>>> mathematical description of reactive sputtering in c
>>> based on berg model described in Journal of Vacuum Science & Technology A: Vacuum, Surfaces, and Films 5, 202 (1987); doi: 10.1116/1.574104

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>>> steady state equations

equation A5 for flux F of nitrogen molecules:

$$F = \frac{p_N}{\sqrt{2k_B \pi T M}} \tag{1}$$

equation A1' for target fractional coverage θ_1:

$$2\alpha_t F(1-\theta_1) - \frac{J}{e} S_N \theta_1 = 0 \tag{2}$$

equation A2' for chamber wall and substrate fractional coverage θ_2:

$$2\alpha_c F(1-\theta_2) + \frac{J}{e} S_N \theta_1 \frac{A_t}{A_c}(1-\theta_2) - \frac{J}{e} S_M (1-\theta_1) \frac{A_t}{A_c}\theta_2 = 0 \tag{3}$$

equation A3 for flow to target:

$$q_t = \alpha_t F(1-\theta_1) A_t \tag{4}$$

>>> steady state equations

equation A4 for flow to surface area A_c of the chamber:

$$q_c = \alpha_c F(1 - \theta_2) A_c \tag{5}$$

equation 2 for flow through pump:

$$q_p = p_N S \tag{6}$$

equation 1 for incoming reactive gas flow:

$$q_0 = q_t + q_c + q_p \tag{7}$$

equation A6 for total sputtering rate Y:

$$R = \frac{J}{e}[S_N \theta_1 + S_M (1 - \theta_1)] \tag{8}$$

\>>> algorithm

solve the equations by assuming a value for p_N. equations are already solved except A1' and A2', they can be written as:

$$\theta_1 = \frac{1}{1 + \frac{JS_N}{2e\alpha_t F}} \tag{9}$$

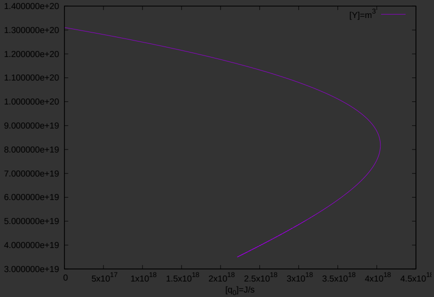
$$\theta 2 = \frac{\frac{e}{J} 2\alpha_c F \frac{A_c}{A_t} + S_N \theta 1}{\frac{e}{J} 2\alpha_c F \frac{A_c}{A_t} + S_N \theta 1 + S_M (1 - \theta_1)} \tag{10}$$

now assume a new (little higher) value for p_N

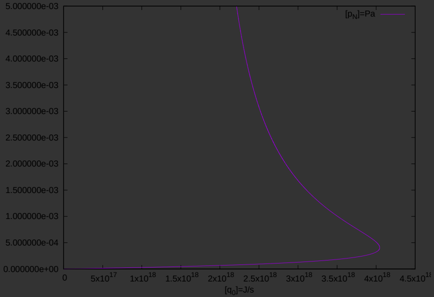
>>> results

for n=5000 iterations, $dp = 10^{-6}$Pa pressurechange, $p_N = 10^{-6}$Pa initial nitrogen partial pressure, T=300Kelvin, $M = 4.651 \cdot 10^{-26} kg$ mass of nitrogen molecule, $S_N = 0.3$ sputtering yield of compound by incoming argon ions, $J = 14\frac{A}{m^2}$ current density of argon ions causing sputtering from target surface, $A_t = 0.127m^2$ target surface, $A_c = 1.27m^2$ exposed chamber surface, $S_M = 1.5$ sputtering yield of elemental metalmaterial by incoming argon ions, $S = 85\frac{l}{s}$ pumping speed, $\alpha_t = 1$ sticking coefficient for nitrogen molecule to titanium target and $\alpha_c = 1$ sticking coefficient for nitrogen molecule to titanium covered part $(1 - \theta_2)$ of chamber wall you can get these relationships: although for Y the lower part seems to be missing and for P_N the higher part seems to be missing

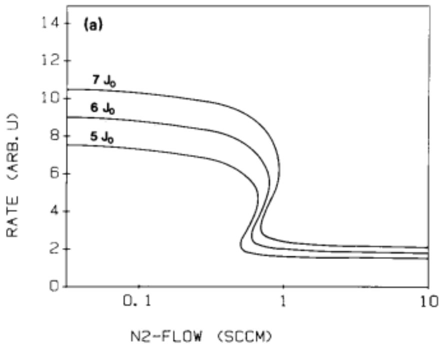
>>> results



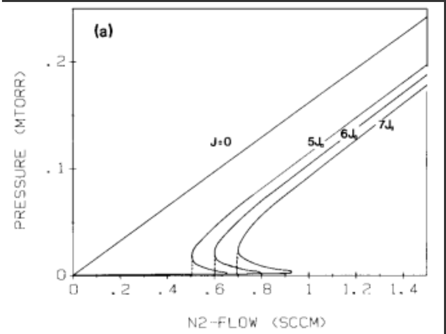
[Y]=m^3
1.400000e+20
1.300000e+20
1.200000e+20
1.100000e+20
1.000000e+20
9.000000e+19
8.000000e+19
7.000000e+19
6.000000e+19
5.000000e+19
4.000000e+19
3.000000e+19
0
5x10^{17}
1x10^{18}
1.5x10^{18}
2x10^{18}
2.5x10^{18}
3x10^{18}
3.5x10^{18}
4x10^{18}
[q$_0$]=J/s



[p$_N$]=Pa
5.000000e-03
4.500000e-03
4.000000e-03
3.500000e-03
3.000000e-03
2.500000e-03
2.000000e-03
1.500000e-03
1.000000e-03
5.000000e-04
0.000000e+00
0
5x10^{17}
1x10^{18}
1.5x10^{18}
2x10^{18}
2.5x10^{18}
3x10^{18}
3.5x10^{18}
4x10^{18}
[q$_0$]=J/s



(a)
7 J$_0$
6 J$_0$
5 J$_0$
RATE (ARB. U)
14
12
10
8
6
4
2
0
0. 1
1
10
N2-FLOW (SCCM)



(a)
J=0
5J$_0$
6J$_0$
7J$_0$
PRESSURE (MTORR)
.2
.1
0
.2
.4
.6
.8
1
1.2
1.4
N2-FLOW (SCCM)