. Experimental curves of the O_2 partial pressure as a function of the O_2 flow rate at N_2 flow rates of (a) 0 and (b) 1.0 sccm.

Deposição de TiO_xN_y

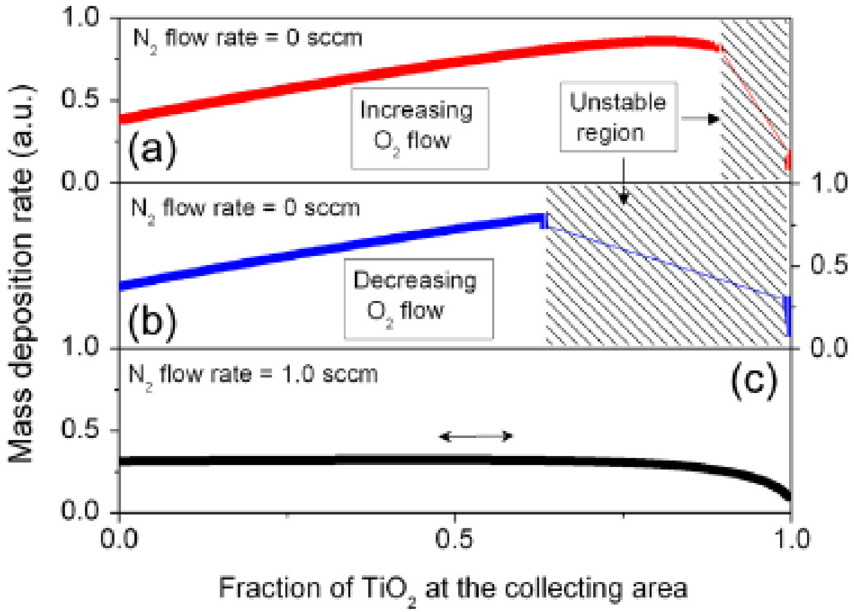


Fig. 7. Numerical solutions of the mass deposition rate as a function of the fraction of TiO_2 at different N_2 flow rates. In (a), reactive deposition is shown with a N_2 flow rate equal to zero and an increasing O_2 flow rate. In (b), reactive deposition is shown with a N_2 flow rate equal to zero and a decreasing O_2 flow rate. In (c), reactive deposition is shown with a N_2 flow rate equal to 1.0 sccm and an increasing and decreasing O_2 flow rate.

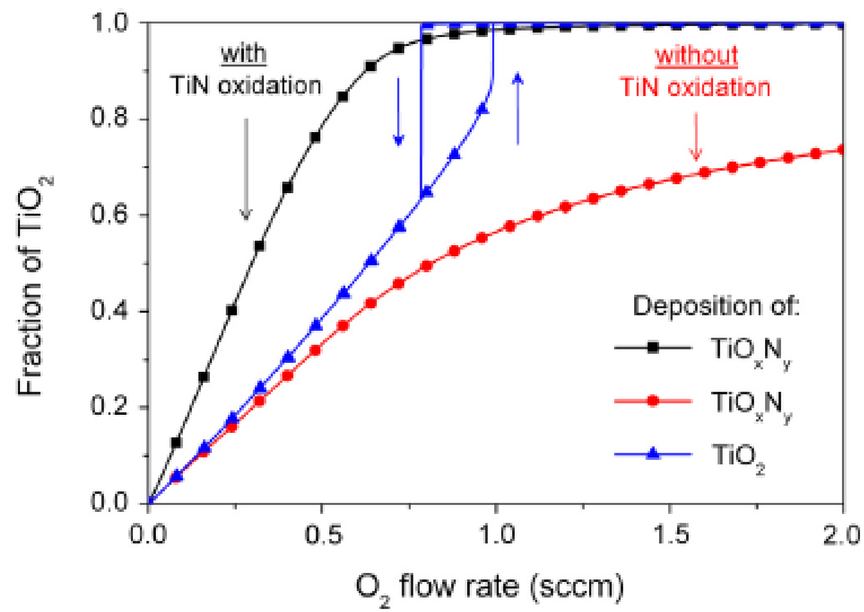
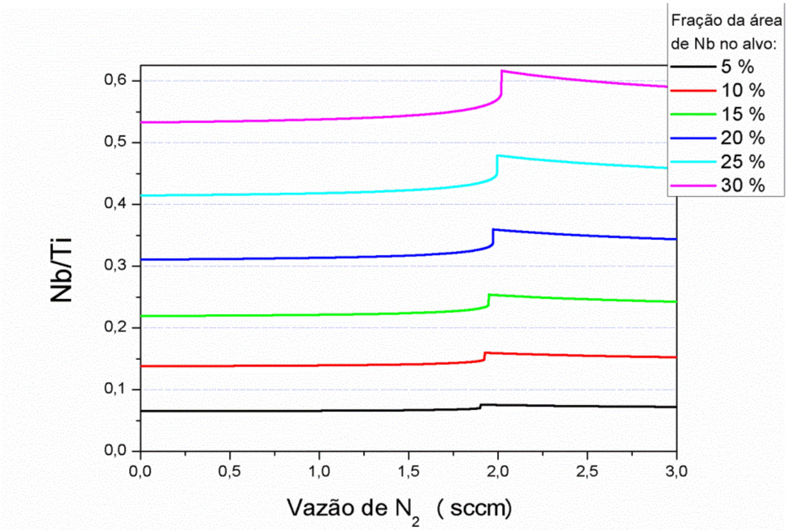
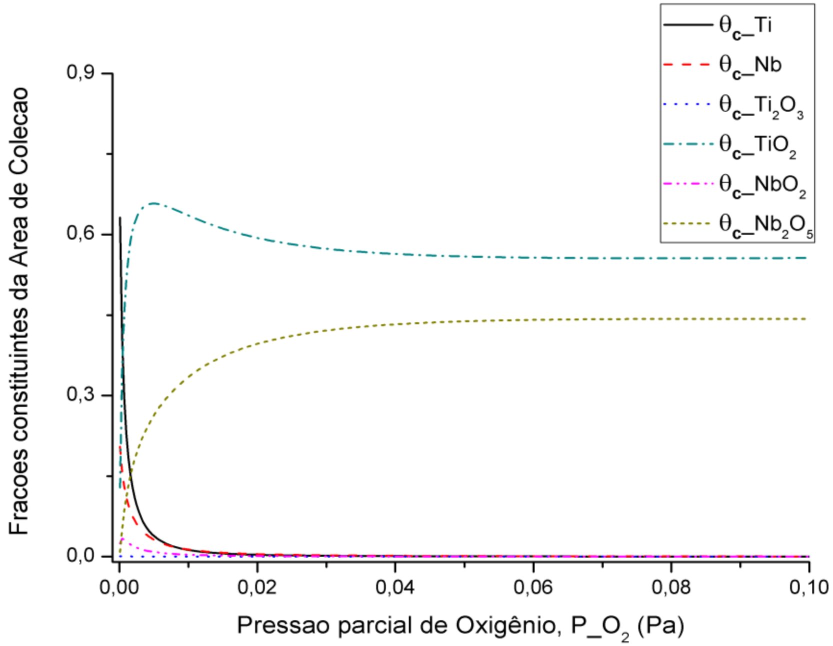
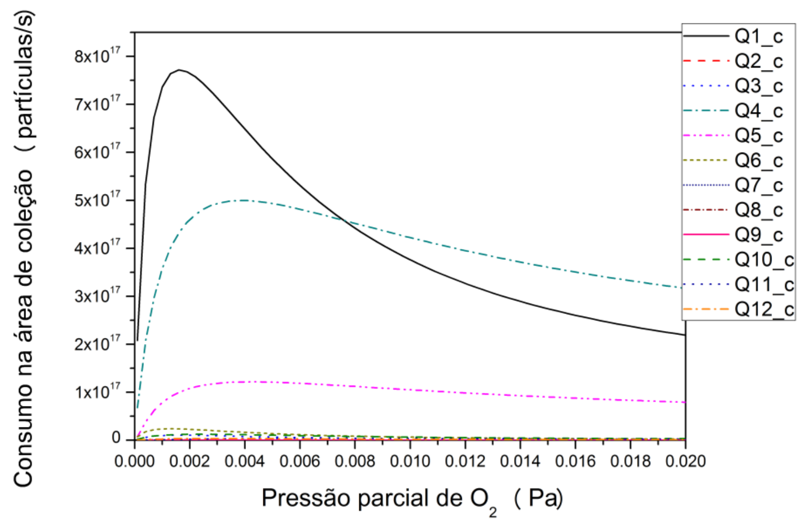


Fig. 8. Fraction of TiO_2 as a function of the O_2 flow rate at different modeling conditions for the collecting area. The numerical simulations for the deposition of TiO_xN_y with and without oxidation of the TiN were conducted at a N_2 flow rate of 1.0 sccm.

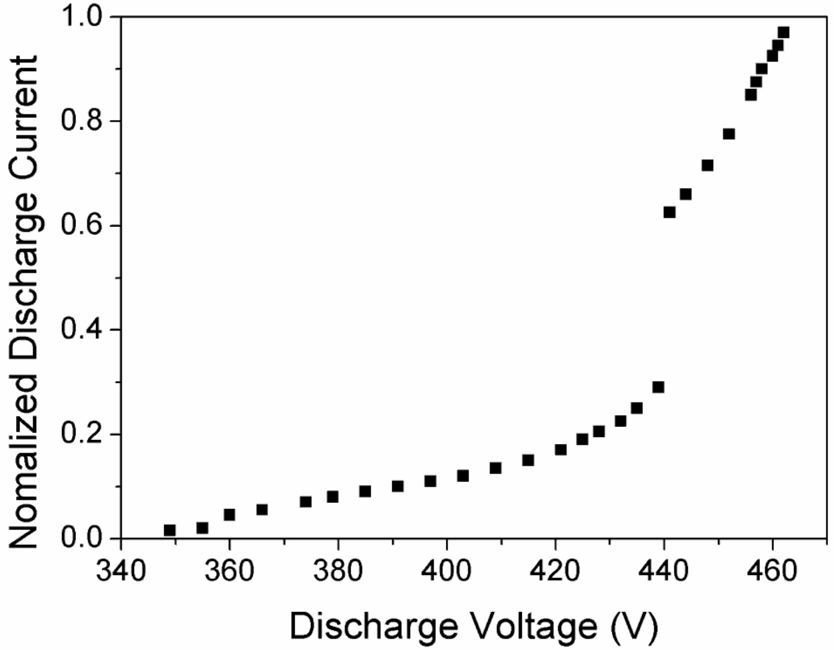
Deposição de TiN e TiO_2 com adição de nióbio

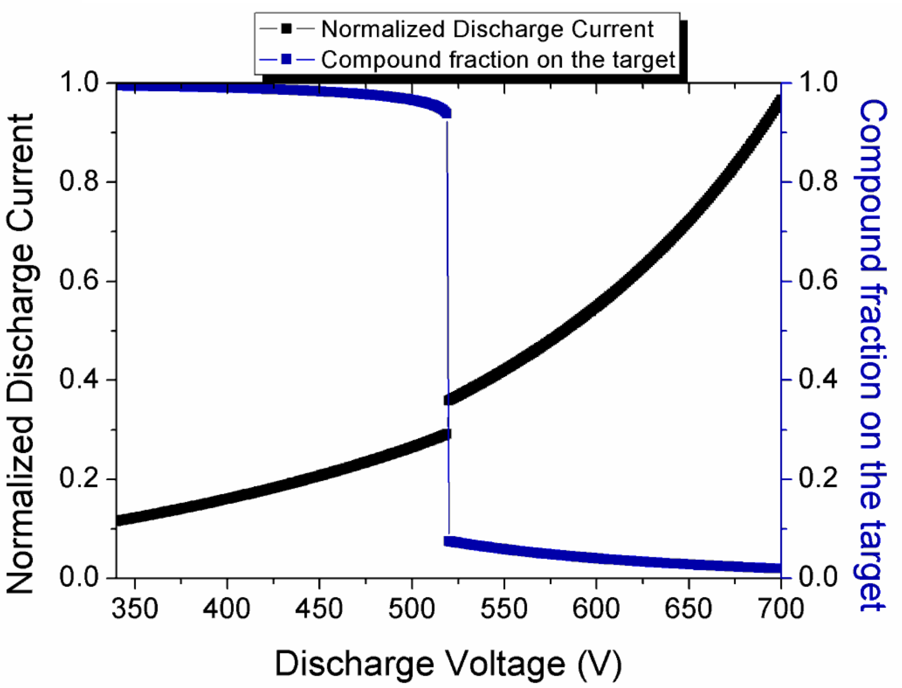






Curvas I-V


Nomalized Discharge Current
Discharge Voltage (V)
0.0
0.2
0.4
0.6
0.8
1.0
340
360
380
400
420
440
460


Normalized Discharge Current
Compound fraction on the target
Normalized Discharge Current
Compound fraction on the target
Discharge Voltage (V)
0.0
0.2
0.4
0.6
0.8
1.0
350
400
450
500
550
600
650
700