## Modelling of reactive HiPIMS discharges: parametric, ionization-region and particle-based approaches

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High power impulse magnetron sputtering (HiPIMS) has become a highly-effective technique of magnetron sputtering, providing high and tuneable degree of ionization of sputtered atoms to enable better control of energy delivered into growing films. In combination with reactive gases, it was proved effective in depositing various oxides, nitrides or oxynitrides with high application potential. Moreover, benefits of reactive HiPIMS, such as high density of films, high depositions rate, narrow hysteresis and less arcing have been reported [1, 2].

The presentation summarizes our effort to model the reactive HiPIMS discharge to explain the relationships between process input parameters (partial pressures, power, pulse length, etc.) and film properties. Our models are based on the well-known Berg model describing the coverage of surfaces by a compound. But, most importantly, they include the key HiPIMS phenomena, such as ionization of sputtered atoms, reactive gas dissociation, ion return to target and gas rarefaction, which are, however, characterized by a shorter timescale compared to the compound coverage processes. We present how the plasma phenomena can be described using a parametric approach [3] and using a simplified ionization-region (global) model [4] and coupled to the compound coverage model. Examples of model predictions and comparisons with experiment will be given (for example, for ZrO2 and WO3 depositions). Finally, a recently developed particle-based model of non-reactive HiPIMS [5], which calculates the spatial distribution of atoms and ions within the HiPIMS discharge will be presented. Its advantages, limitations, and potential extensions to a reactive HiPIMS model will be discussed.

- [1] J. Vlček, J. Rezek, J. Houška, T. Kozák, J. Kohout, Vacuum. 114 (2015) 131–141.
- [2] J. Čapek, S. Kadlec, J. Appl. Phys. 121 (2017) 171911.
- [3] T. Kozák, J. Vlček, J. Phys. D: Appl. Phys. 49 (2016) 055202.
- [4] J. Rezek, T. Kozák, N. Kumar, S. Haviar, J. Phys. D: Appl. Phys. 54 (2021) 125202.
- [5] T. Kozák, Plasma Sources Sci. Technol. 32 (2023) 035007.