

A global model study of a reactive high

power impulse magnetron sputtering

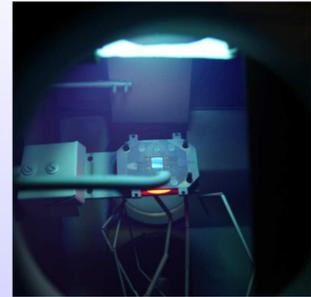
(HiPIMS) N₂/Ar discharge

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The global (volume averaged) model

- A global model (Gudmundsson, 2008) is applied to study a reactive high power impulse magnetron sputtering (HiPIMS) N₂/Ar discharge
- The discharge consists of (Thorsteinsson and Gudmundsson, 2009a,b):
 - Electrons, Maxwellian-like energy distribution (0.0259 – 10 V)
 - vibrational levels of the ground state nitrogen molecule N₂(X¹Σ_g⁺, v = 0 – 6) (0 – 1.68 eV)
 - metastable nitrogen molecule N₂(A³Σ_u⁺) (6.17 eV)
 - nitrogen atoms N(⁴S), N(²D) (2.38 eV) and N(²P) (3.58 eV)
 - nitrogen ions N₂⁺ (15.6 eV) and N⁺ (14.5 eV)
 - argon atoms Ar(3s²3p⁶), Ar^m (1s₅ and 1s₃) (11.6 eV), Ar^r (1s₄ and 1s₂) (11.7 eV), excited argon atoms 4p states Ar(4p) (13.2 eV)
 - argon ions Ar⁺ (15.8 eV)
 - titanium atom Ti(a³F) and titanium ion Ti⁺ (6.83 eV)

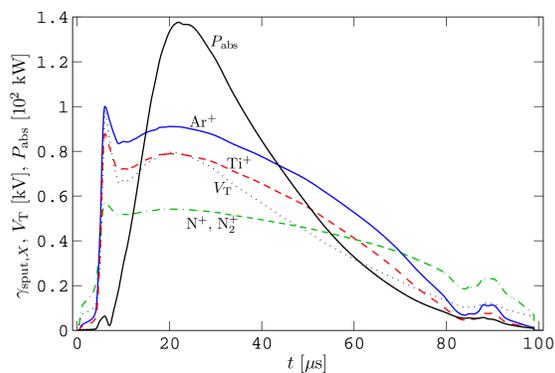


Figure 1: The temporal evolution of the sputtering yields $\gamma_{\text{sput},X}$, the absorbed power P_{abs} and the target voltage V_T .

- Sputtering of metal atoms from the target by bombardment of positive ions with the rate coefficients

$$k_{\text{sput},X} = u_B h_L \frac{R_T^2}{R^2 L} \gamma_{\text{sput},X} \quad (1)$$

where $\gamma_{\text{sput},X}$ is the sputtering yield for sputtering by positive ion X

- The sputtering yields are dependent on the ion energy, so the temporal evolution of the target voltage V_T must be known
- We use experimentally obtained current–voltage characteristics for the power P_{abs} and the target voltage V_T , that were measured for a pure Ar HiPIMS discharge (Gudmundsson et al., 2002)

Results and discussion

- The chamber is assumed to be made of stainless steel, cylindrical with $R = 15$ cm and $L = 15$ cm and the target is made of titanium of radius $R_T = 15$ cm
- The discharge pressure is 10 mTorr and the total gas flow is $Q = 42$ sccm which is 95% argon ($Q_{\text{Ar}} \approx 40$ sccm, $Q_{\text{N}_2} \approx 2$ sccm) and the gas temperature is assumed to be $T_g = 430$ K

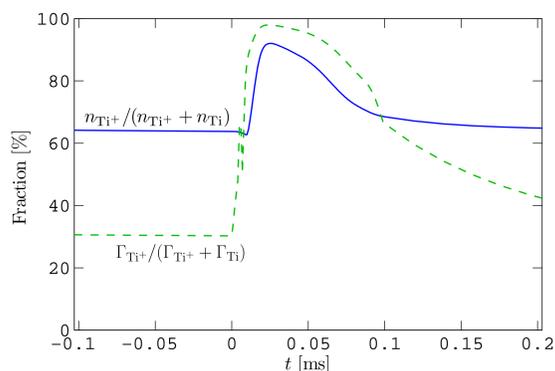


Figure 2: The temporal evolution of the ionized metal fraction $n_{\text{Ti}^+}/(n_{\text{Ti}^+} + n_{\text{Ti}})$ and the fraction of ionized metal flux at the substrate $\Gamma_{\text{Ti}^+}/(\Gamma_{\text{Ti}^+} + \Gamma_{\text{Ti}})$ at and around the tenth pulse period.

- The power is assumed to be deposited uniformly to a reduced volume V_p below the target that is cylindrical in shape and assumed to have the dimensions $R_p = 15$ cm and $L_p = 7.5$ cm
- The pulse length is roughly 100 μs (FWHM of about 32 μs) and the repetition frequency is 500 Hz (i.e. a period of $T = 2$ ms)
- The fraction of ionized metal flux at the substrate is significantly larger than the ionized metal fraction when the power is on but significantly smaller when it is off

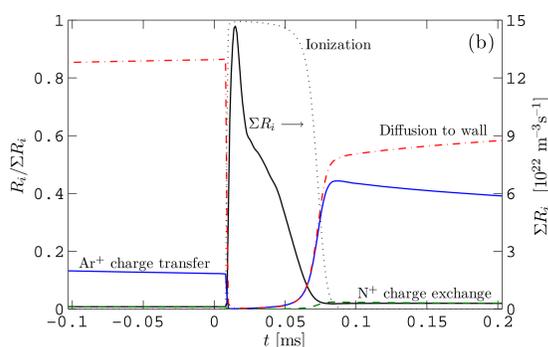
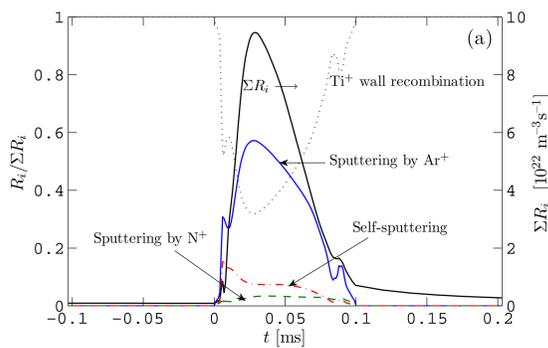


Figure 3: The temporal evolution of (a) the creation of Ti and (b) the loss of Ti atoms over 300 μs at and around the tenth pulse.

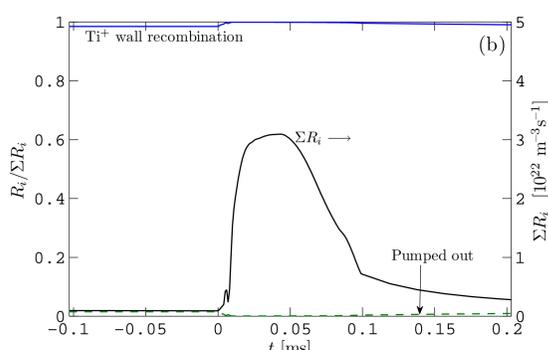
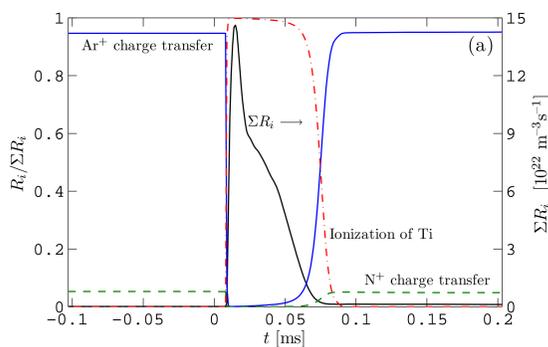


Figure 4: The temporal evolution of (a) the creation of Ti⁺ and (b) the loss of Ti⁺ ions over 300 μs at and around the tenth pulse.

- The most important reactions for creation of Ti atoms, are wall recombination of Ti⁺ and sputtering by Ar⁺, Ti⁺ and N⁺
- The most important reactions for the loss of Ti atoms are electron impact ionization, diffusion to the wall, and Ar⁺ and N⁺ charge transfer
- Electron impact ionization is the dominating reaction in the creation of Ti⁺ ions while the power is on but Ar⁺ – Ti charge transfer is the dominating reaction after the power is turned off
- Ti⁺ ions are almost entirely lost to wall recombination

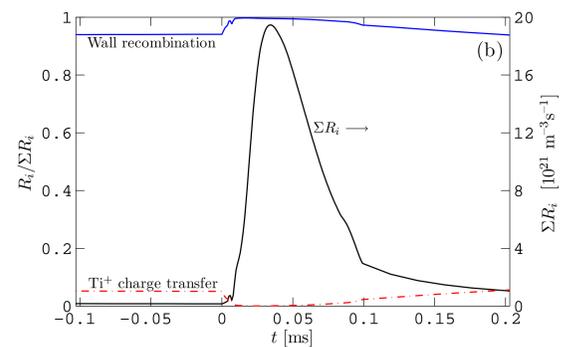
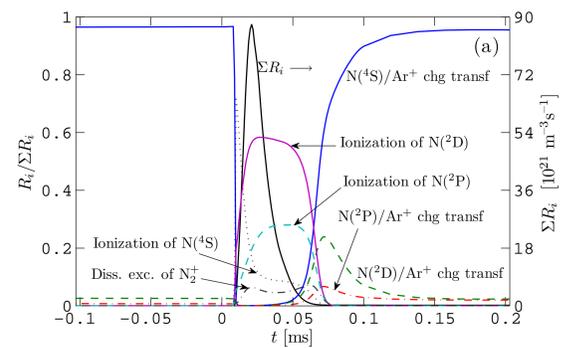


Figure 5: The temporal evolution of (a) the creation of N⁺ and (b) the loss of N⁺ ions over 300 μs at and around the tenth pulse.

- Electron impact ionization is most important in N⁺ production when the power is on, and N – Ar⁺ charge transfer when the power is off
- The excited atoms are extremely important for the ionization of N⁺, ionization of N(²D) and N(²P) being dominant in comparison to ionization of the ground state N(⁴S) atom for most of the on-period
- Electron impact ionization of N(⁴S) is only most important for the first few μs after the power has been turned on
- The excited atoms are much less important during the off period when essentially all N⁺ ions are created by Ar⁺ – N charge transfer

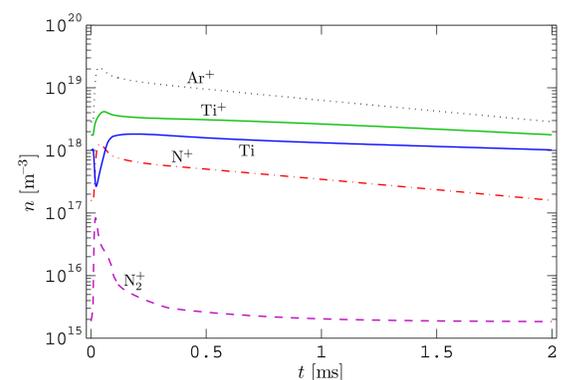


Figure 6: The temporal evolution of the densities of titanium atoms and positive ions over the tenth pulse period.

Conclusions

- A global (volume averaged) model of an N₂/Ar discharge was applied to study the reaction mechanism in a HiPIMS discharge with a titanium target

Acknowledgments

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