Kinetic Monte Carlo simulation of film growth deposited by HiPIMS and evaluation of film properties

HiPIMS Today
Recent Developments in
High-Power Impulse Magnetron Sputtering
January 25th -27th, 2022

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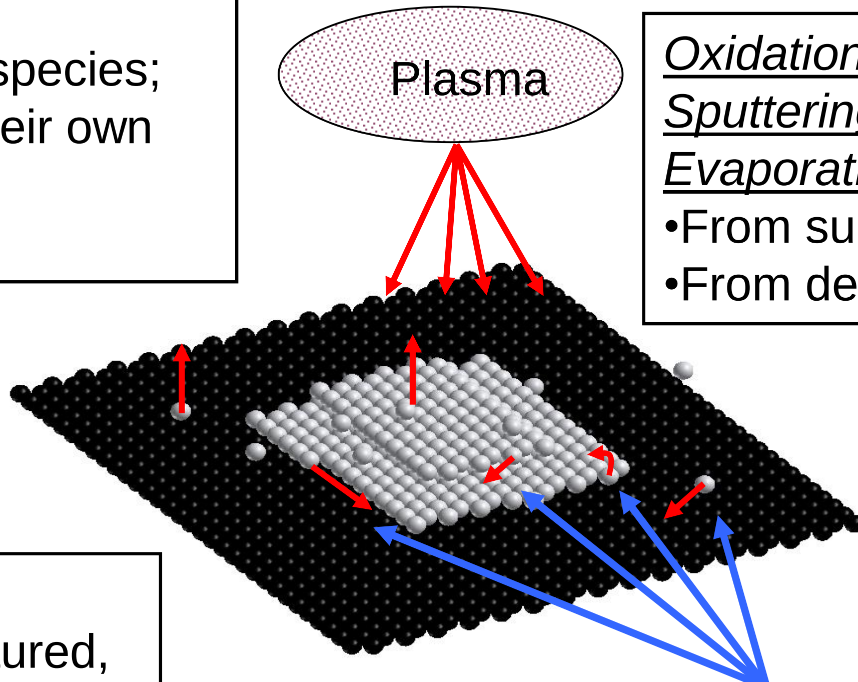
OUTLINE

- Film growth model in kMC package NASCAM
- Film properties as a function of discharge power
- Metal filling by HiPIMS
- Conclusions

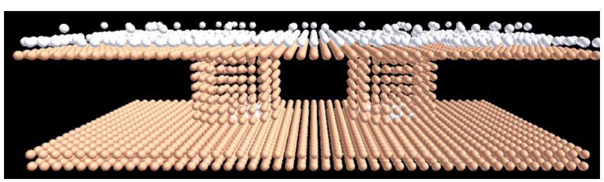
Description of the model: overview

Deposition:
Metallic and reactive species;
Incident atoms with their own
•Energy distribution,
•Angular distribution.



Oxidation;
Sputtering;
Evaporation:
•From substrate
•From deposited film

Substrate:
- flat as well as textured,
- tilting and rotation.
- Substrate movement,
- Masked deposition.

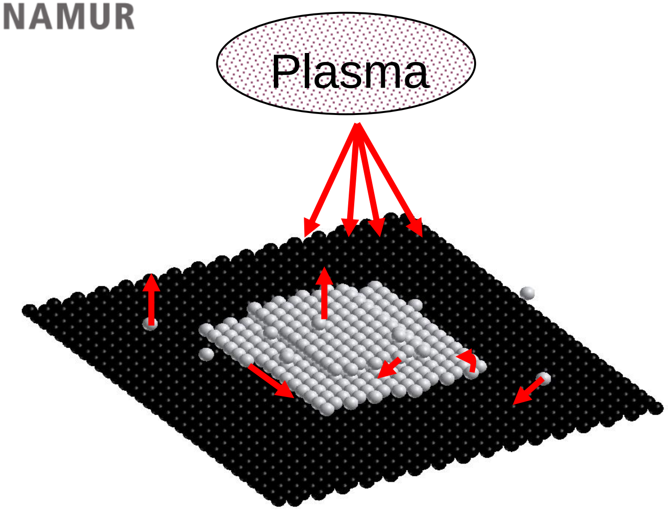


All kinds of diffusion events:
•Diffusion on the substrate
•Diffusion on the deposited film
•Jumps from one layer to another

NASCAM V 4.7.X features

- > 1e^6 atom begin deposited
- One or two metallic, one reactive (O, N, …) and one neutral species
  - neutral or/and ionized
- Flat or corrugated substrate
- Evaporation, sputtering, reactive mode, ….
- Interface with gas/plasma simulation codes
- Plugins:
  - Optic
  - Porosity
  - Roughness
  - …..

Application to HiPIMS



What we need for the film growth simulations?

- List of condensing species,
- Relative amount of each specie (percentage of ions),
- Parameters of their fluxes, energy and angular distribution.

Two separate fluxes for neutrals and ions:

- neutrals: lower average energy and broad angular distribution,
- Ions: higher average energy and narrow angular distribution.

Energy transfer from incident particles to growing film:

- higher film density,
- Sputtering and re-deposition.

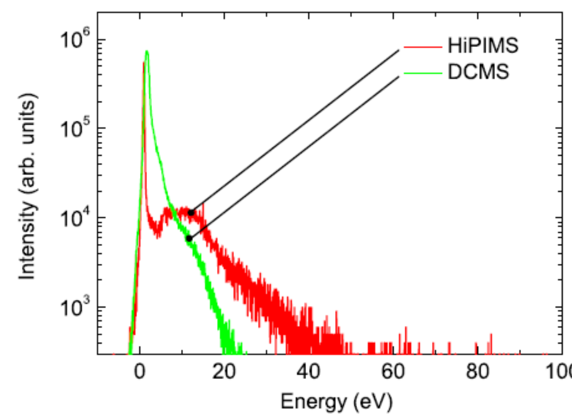
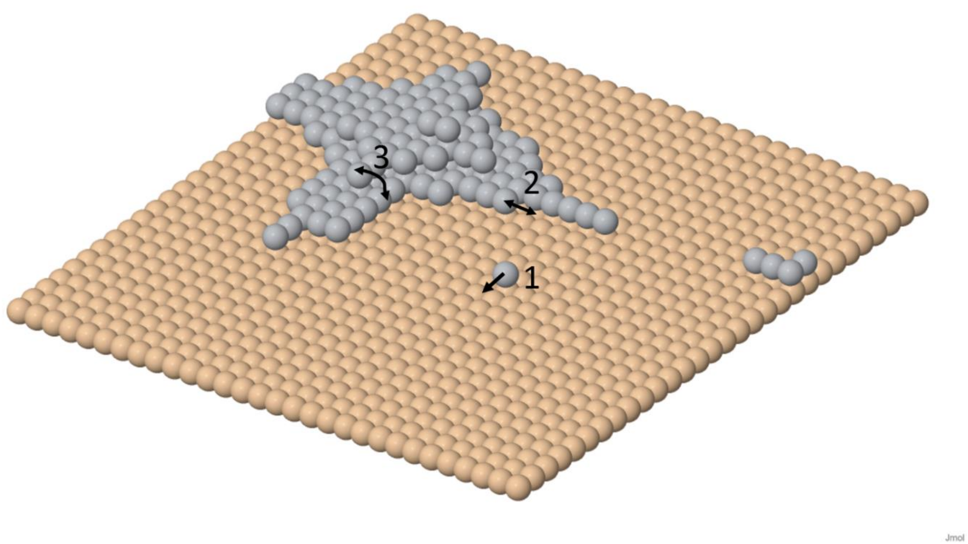


FIG. 3. Comparison between Ti^+ ion-energy distributions from HiPIMS and direct current magnetron sputtering (DCMS) measured at 0.80 Pa Ar under equivalent process conditions at the same average power. The

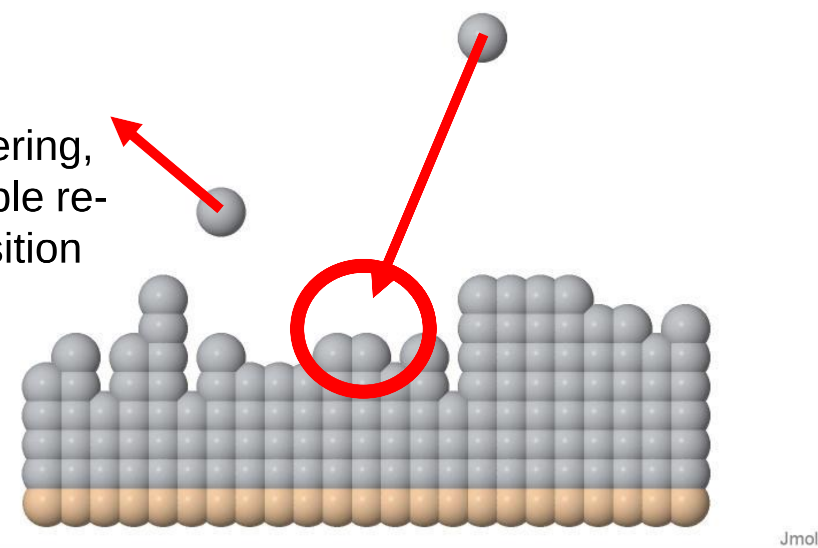
D. Lundin et al.: An introduction to thin film processing using high-power impulse magnetron sputtering J. Mater. Res., Vol. 27, No. 5, Mar 14, 2012

Processes in the film

- Thermally activated – diffusion, rate ~ $exp(-E_a/k_BT)$
- Activated by collisions and energy transfer -
  - displacement of atoms,
  - sputtering,
  - re-deposition.



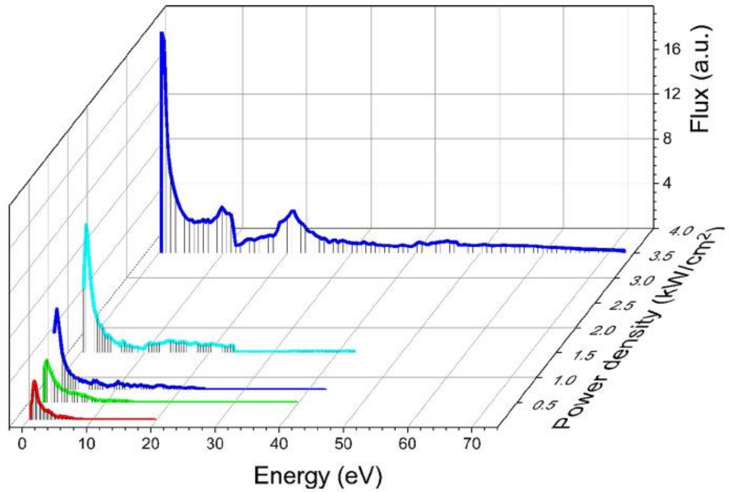
Sputtering, possible re-deposition



Energy transfer, displacements of atoms and re-arrangement

Film properties as a function of discharge power

Ruhr University Bochum, Institute of Energy and Climate Research
Fraunhofer IST, University of Mons, University of Namur



Peak power densities, average discharge power variation from dcMS-like to HiPIMS.

No.	(P/A) peak (kW/cm^2)	<P > (W)	Type of plasma
1	3.43	420	HiPIMS
2	1.55	219	HiPIMS
3	0.79	137	dcMS-like
4	0.55	106	dcMS-like
5	0.17	34	dcMS-like

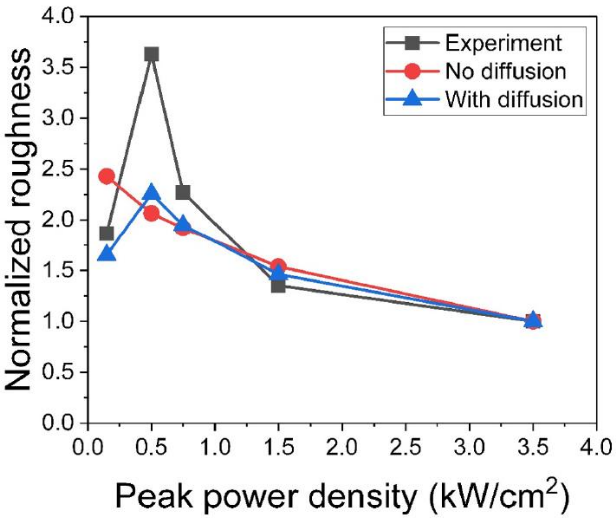
Averaged energy deposited per atom for different deposition conditions.

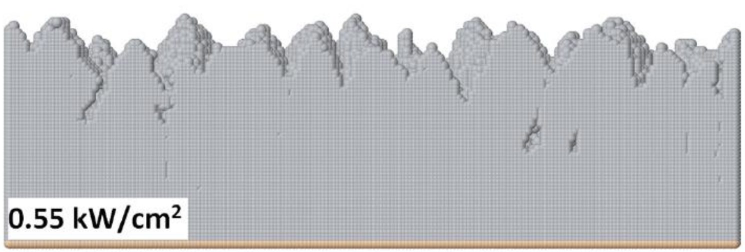
Peak power density (kW/cm^2)	0.17	0.55	0.79	1.55	3.43
Averaged energy deposited per atom (eV/atom)	2.1	2.4	3.4	5.4	14.1

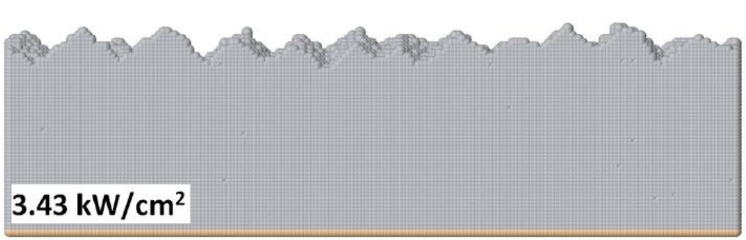
What is necessary to know to make simulations.
Fluxes of species
- ions : energy distribution – from measurements, angular distribution - analytical estimations,
- neutrals : SiMTra

P. Moskovkin, C. Maszl, R. Schierholz, W. Breilmann, J. Petersen, A. Pflug, J. Muller, M. Raza, S. Konstantinidis, A. von Keudell, S. Lucas, Link between plasma properties with morphological, structural and mechanical properties of thin Ti films deposited by high power impulse magnetron sputtering, Surface and Coating Technologies 418 (2021) 127235

Simulation results – evolution of film roughness with an increase of discharge power density







Why roughness is low at low discharge power density – role of surface diffusion

Deposition rate :

- 0.17 kW/cm^2 – 4 nm/min
- 0.55 – 3.43 kW/cm^2 - ~15 nm/min

When surface diffusion becomes important : deposition rate expressed in mono layer per second is less than or comparable to diffusion rate $\omega = \omega_0 \, exp(-E_a/k_B T)$

Deposition rate is low at W=0.17 kW/cm^2 : roughness is low because of diffusion.
At W>1 kW/cm^2 roughness is low because of ion bombardment.
At W=0.55 kW/cm^2 roughness is maximum as neither diffusion nor ion bombardment are effective.

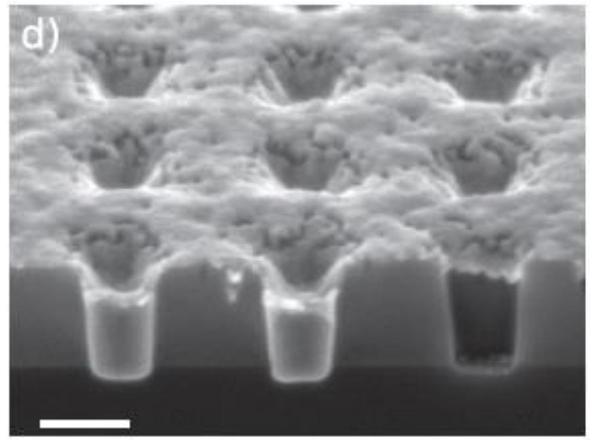
Metal filling by HiPIMS

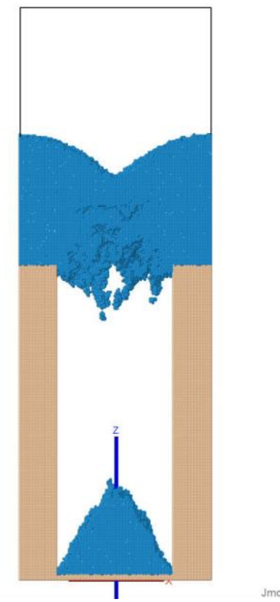
Uppsala University
University of Namur

Deposition of Cu on a surface with holes, diameter of holes 100-150 nm, aspect ratio ~ 2.

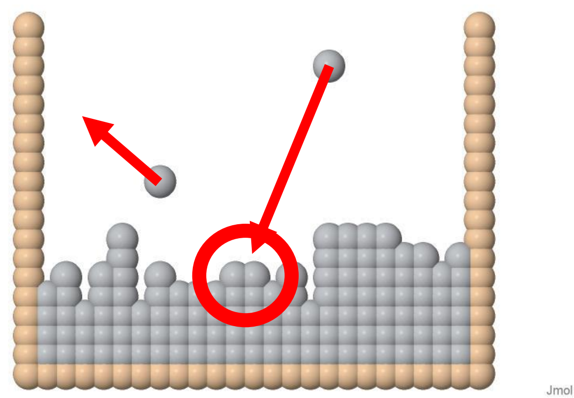
Working pressure 0.5 Pa and 1.0 Pa.

Bias – from 0 to -400 V



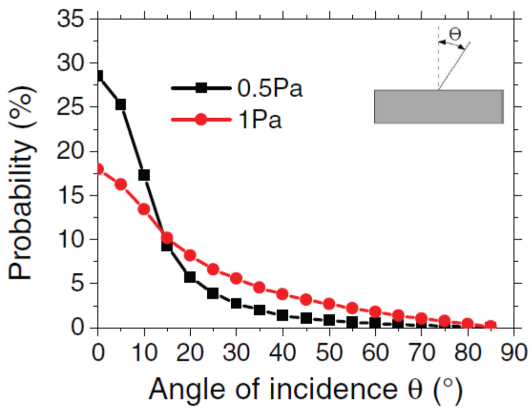


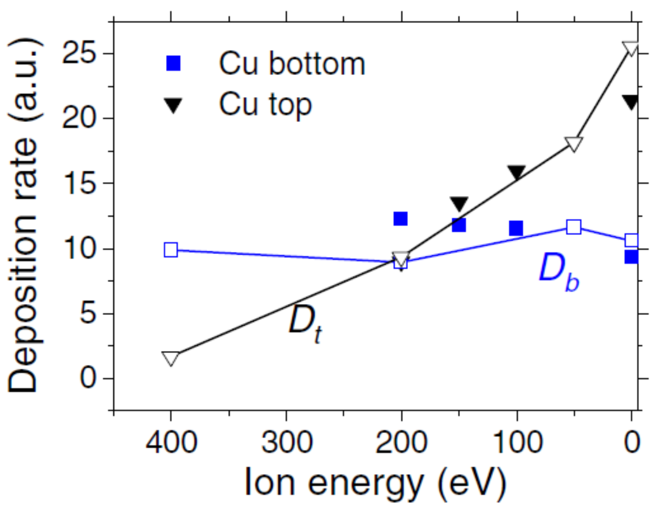
Fluxes of species
- ions : fixed energy which is equal to bias, angular distribution
- normal to the surface,
- neutrals : SiMTra

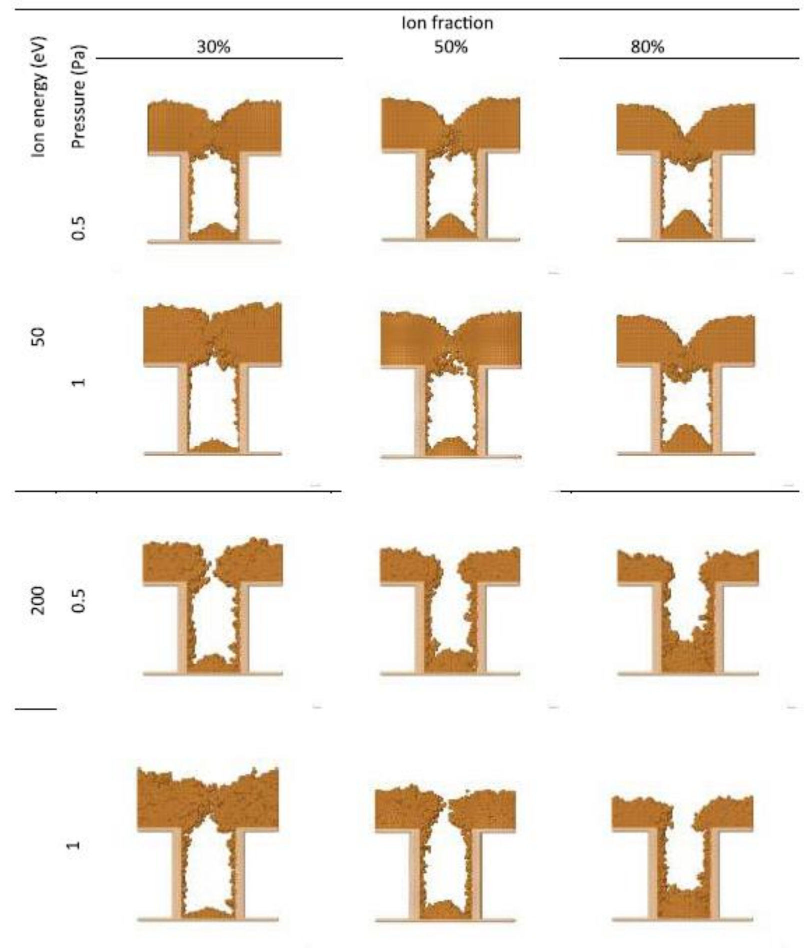


L. Jablonka, P. Moskovkin, Z. Zhang, S.-L. Zhang, S. Lucas, T. Kubart, Metal filling by high power impulse magnetron sputtering, *J. Phys. D: Appl. Phys.* 52 (2019) 365202

Metal filling by HiPIMS







Dt **and** ***Db are*** **deposition rates on the top surface and at the feature bottom.**
Open symbols indicate experimental data, full symbols simulated results

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Conclusions

- Atomistic simulations can help in planning experiments and understanding their results
- Kinetic Monte Carlo approach has shown its applicability and usefulness for film growth simulations, from electron beam evaporation to HiPIMS and ion assisted deposition
- After film growth simulation one can use simulated structures to analyse film properties:
  - Morphology,
  - Electrical,
  - Optical,
  - …

Thank you

https://www.incosol4u.com/nascam-general