Metal ion escape in high-power impulse magnetron sputtering discharges

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Abstrac

When the magnetron sputtering discharge is driven by high power unipolar pulses of low repetition frequency and low duty cycle, it is referred to as high power impulse magnetron sputtering (HiPIMS). HiPIMS operation results in increased ionization of the sputtered species and lower deposition rate than the dc magnetron sputtering discharge, when operated at the same average power. The HiPIMS discharge can costitute a large fraction of ionized sputtered material. This means that, at least some fraction, often a significant fraction, of the ions involved in the sputter process are ions of the target material. This also implies that a large fraction of the ions of the sputtered species can be attracted back to the target and is not deposited on the substrate to form a film or coating. Self-sputtering and the self-sputter yield are therefore expected to play a significant role in HiPIMS operation, and have a decisive impact on the film deposition rate, at least for metal targets. We have applied the ionization region model (IRM) to model HiPIMS discharges in argon with a number of different target materials, to study various processes, such as working gas rarefaction and refill processes, the electron heating mechanisms, ionization probability and back-attraction of the sputtered species, and recycling mechanisms. We find that metal ions in metal-rich discharges (high sputter yield) can escape more easily to the substrate region compared to metal ions in argon-dominated discharges (low sputter yield).

Introduction

Magnetron sputtering is a versatile and widely applied physical vapor deposition technique where the film-forming material is sputtered from a cathode target by ion bombardment [1]

A variation of the magnetron sputtering technique is high power impulse magnetron sputtering (HiPIMS) where the discharge is driven by high power pulses delivered at low repetition frequency, and with low duty cycle [2]

Low deposition rate is the main drawback of this sputter technology and hampers its use for industrial applications

The main reason for the low deposition rate of the HiPIMS discharge is suggested to be due to the back-attraction of the ions of the sputtered species to the cathode target

Increased deposition rate in HiPIMS often comes at the cost of a lower ionized flux fraction of the sputtered material

Two internal parameters are of importance

- $\alpha_{\rm t}$ ionization probability
- $\beta_{\rm t}$ back-attraction probability

The ionization region model (IRM) is a time-dependent volume averaged plasma chemical model of the ionization region (IR) of the HiP-IMS discharge [3]

The IRM gives the temporal evolution of the densities of ions, neutrals and electrons

Results and discussion

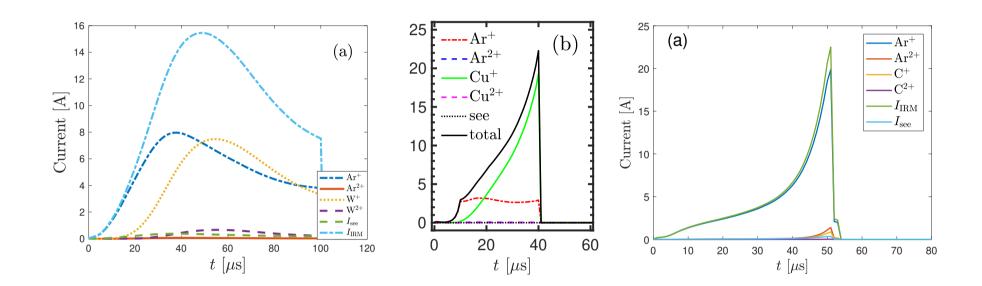


Figure 1: The current composition at the target surface for a discharge with (a) tungsten [4], (b) copper [5], and (c) graphite target [6], determined by the ionization region model.

Figure 1 shows the temporal evolution of the discharge current composition at the target surface for three different target materials

With Cu target Cu⁺ ions dominate the discharge, with graphite target Ar⁺ ions dominate the discharge, and a discharge with tungsten target shows a mix of W⁺ and Ar⁺ ions

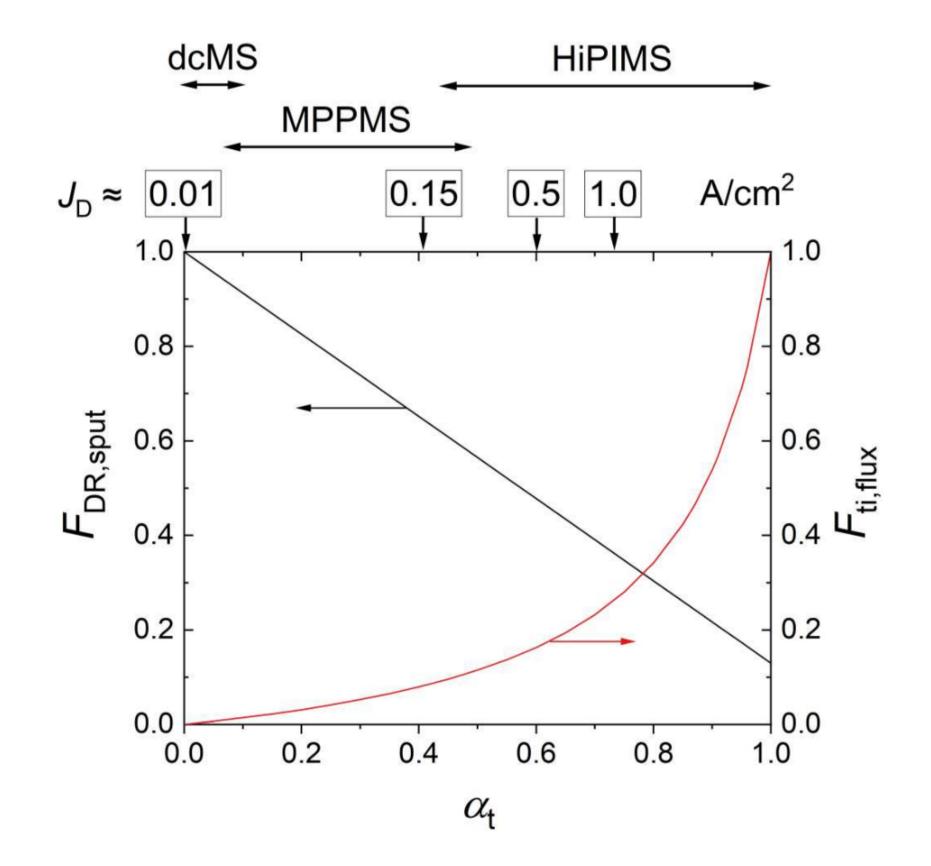


Figure 2: An illustration of the "HiPIMS compromise" for a discharge in argon with titanium target: the necessary choice between a high degree of ionization and a high deposition rate. The black curve (left axis) shows the flux available for deposition. The red curve (right axis) shows the ionization fraction in that flux. A value of $\beta_t = 0.87$ is assumed here. At the top of the panel, some typical discharge current densities at the target are drawn at the appropriate α_t values [7].

There are two measures of how good a HiPIMS discharge is:

• The fraction $F_{\mathrm{DR,sput}}$ of all the sputtered material that reaches the diffusion region (DR)

ullet The fraction $F_{
m ti,flux}$ of ionized species in that flux

There is a trade off, an inescapable conflict between the goals of higher $F_{\mathrm{DR,sput}}$ and higher $F_{\mathrm{ti,flux}}$, what we refer to as the HiPIMS compromise

Figure 2 shows $F_{\rm DR,sput}$ and $F_{\rm ti,flux}$ as functions of $\alpha_{\rm t}$ at assumed fixed value of $\beta_{\rm t}=0.87$

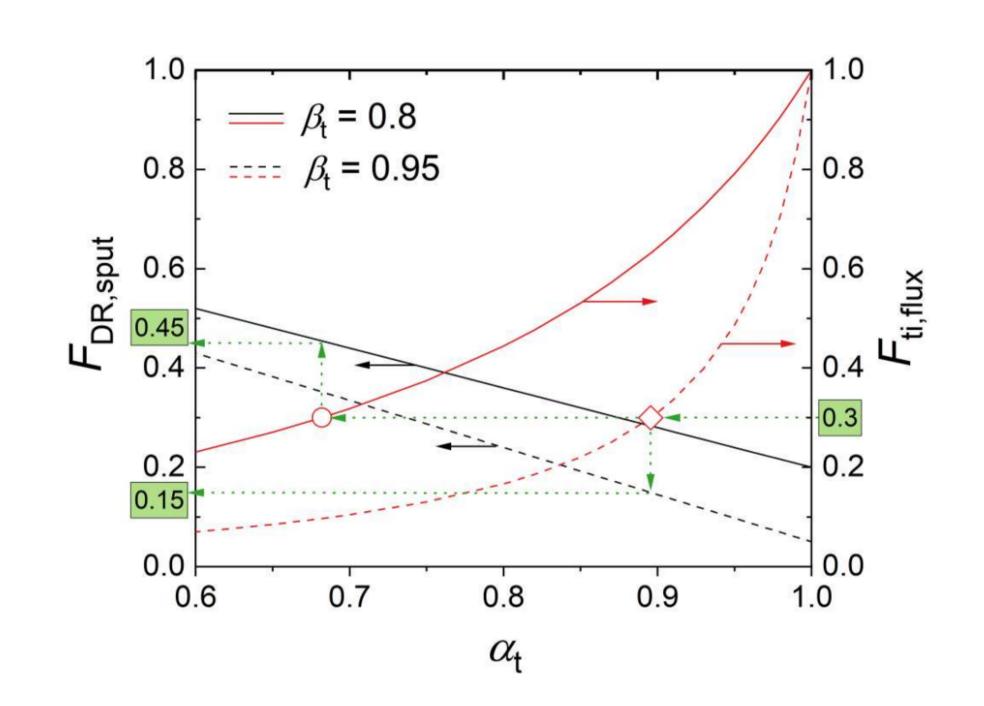


Figure 3: An illustration of that a factor of three improvement in the deposition rate (left-hand axis) can be achieved, by reducing β_t within a realistic range from 0.95 (dashed lines) to 0.8 (solid lines) for a discharge in argon with titanium target. F_{flux} (right-hand axis) is here maintained at 0.30 [7].

For a particular application an ionized flux fraction of 30 % is suitable but $0.8 \le \beta_t \le 0.95$

It is illustrated in Figure 3 that if the back-attraction can be reduced to $\beta_t = 0.8$ the deposition rate is increased

The solid lines show that reducing the back-attraction to $\beta_t = 0.8$ where $\alpha_t = 0.69$ is sufficient to maintain $F_{ti,flux} = 0.30$ (red circle) $F_{DR,sput} = 0.45$ or a factor of three increase in the deposition rate

The questions that remain:

- What determines the back-attraction probability?
- How can we vary the ionization probability α_t and maybe more importantly the back-attraction probability β_t ?

Figure 4 shows the back-attraction probability β_t determined by IRM, versus the self-sputter yield for various target materials

The data indicate that the back-attraction probability decreases roughly linearly with increased self-sputter yield









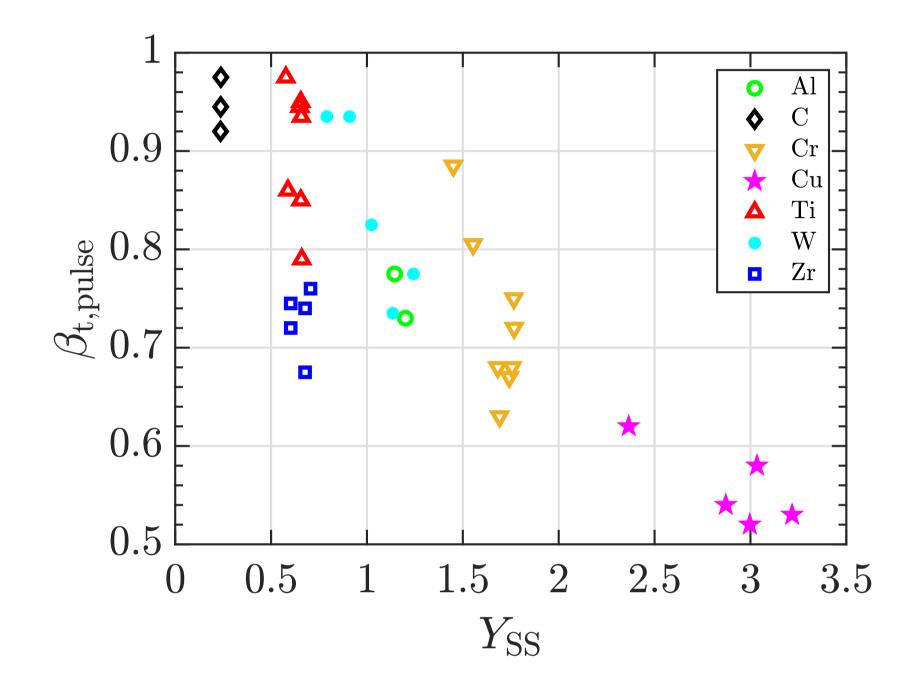


Figure 4: The back-attraction probability β_t versus the self-sputter yield for various target materials modeled by the IRM [8].

Conclusions

There is an inescapable conflict between the goals of higher deposition rate and higher fraction of ionized species in the sputtered material flux

We have applied the ionization region model to determine the backattraction probability for HiPIMS discharges with a number of different cathode targets, spanning a wide range in atomic mass

The back-attraction probability appears to decrease with increased sputter yield of the target material

References

- [1] J. T. Gudmundsson. *Plasma Sources Sci. Technol.*, **29**(11), 113001, 2020
- [2] J. T. Gudmundsson *et al. J. Vac. Sci. Technol. A*, **30**(3), 030801, 2012.
- [3] Chunqing Huo et al. J. Phys. D: Appl. Phys., **50**(35), 354003, 2017.
- [4] S. Suresh Babu et al. Plasma Sources Sci. Technol., 31(6), 065009,
- [5] J. T. Gudmundsson et al. Surf. Coat. Technol. 442, 128189, 2022.
- [6] H. Eliasson *et al. Plasma Sources Sci. Technol.*, **30**(11), 115017, 2021
- [7] N. Brenning et al. J. Vac. Sci. Technol. A, 38(3), 033008, 2020.
- [8] K. Barynova et al. Plasma Sources Sci. Technol., 34(6), 06LT01, 2025.