

Experiments and modelling of high power impulse magnetron sputtering discharges with metallic target

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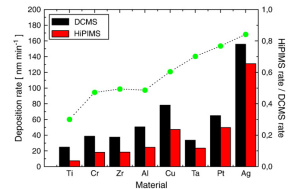
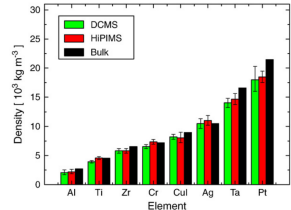
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Introduction – Magnetron sputtering

- In a high power impulse magnetron sputtering (HiPIMS) the discharge is driven by high power pulses of low repetition frequency, and with low duty cycle
- The film mass density is higher, the films exhibit better crystallinity, and overall improved film properties, when deposited with HiPIMS
- There is a drawback: The deposition rate is lower for HiPIMS when compared to dcMS operated at the same average power
- Many of the ions of the target material are attracted back to the target surface by the cathode potential



From Samuelsson et al. (2010) SCT 202-591



Overview

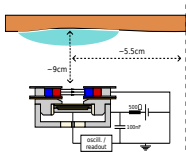
- Ionized flux fraction – measurements
- The ionization region model (IRM)
- Deposition rate vs ionized flux fraction
- Summary



Ionized flux fraction – measurements



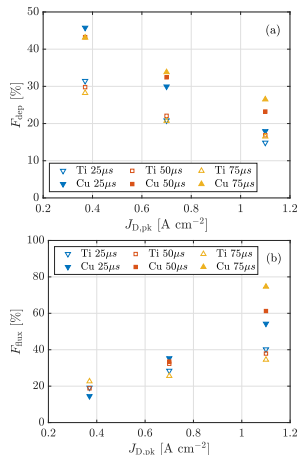
Ionized flux fraction – measurements



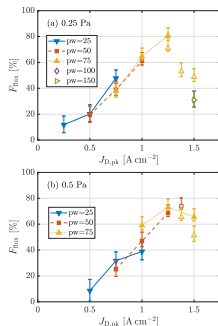
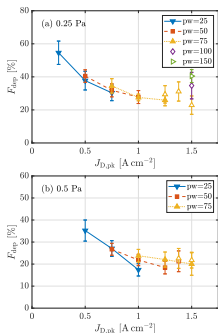
- The ionized flux fraction and the deposition rate fraction – measured by an ion meter in HiPIMS discharges with Cu and Ti targets and working gas pressure of 0.3 Pa

Cu: Fischer et al. (2023) PSST **32** 125006

Ti: Shimizu et al. (2021) PSST **30** 045006



Ionized flux fraction – measurements

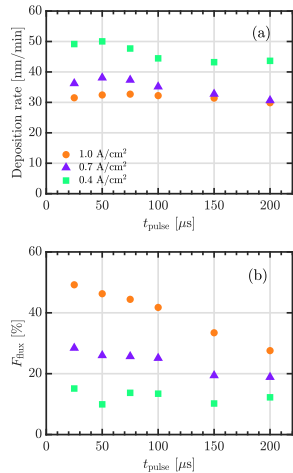


From Fischer et al. (2023) PSST **32** 125006

- The measured normalized deposition rate (left) and ionized flux fraction (right) as a function of the peak discharge current density $J_{D,peak}$ for working gas pressure of (a) 0.25 Pa and (b) 0.5 Pa

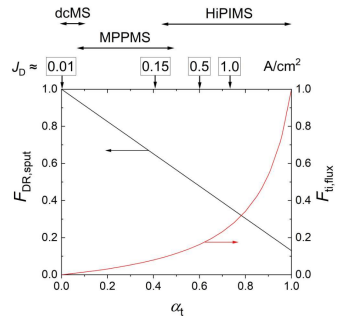
Ionized flux fraction – measurements

- The deposition rate (upper) and the ionized flux fraction (lower) versus the pulse length
- For peak discharge current density of 0.4 A/cm^2 , 0.7 A/cm^2 , and 1.0 A/cm^2 and argon working gas pressure of 0.3 Pa
- The target was 150 mm diameter chromium disk
- The pulse repetition frequency was adjusted to maintain a constant time-averaged power of 1.5 kW



Ionized flux fraction – measurements

- The measurements show a decrease in deposition rate and an increase in the ionized flux fraction with increased discharge current density
- There are two measures of how good a HiPIMS discharge is:
 - the fraction $F_{\text{DR,sput}}$ of all the sputtered material that reaches the diffusion region (DR)
 - the fraction $F_{\text{ti,flux}}$ of ionized species in that flux
- There is a trade off between the goals of higher $F_{\text{DR,sput}}$ and higher $F_{\text{ti,flux}}$



From Brenning et al. (2020) JVSTA **38** 033008

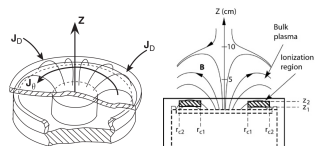
The ionization region model (IRM)



Ionization region model

- The ionization region model (IRM) is a time-dependent volume averaged plasma chemical model of the ionization region (IR) of the HiPIMS discharge
- The IRM gives the temporal evolution of the densities of ions, neutrals and electrons
- The IRM gives also two internal parameters that are of importance
 - α_t – ionization probability
 - β_t – back-attraction probability

Detailed model description is given in Huo et al. (2017) JPD **50** 354003



The definition of the volume covered by the IRM

- The IR is defined as an annular cylinder of width $w_{rt} = r_{c2} - r_{c1}$ and thickness $L = z_2 - z_1$, extends from z_1 to z_2 axially away from the target

Ionization region model

- The temporal development is defined by a set of ordinary differential equations giving the first time derivatives of
 - the electron energy
 - the particle densities for all the particles (except electrons)
- The species assumed in the non-reactive-IRM are
 - cold electrons e^C , hot electrons e^H
 - argon atoms $Ar(3s^23p^6)$, warm argon atoms in the ground state Ar^W , hot argon atoms in the ground state Ar^H , Ar^m ($1s_5$ and $1s_3$) (11.6 eV), argon ions Ar^+ (15.76 eV), doubly ionized argon ions Ar^{2+} (27.63 eV)
 - Metal atoms, sometimes metastable states, metal ion M^+ , and doubly ionized metal ions M^{2+}

Detailed model description is given in Huo et al. (2017) JPD **50** 354003



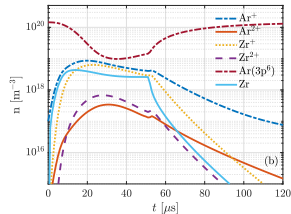
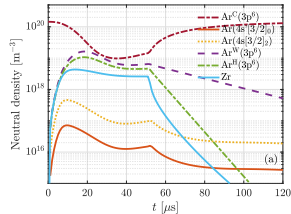
Ionization region model

- As an example the particle balance equation for the metal ion M^+ is

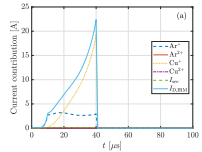
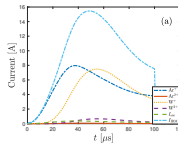
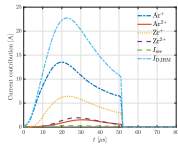
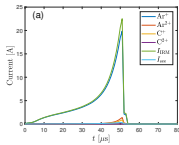
$$\begin{aligned}
 \frac{dn_{M^+}}{dt} = & \underbrace{k_{iz,M}^c n_{e,c} n_M + k_{iz,M}^h n_{e,h} n_M}_{\text{electron impact ionization}} + \underbrace{k_{P,iz} n_{Ar^m} n_M}_{\text{Penning ionization}} \\
 & + \underbrace{k_{chexc,1} n_M n_{Ar^+} + k_{chexc,2} n_{M^{2+}} n_{Ar}}_{\text{charge exchange}} - \underbrace{k_{iz,M^+}^c n_{e,c} n_{M^+} + k_{iz,M^+}^h n_{e,h} n_{M^+}}_{\text{electron impact ionization to create } M^{2+}} \\
 & - \underbrace{\frac{\Gamma_{M^+}^{RT} + \Gamma_{M^+}^{BP} (S_{IR} - S_{RT})}{\nu_{IR}}}_{\text{ion flux out of the ionization region}}
 \end{aligned}$$

Ionization region model studies of HiPIMS

- The temporal evolution of the neutral and ion densities in a discharge with zirconium target
- Ar^+ ions dominate the discharge – but Zr^+ ions are not far off
- Ar^{2+} and Zr^{2+} ions have much lower densities
- Working gas rarefaction is very apparent



Ionization region model



C: PSST (2021) **30** 115017 Zr: JVSTA (2024) **42** 043007 W: PSST (2022) **31** 065009 Cu: SCT (2022) **442** 128189

- The temporal evolution of the discharge current composition at the target surface for four different targets
- With Cu target Cu^+ ions dominate, with graphite target Ar^+ ions dominate
- For Zr and W targets there is a mix of Ar^+ and metal ions

Deposition rate vs ionized flux fraction



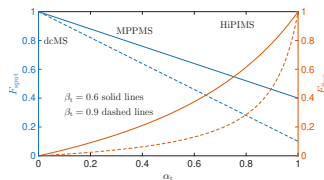
Deposition rate vs ionized flux fraction – α_t and β_t

- We can relate the measured quantities normalized deposition rate $F_{\text{DR,sput}}$ and the ionized flux fraction $F_{\text{ti,flux}}$

$$F_{\text{DR,sput}} = \frac{\Gamma_{\text{DR}}}{\Gamma_0} = (1 - \alpha_t \beta_t)$$

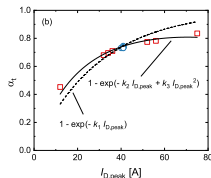
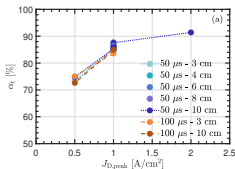
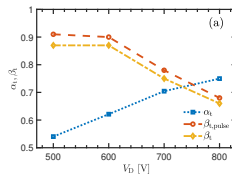
$$F_{\text{ti,flux}} = \frac{\Gamma_{\text{DR,ions}}}{\Gamma_{\text{DR,sput}}} = \frac{\Gamma_0 \alpha_t (1 - \beta_t)}{\Gamma_0 (1 - \alpha_t \beta_t)} = \frac{\alpha_t (1 - \beta_t)}{(1 - \alpha_t \beta_t)}$$

to the internal parameters back
attraction probability β_t and ionization
probability α_t



Deposition rate vs ionized flux fraction – α_t and β_t

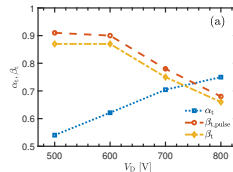
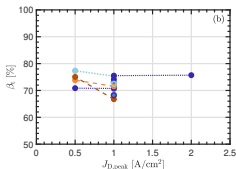
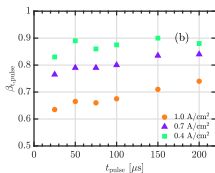
- The internal discharge parameters α_t and β_t from the ionization region model (IRM)

Ti: JPD **55** 015202Zr: JVSTA **42** 043007W: PSST **31** 065009

- The ionization probability α_t increases with increased peak increased discharge current density
- The peak discharge current increases with increased discharge voltage

Deposition rate vs ionized flux fraction – α_t and β_t

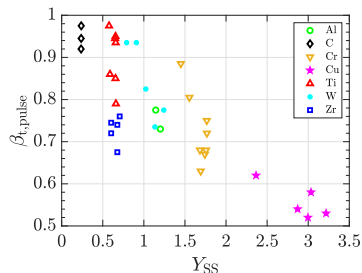
- The internal discharge parameters α_t and β_t from the ionization region model (IRM)



- The back-attraction probability β_t has less clear dependence on the peak discharge current density – decreases with increased peak discharge current density for Cr and W – no clear trend for Zr

Deposition rate vs ionized flux fraction – α_t and β_t

- What determines the back-attraction probability ?
- How can one influence the back-attraction probability ?
- The back-attraction probability $\beta_{t,pulse}$, 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



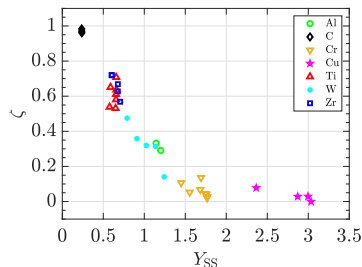
From Barynova et al. (2025) PSST **34** 06LT01

Deposition rate vs ionized flux fraction – α_t and β_t

- The fraction of the ion current carried by Ar^+ ions can be estimated using

$$\zeta = \frac{J_{\text{Ar}^+}}{J_{\text{Cr}^+} + J_{\text{Ar}^+}} = \frac{1 - \alpha_t \beta_t Y_{\text{SS}}}{1 + \alpha_t \beta_t (Y_{\text{tg}} - Y_{\text{SS}})}$$

- It is almost 100 % for a discharge with graphite target and falls to almost zero for a discharge with copper target
- A HiPIMS discharge with graphite target is operated on working gas recycling and a discharge with a copper target operates on self-sputter recycling, while discharges with titanium, tungsten, and zirconium targets operate on a mixture



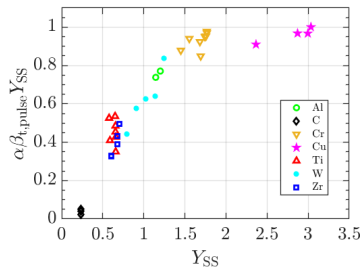
Deposition rate vs ionized flux fraction – α_t and β_t

- The condition for sustained self-sputtering

$$\alpha_t \beta_t Y_{SS} \geq 1$$

Hosokawa et al. (1980) IVC-8 and Anders et al. (2007) JAP **102** 113303

- For sustained self-sputtering the noble working gas is only needed to get the process started
- Since $\alpha_t < 1$ and $\beta_t < 1$ the condition $Y_{SS} > 1$ is necessary
- This parameter increases with increased self-sputter yield and approaches sustained self-sputtering for a chromium and copper targets



Summary



Summary

- The discharge current composition at the target surface depends on the target material
- There is an inescapable conflict between the goals of higher deposition rate and higher fraction of ionized species in the sputtered material flux
- The back-attraction probability appears to depend on the self-sputter yield – it is lower for higher self-sputter yield
- The main contributor to working gas rarefaction for low sputter yield target is electron impact ionization, while for targets with high sputter yield kick-out by the sputtered species is the main contributor



Thank you for your attention

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The slides can be downloaded at

<http://langmuir.raunvis.hi.is/~tumi/ranns.html>



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