Modeling of the Reactive High Power Impulse Magnetron Sputtering (HiPIMS) process

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Abstract

Reactive high power impulse magnetron sputtering (HiPIMS) provides both a high ionization fraction of the sputtered material and a high dissociation fraction of the molecular gas. We demonstrate this through an ionization region model (IRM) of the reactive Ar/O_2 HiPIMS discharge with a titanium target. We explore the influence of oxygen dilution on the discharge properties such as electron density, the ionization fraction of the sputtered vapor and the oxygen dissociation fraction. The discharge current waveform is highly dependent on the reactive gas flow rate, pulse repetition frequency and discharge voltage. The discharge current increases with decreasing repetition frequency and increasing flowrate of the reactive gas.

Introduction

The high power impulse magnetron sputtering (HiPIMS) discharge is a recent addition to plasma based sputtering or physical vapor deposition (PVD) technology.

In HiPIMS, high power is applied to the magnetron target in unipolar pulses at low duty cycle and low repetition frequency while keeping the average power about 2 orders of magnitude lower than the peak power [1]. This results in a high plasma density, and high ionization fraction of the sputtered vapor.

Reactive sputtering, where metal targets are sputtered in a reactive gas atmosphere to deposit compound materials, including transparent conductive oxides, permeation barrier coatings, hard coatings, etc., is of utmost importance in various technologies. In reactive sputtering processes a reactive gas (e.g., O_2, N_2, CH_4, etc.) is mixed to the noble working gas to synthesize a compound film.

The high electron density in the HiPIMS discharge is expected to enhance the dissociation of the molecular gas, which is sometimes considered beneficial for the oxide, nitride, or carbide deposition.

The presence of reactive gas can lead to the formation of compound material on the target surface, often referred to as target coverage or target poisoning. Due to this target coverage the reactive sputtering process is inherently unstable, and is commonly represented in a familiar hysteresis curve that shows, e.g., the deposition rate or the target voltage versus the flow rate of the reactant.

Experimental findings

For the reactive HiPIMS discharge striking differences are observed and those seem to depend on the mode of operation, the reactive gas and the target material. The discharge current waveform changes in shape as well as in the peak value when the target surface enters the compound mode.

For Ar/O_2 discharge with Ti target at the higher repetition frequencies the familiar non-reactive current waveform is observed. As the repetition frequency is lowered from 50 Hz to 20 Hz there is an increase in the current which transits into a different waveform as the repetition frequency is decreased further [2].

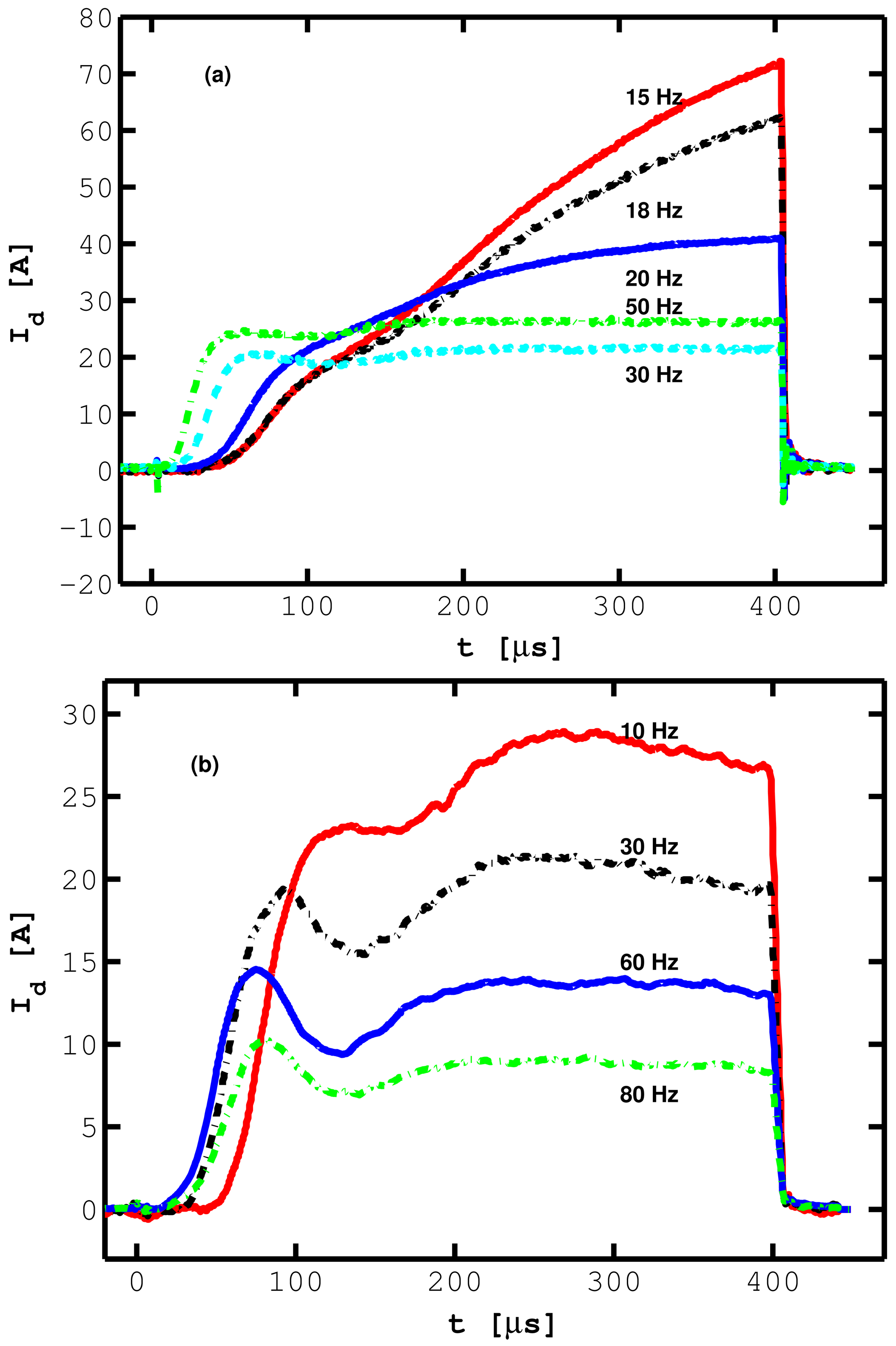

Figure 1: The discharge current for various repetition frequencies. (a) Ar/O_2 discharge with titanium target. The discharge pressure is roughly 0.6 Pa, the oxygen flow rate 2 sccm, and the pulse voltage is 600 V. (b) Ar/N_2 discharge with titanium target. The discharge pressure is roughly 0.6 Pa, the nitrogen flow rate 2 sccm, and the pulse voltage is 550 V.

The waveform observed at low repetition frequency is similar to the one observed at high reactive gas flow rate. This indicates that oxidation takes place during the long pause between the pulses.

For Ar/N_2 discharge with Ti target the discharge current keeps its shape but it remains as for the non-reactive case as the current increases, except for the delay to the onset of the current which increases slightly [3].

Modeling findings

An ionization region model (IRM) of the reactive Ar/O_2 high power impulse magnetron sputtering (HiPIMS) discharge is developed and applied to study the temporal behavior of the discharge plasma paremeters.

The main feature of the model is that an ionization region (IR) is defined next to the race track [4]. This global model provides a flexible modeling tool to explore, e.g., the temporal variations of the ionized fractions of the working gas and the sputtered vapor, the electron density and temperature.

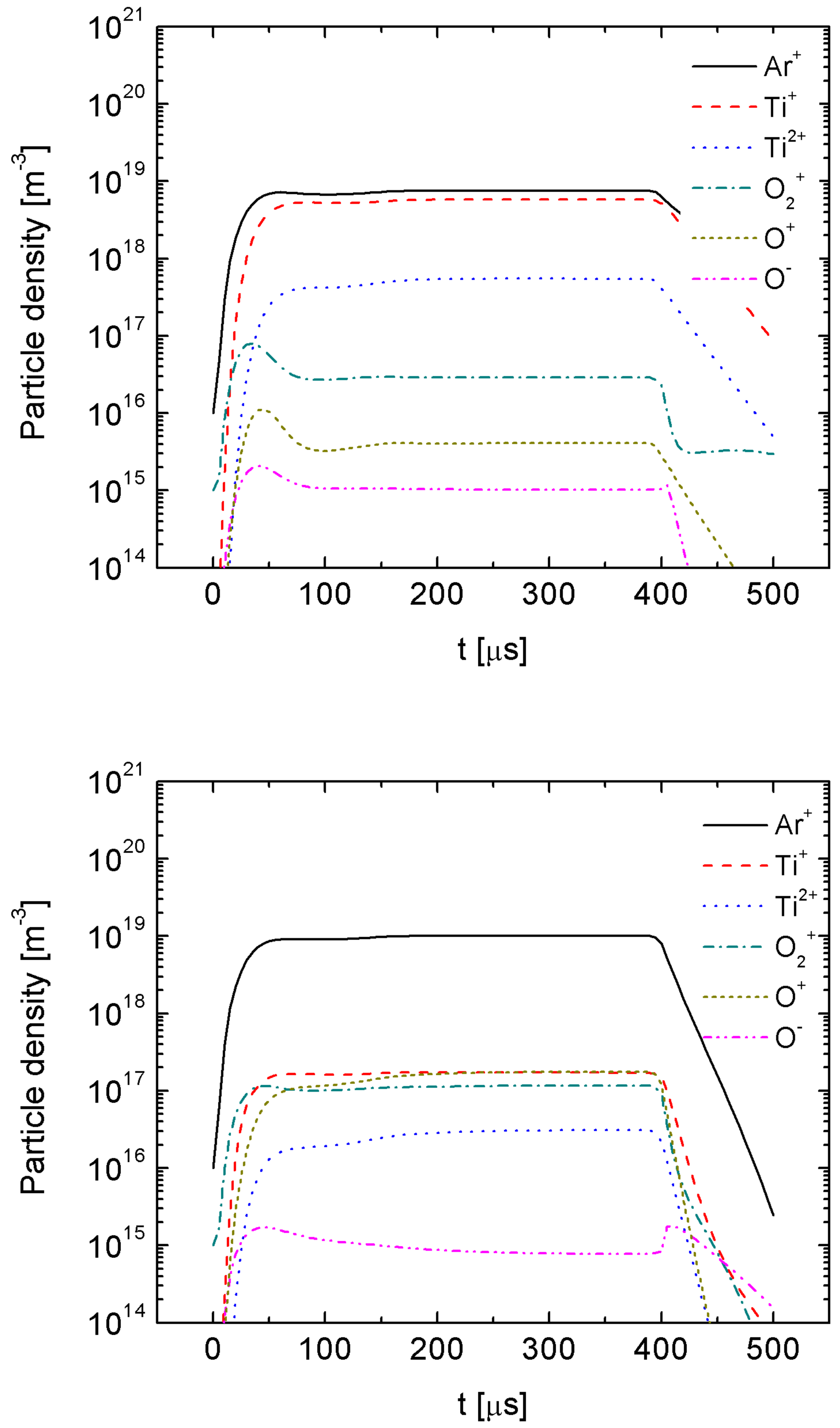

Figure 2: The discharge current showing the contribution of the various charged particles for 5 $\%O_2$ fractional flowrate in Ar/O_2 discharge with Ti target in (a) metal mode and (b) poisoned mode.

The species assumed in the IRM are electrons, ground state argon atoms Ar, hot argon atoms in the ground state Ar^H, warm argon atoms in the ground state Ar^W, metastable argon atoms Ar^m, argon ions Ar^+, doubly ionized argon ions Ar^{2+}, metal neutrals M, singly ionized metal ions M^+ and doubly ionized metal ions M^{2+}. The oxygen discharge consists of oxygen molecule in the ground state $O_2(X^3\Sigma_g^-)$, the metastable oxygen molecules $O_2(a^1\Delta_g)$ and $O_2(b^1\Sigma_g)$, the oxygen atom in the ground state $O(^3P)$, the metastable oxygen atom $O(^1D)$, the positive ions O_2^+ and O^+, and the negative ion O^-.

The IRM is a semi-empirical model in the sense that it uses a measured discharge current waveform as a main input parameter. For this study we use the measured curve for Ar/O_2 with Ti target at 50 Hz seen in figure 1 (a).

Figure 2 shows the particle density of the charged particles in 400 μs pulse in metal mode and poisoned mode. In metal mode the Ar^+ and Ti^+ ions dominate the discharge while Ti^{2+}-ions have roughly an order of magnitude lower density, but in poisoned mode Ar^+ dominate and Ti^+, O^+, and O_2^+, have similar densities roughly two orders of magnitude lower.

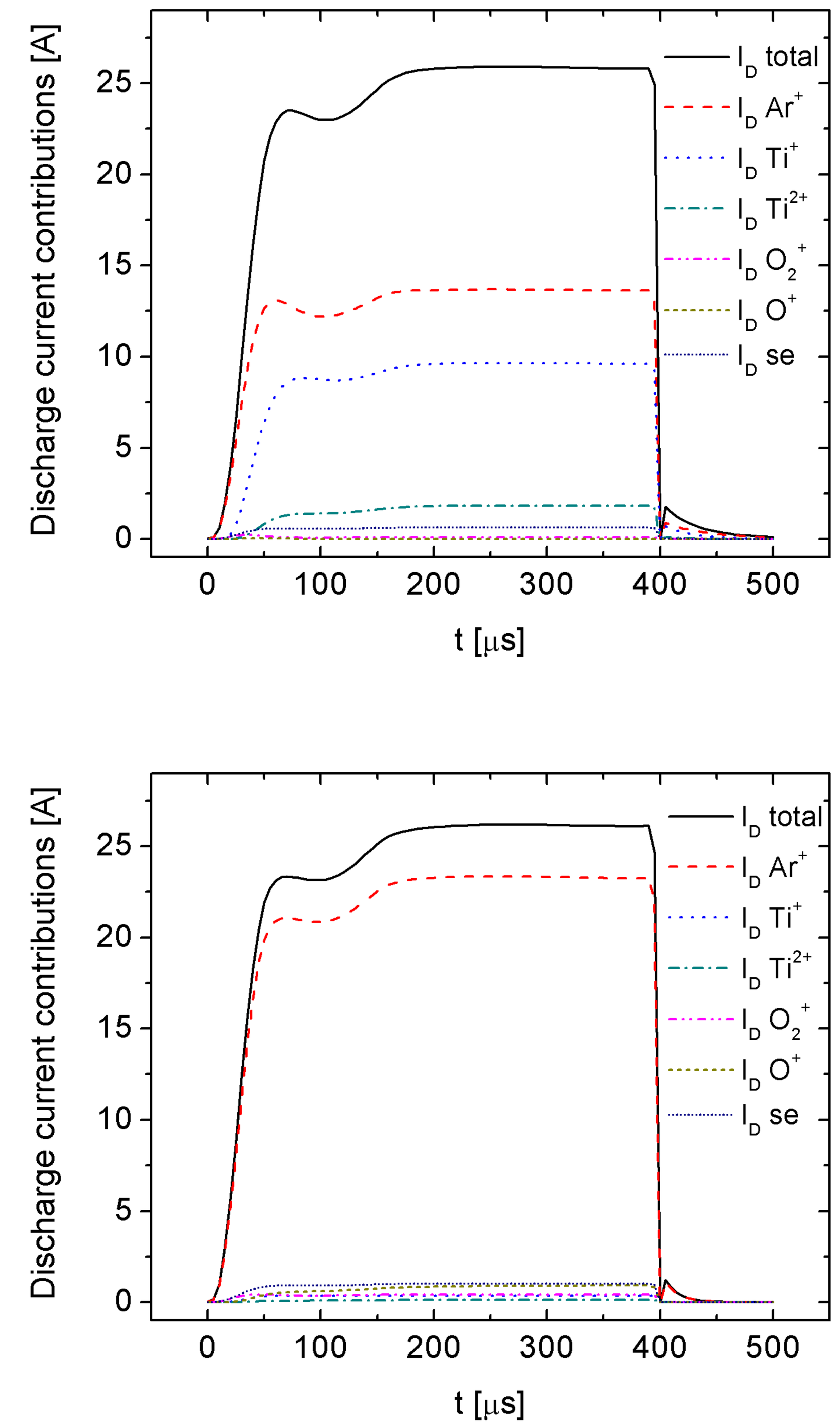

Figure 3: The discharge current showing the contribution of the various charged particles for 5 $\%O_2$ fractional flowrate in Ar/O_2 discharge with Ti target in (a) metal mode and (b) poisoned mode.

Figure 3 shows the charged particles contribution to the discharge current in a 400 μs pulse in metal mode and poisoned mode. In the metal mode Ar^+-ions and secondary electrons contribute mainly to the current. In the poisoned mode Ar^+-ions contribute over 90 % of the current.

Conclusions

- Experimantally an increase in the discharge current is observed when reactive molecular gas is added to the HiPIMS discharge. This current increases with increased reactive gas partial pressure and lowered repetition frequency.
- We have developed an ionization region model to explore the processes in a reactive high power impulse magnetron sputtering discharge.

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