Modelisation of thin film deposition by KMC Plathinium, Antibes, 9/2019

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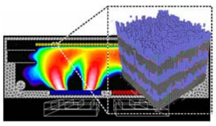


1.5 hours lecture

- Concepts
- Illustration of concepts with NASCAM (google NASCAM for info)

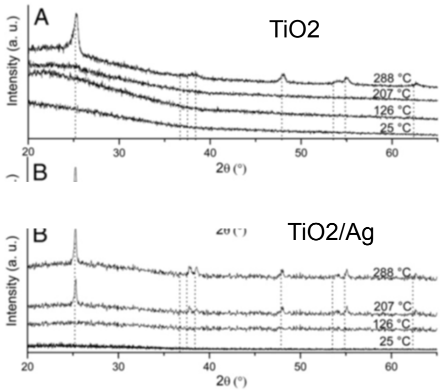
- You received either NASCAM or a link to download it
- It runs under windows and JAVA (32 or 64 bits)
- The licence key is valid for one month.
- You are welcome to request an extension of the licence.

A little story (TiO_2 magnetron sputtering)

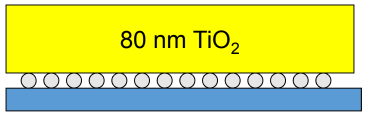
Superhydrophilicity and photocatalytic activity of TiO2 are related to the crystallisation film in anatase structure

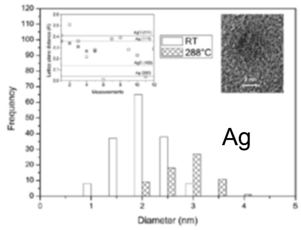
Heat, anneal

Lower the nucleation energy for a specific phase.



H. Limage, … S. Lucas, Surf. And Coat. Techn., 2011 (206)3774





By Magn. Sputtering

A little story

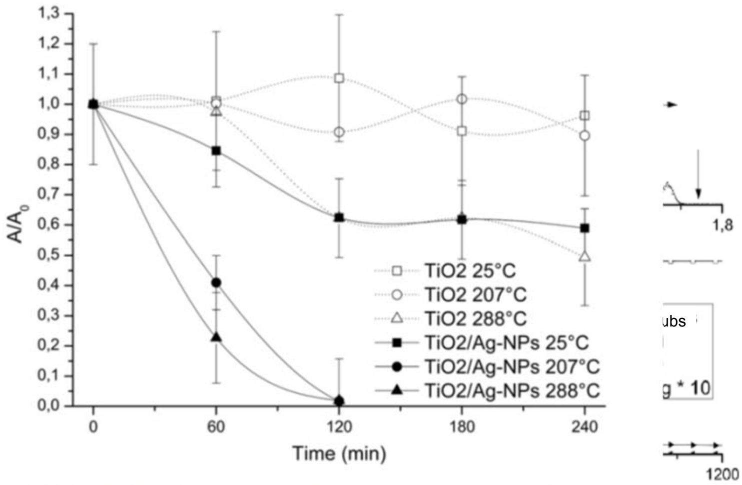
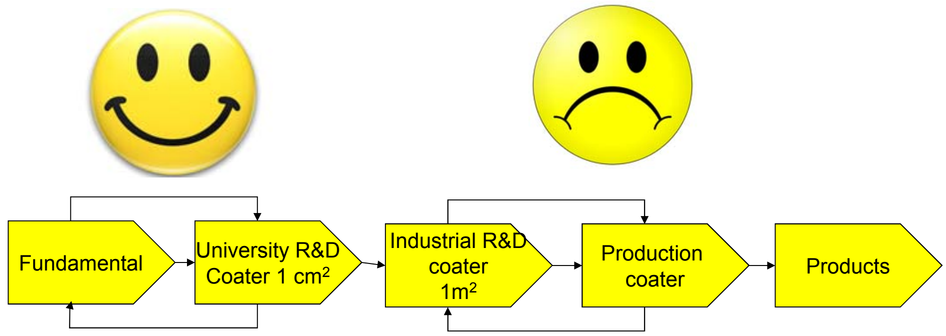


Fig. 7. Evolution of palmitic acid degradation as measured by absorbance ratio versus UV exposure time.

H. Limage, … S. Lucas, Surf. And Coat. Techn., 2011 (206)3774

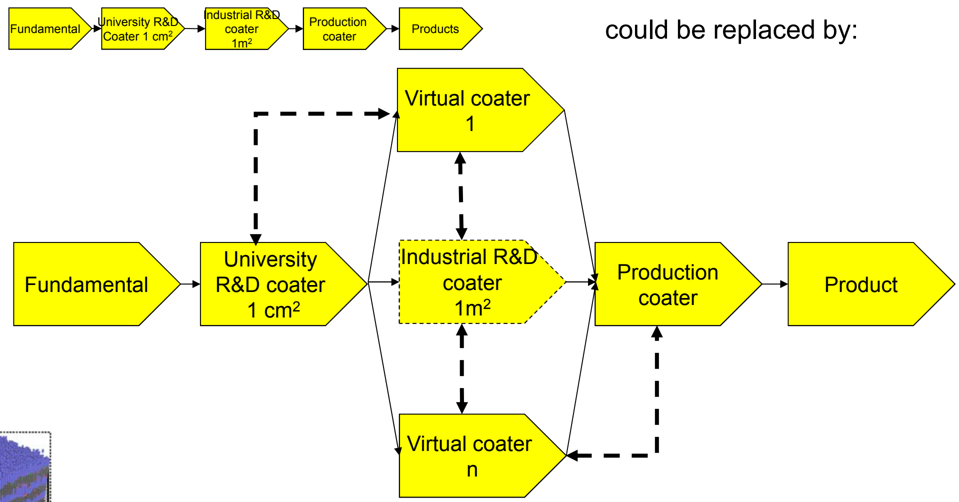
A little story: paradigm

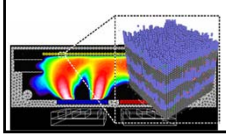


We need more predictive tools

- Was it predictable ?
- Could we have guessed the upscaling parameters (coater setup) ?
- Is there only one suitable set of coater's parameters ?

Redefining the product development model





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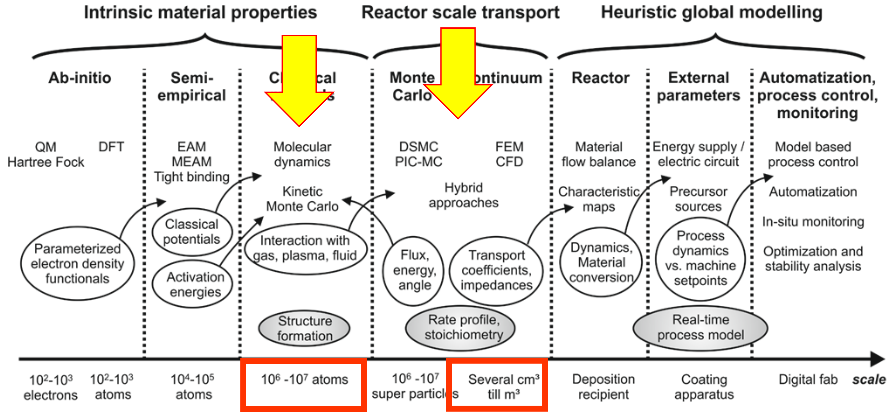
Multi scale simulation in thin film deposition

Complementary modelling approaches and scales



Courtesy of A. Pflug, IST

→ Chapter „Deposition technology (thin films)" in Georg Schmitz, Ulrich Prahl (Ed.): Handbook of Software Solutions for ICME, Wiley VCH, in press (expected for 2016).

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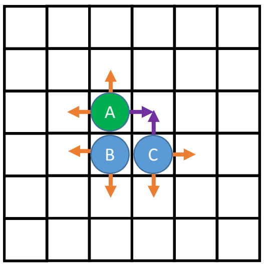
Kinetic Monte Carlo method (kMC)

- kMC method was developed to mimic the time evolution of a system containing large number of atoms for a relatively long period of time
- The evolution of the system is driven by the probabilities of different "elementary" ***events*** (e;g. moves)
- The event rates are defined as $w = w_0 exp(-U/kT)$, where w_0 can be estimated as $2kT/h \sim 10^{12}$-10^{13}, U – energy barrier for an atom for the movement, T – temperature, k – Boltzmann constant, h Planck constant
- At each time step an atom and the direction of its movement are chosen in accordance with the probability of such movement
- Time increment at each time step is equal to $\Delta t=(\Sigma w_i)^{-1}$, where it is necessary to sum over all possible "jumps" of atoms in the system

Kinetic Monte Carlo method

Example:

$N_{ev} = 8$



Ea_detach (6) > **Ea_nn_inc** (2)

$$w_j = w_0 \exp(-E_j / k_B T),$$

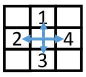
Probability to have a *j*-kind event:

$$p_j = N_j w_j / R$$

Total rate

Nbre of possible jumps

diffusion directions

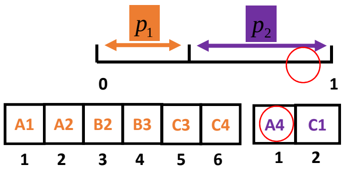


event 1: A1, A2, B2, B3, C3, C4

event 2: A4, C1

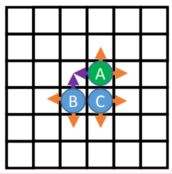
1st rng

2nd rng



⇒

final configuration and corresponding new possible movements

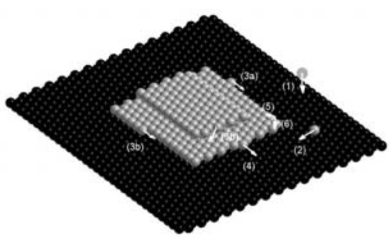


Example of calculation of event rate

$$T = 0,03\ eV = 0,03 * 11600 = 348\ K = 75°C$$

$$Ea\_diff = 0,5\ eV$$

$$W = W_0 . e^{-\frac{Ea}{k_B . T}}$$



$$W_0 = \frac{2.k_B.T}{h} = 1,45x10^{13} / s$$

$$W = W_0 . e^{-\frac{Ea}{k_B . T}} \approx 8x10^5 / s$$

Some order of magnitude

Ea_diff,(eV): 0.51	- rate 5.78e+005 (1/s)
Ea_nn_dec,(eV): 1.90	- rate 3.12e-015 (1/s)
Ea_nn_inc,(eV): 1.90	- rate 3.12e-015 (1/s)
Ea_detach,(eV): 1.95	- rate 5.90e-016 (1/s)
Ea_up,(eV): 2.00	- rate 1.11e-016 (1/s)
Ea_down,(eV): 2.00	- rate 1.11e-016 (1/s)
Ea_detrap,(eV): 4.50	- rate 7.18e-053 (1/s)
Ea_sub_evap,(eV): 4.50	- rate 7.18e-053 (1/s)
Ea_lay_evap,(eV): 4.50	- rate 7.18e-053 (1/s)

Not required if deposition at RT

$$T = 0,03\ eV = 0,03*11600 = 348\ K = 75°C$$

From literature

- MD simulations
- Bond counting

From experimentation, observation, knowledge

….

Introduction to NASCAM

- Introduction and motivation
- Basis of NASCAM
- What we can do by NASCAM – examples
- Film growth simulation based on the input data from the EOSS simulation run
- Analysis of the optical properties of the film by NASCAM's plug-ins

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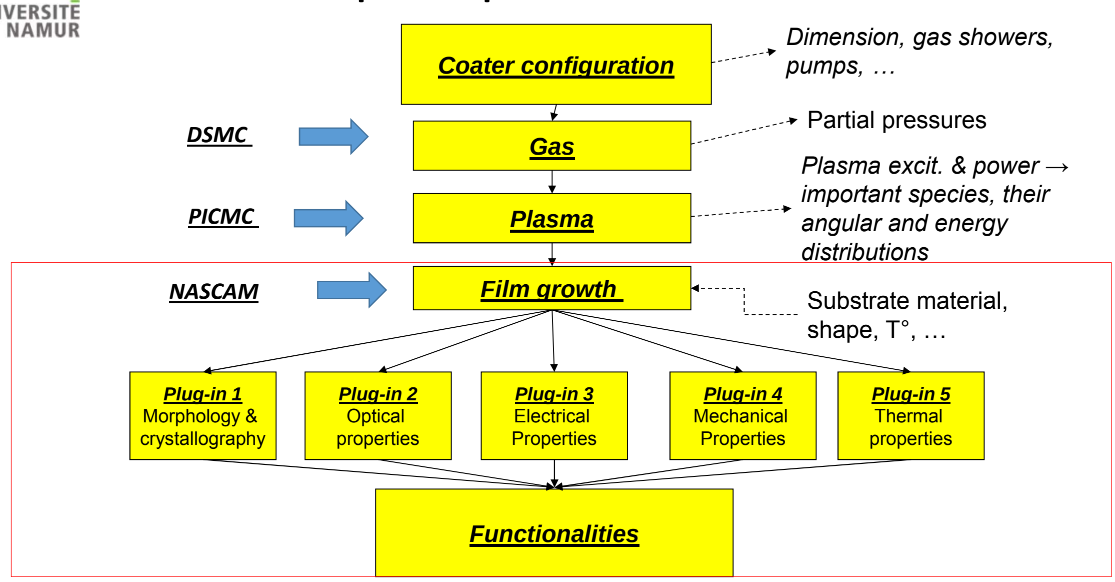
The concept of plasma VIRTUAL COATER^{TM}



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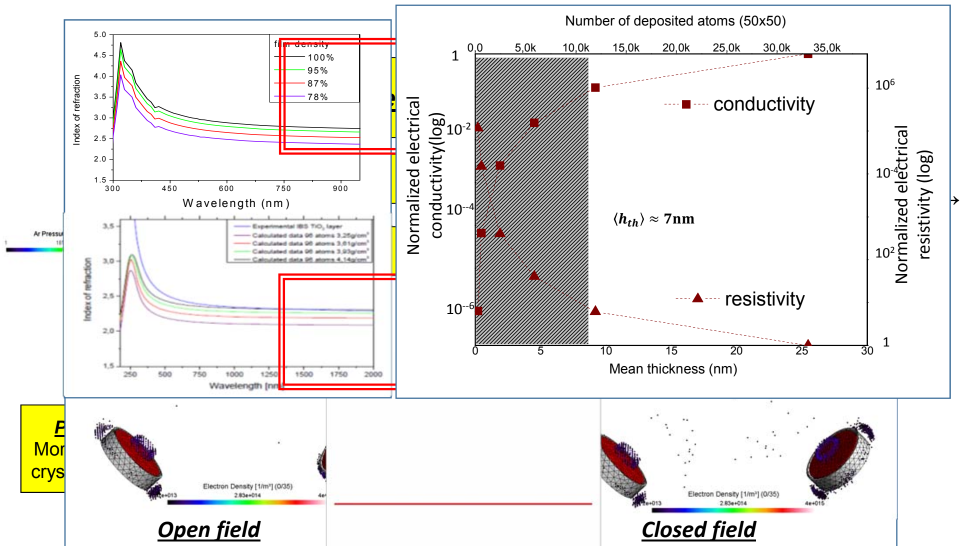
The concept of plasma VIRTUAL COATER^{TM}



A. Pflug, Fraunhofer ISI, Braunschweig, Germany
R. Tonneau, S. Lucas, University of Namur, Namur, Belgium

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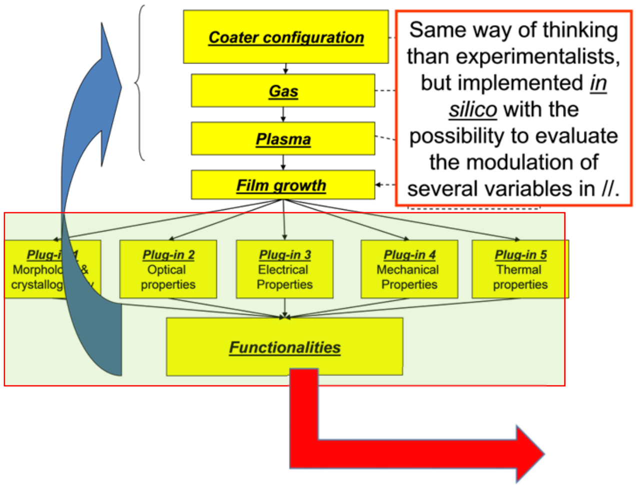
The concept of plasma VIRTUAL COATER^{TM}

NASCAM as a part of VIRTUAL COATER^{TM}

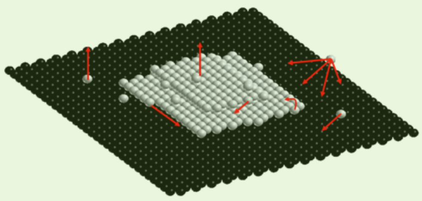
The concept of plasma VIRTUAL COATER^{TM}



Film growth model

We take into account

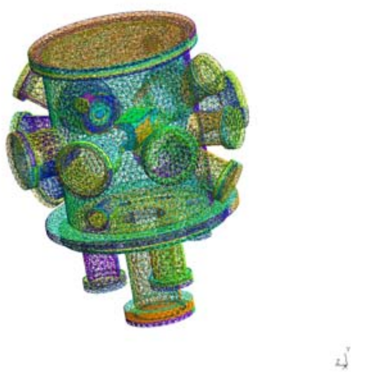
- Deposition
- Free diffusion
- Atom attachment
- Island formation and growth
- Evaporation
- …

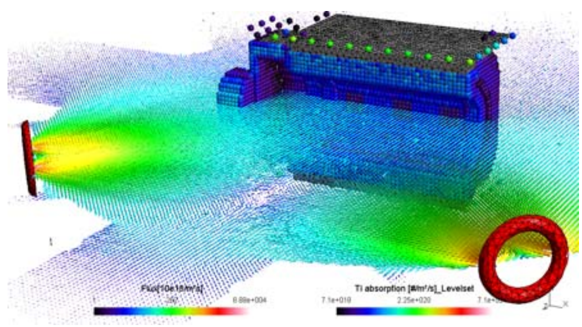


In order to get:

- Film structure
- Morphology
- Properties (roughness, hardness, optical properties, …)

Motivation: simulation of the entire plasma process + film deposition

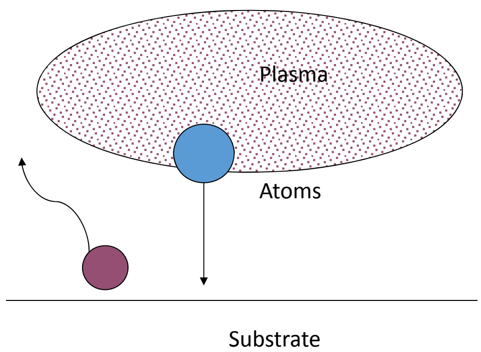


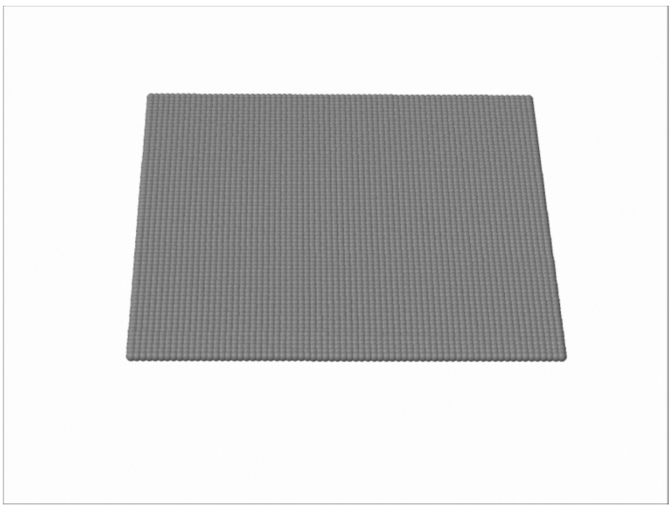


Description of the model

- Deposition of atoms, ions of different species,
- Each specie has its own energy and angular distribution,
- Deposited atoms can diffuse, forming islands, nano particles,
- Incident atoms can transfer energy and momentum to the film.
- Reaction on the surface, e.g. oxidation
- Growth of grains with different orientations -> for future

Example 1, Nucleation





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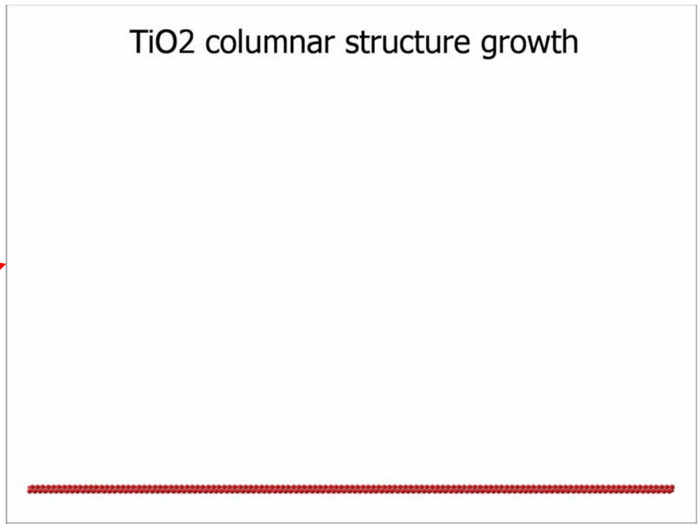
Example 2, columnar growth



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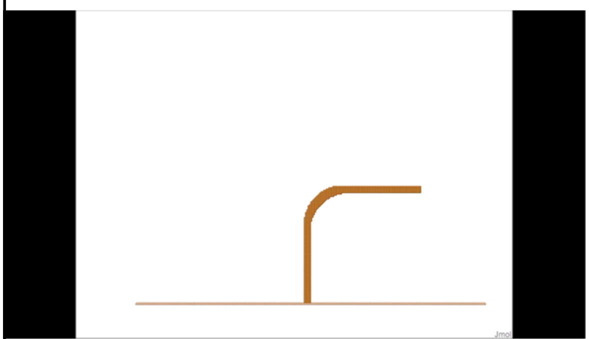
Example 3. Deposition on non flat surfaces



NASCAM V 4.7.X

- One or two metallic, one reactive (O, N, …) and one neutral species
- TiO2, SiO2, Ta2O5, … + multi layer structures
- Flat or corrugated substrate (can come from SEM pictures)
- More that 1e^{6} atoms to deposit
- Evaporation, sputtering, “CVD”, ….
- Interface with gas/plasma simulation codes
- Plugins:
  - Optical, Porosity, Roughness, …..

Nucleation studies

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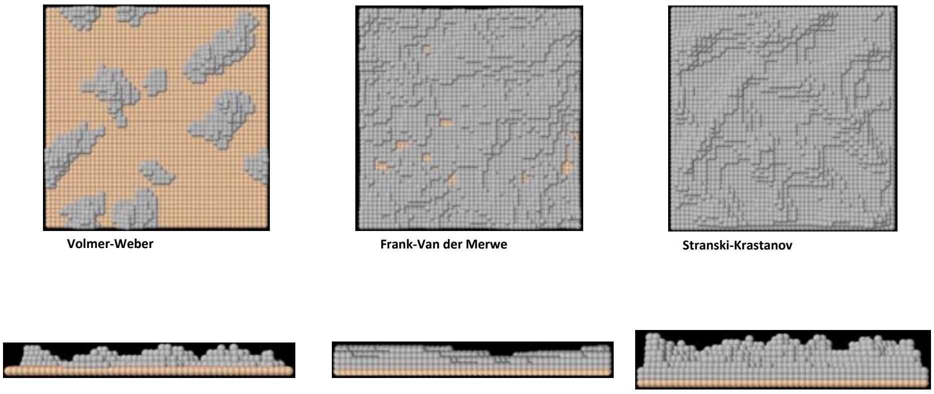
Metal deposition: playing with Ea_up & down

Metal deposition on insulators



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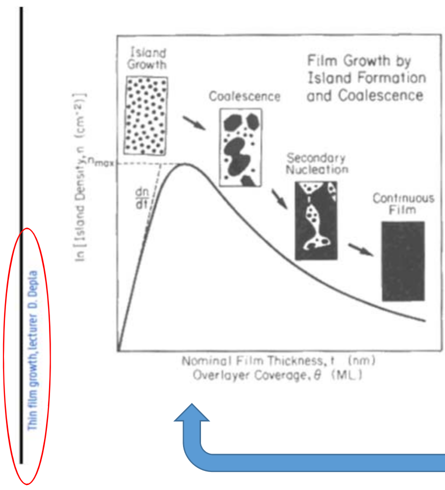
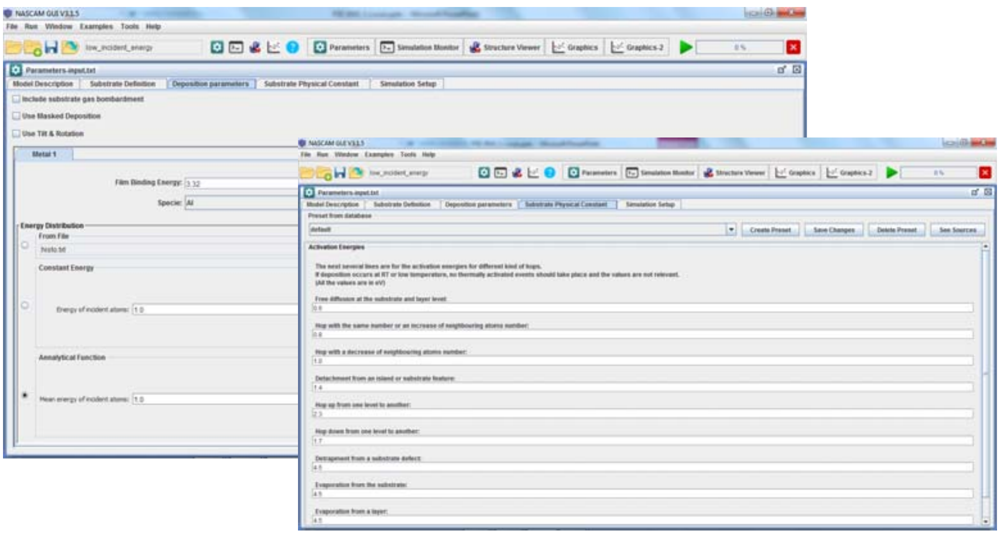
Nucleation



Can we tune this experimentally ?

Case 1: effect of deposition rate

Low energy (1 eV on average)



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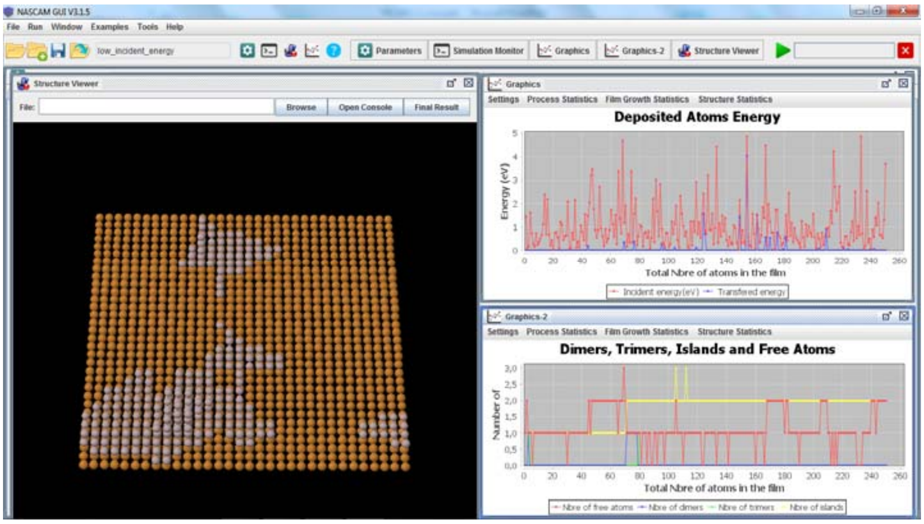
Low energy (1 eV on average)



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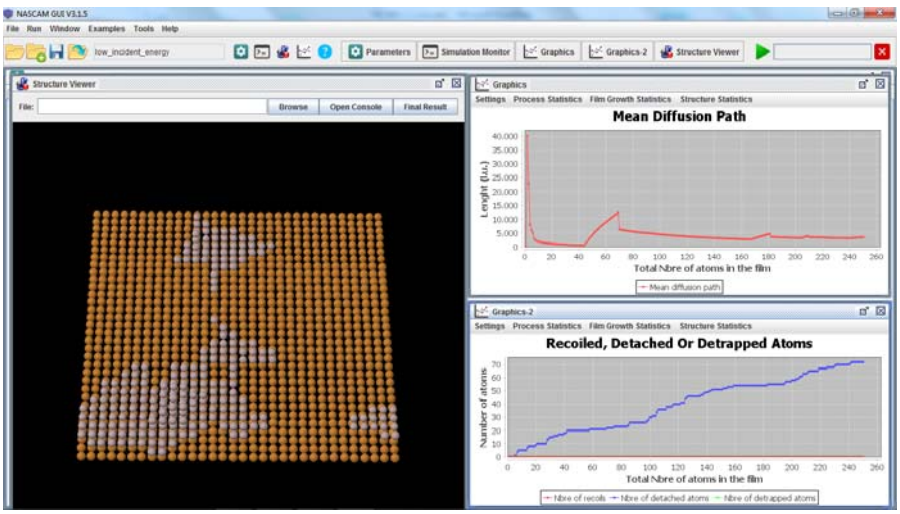
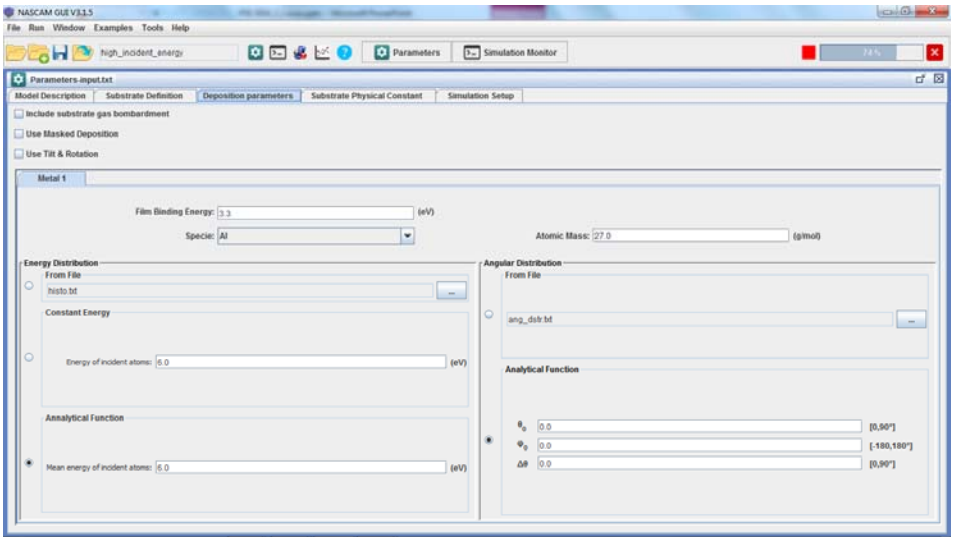
Low energy (1 eV on average)



High energy (6 eV on average)



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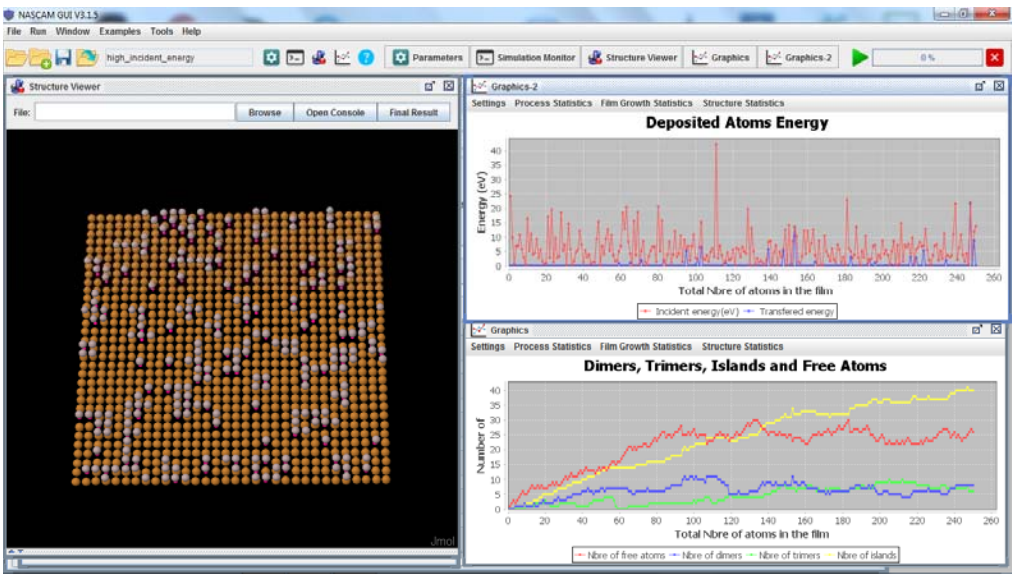
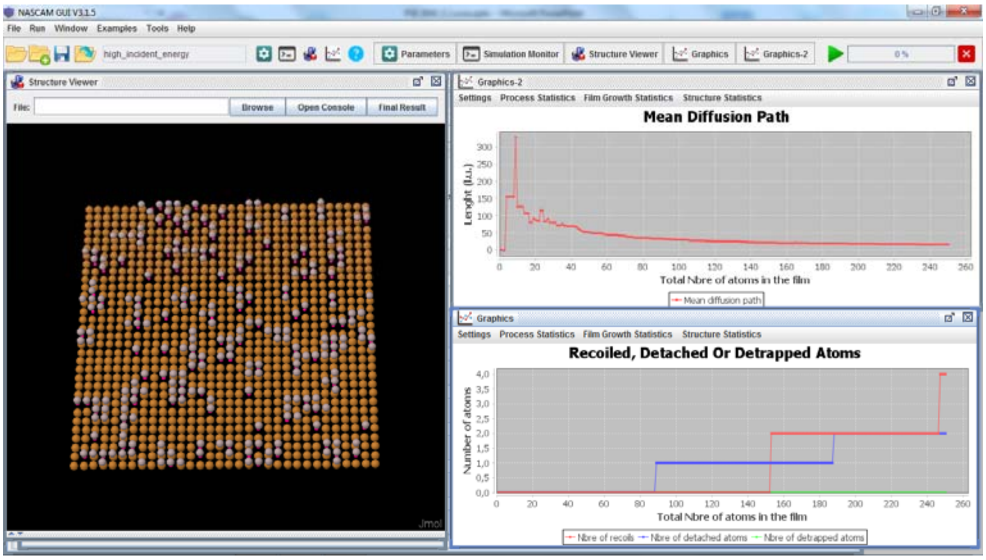
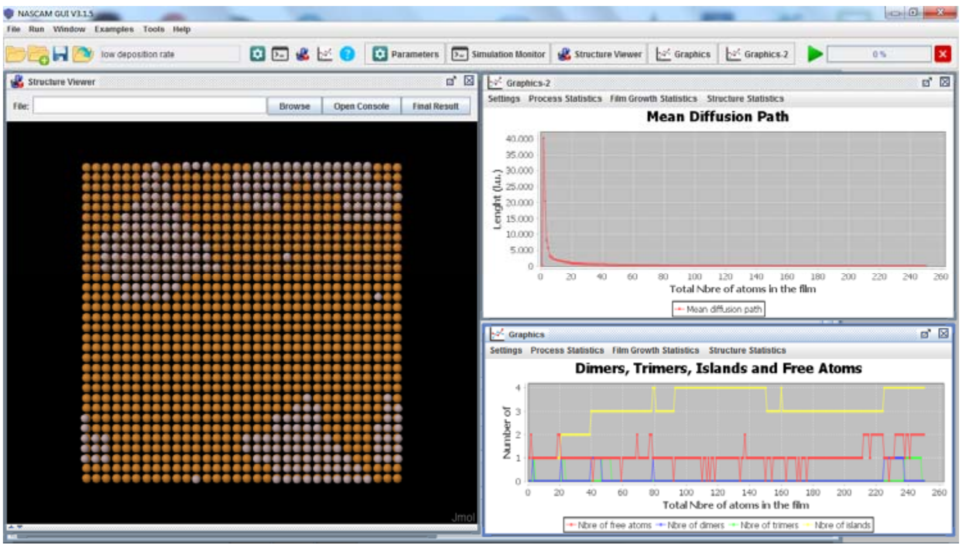
High energy (6 eV on average)



High energy (6 eV on average)



Low deposition rate (0.002 ML/s)



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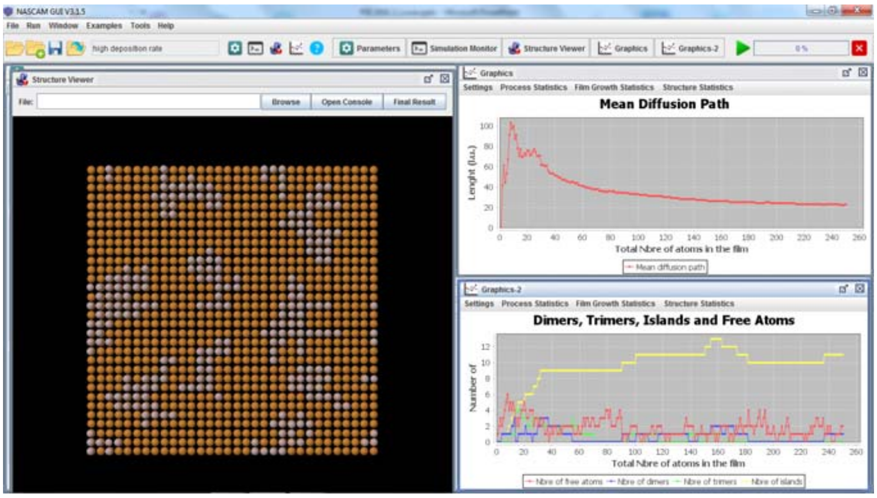
High deposition rate (2 ML/s)



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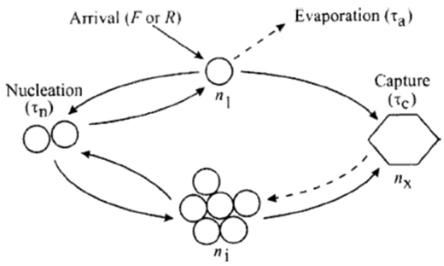
Nucleation is a complex process of capturing of adatoms by clusters(islands) and of exchange of atoms between clusters

Important assumption! There exist a critical cluster size ***i****: all clusters with a smaller size are unstable and quickly dissolve after formation; all clusters with a large sizes are stable.



$A_1 + A_1 \leftrightarrow A_2$
$A_2 + A_1 \leftrightarrow A_3$
$A_3 + A_1 \leftrightarrow A_4$
…
$A_{n-1} + A_1 \leftrightarrow A_n$

Walton equation : $\Omega n_{i^*} \sim (\Omega n_1)^{i^*} \exp\left(-\frac{E_{i^*}}{kT}\right)$, Ω is a lattice site area, n_{i^*} and n_1 are number of critical clusters and adatoms, ***i**** is a size of a critical cluster, E is a formation energy of a cluster

n1, n_i*, N: surface density of adatoms, critical islands, and stable islands, units - 1/m2
L - characteristic diffusion length, m,
F - deposition flux, 1/(m2*s),
D - diffusion coefficient of adatoms, m2/s,
Omega:lattice site area, units - m2.

Calculation of number of clusters. 2D case

Number of islands grows because critical islands (n_{i^*}) capture adatoms (n_1) :

$$\frac{dN}{dt} = \sigma_{i^*} D n_1 n_{i^*},$$

σ_{i^*} is a capturing capability, D is a diffusion coefficient of adatoms

Evolution of adatoms is governed by the same equation – income due to the deposition, lost because of capturing by critical islands and other islands:

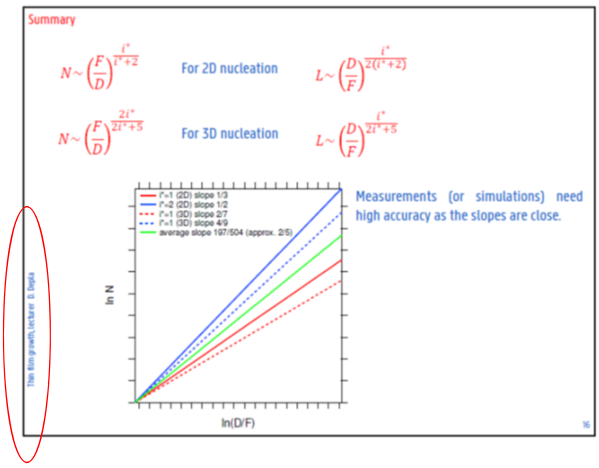
$$\frac{dn_1}{dt} = F - \sigma_{i^*} D n_1 n_{i^*} - \bar{\sigma} D n_1 N;$$ in steady state regime $F = \bar{\sigma} D n_1 N$

These three equations + Walton equation $\Omega n_{i^*} \sim (\Omega n_1)^{i^*} \exp\left(-\frac{E_{i^*}}{kT}\right)$ give us number of islands:

$N \sim \left(\frac{F}{D}\right)^{\frac{i^*}{i^*+2}}$ or characteristic diffusion length $L \sim N^{-0.5} \sim \left(\frac{D}{F}\right)^{\frac{i^*}{2(i^*+2)}}$

Characteristic diffusion length is defined as the typical length adatoms can diffuse before they are capture by existing islands or form a new nucleus

Calculation of the nucleation density based on the kinetic modelling



2D nucleation, simulation by NASCAM

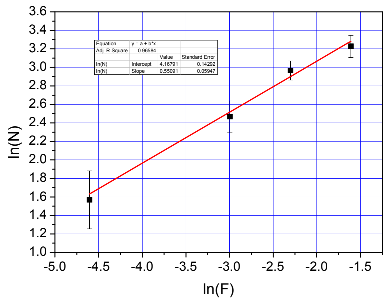
Substrate 200x200, 4000 atoms;
Deposition rates: from 0.01 to 0.2 ML/s
$E_{diffusion}$ = 0.45 eV, T = 0.03 eV = 100 C
No detachment

F = 0.01ML/s
<N> = 4.8 islands

F = 0.05ML/s
<N> = 11.8 islands

F = 0.1ML/s
<N> = 19.4 islands

F = 0.2ML/s
<N> = 25.2 islands



5 simulations for each case;
Slope = 0.55
Critical size = 2.4 atoms

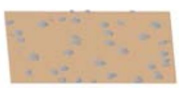
3D nucleation, simulation by NASCAM

Substrate 200x200, 4000 atoms;
Deposition rates: from 0.01 to 0.2 ML/s
$E_{diffusion}$ = 0.45 eV, T = 0.03 eV = 100 C
No detachment

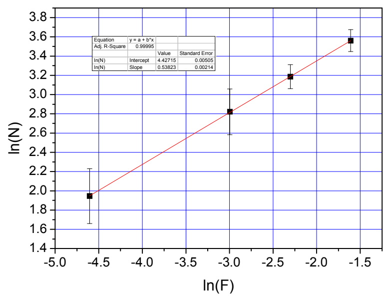
F = 0.01ML/s
<N> = 7.0 islands

F = 0.05ML/s
<N> = 16.8 islands

F = 0.1ML/s
<N> = 24.2 islands



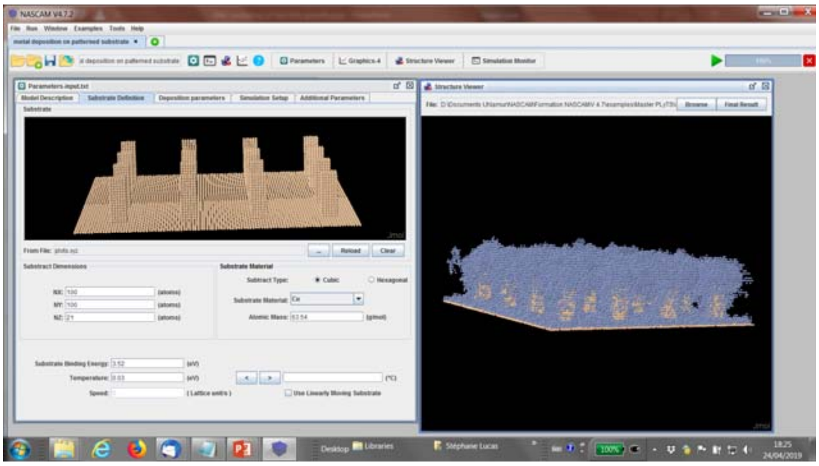
F = 0.2ML/s
<N> = 35.2 islands



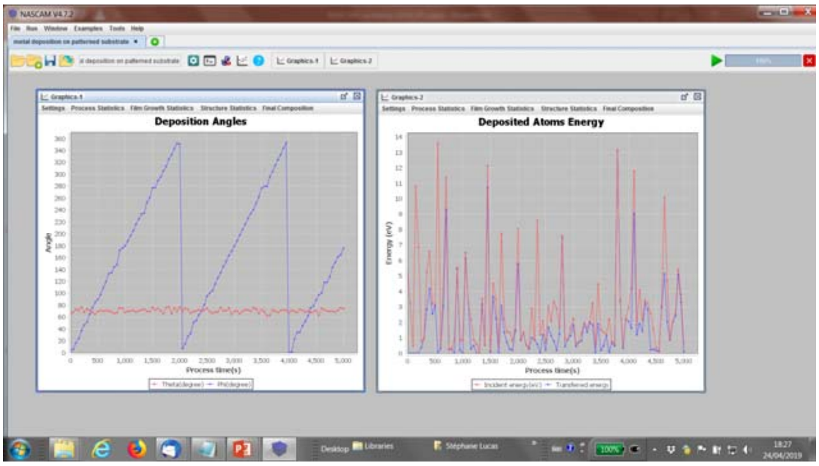
5 simulations for each case;
Slope = 0.54
Critical size = 2.9 atoms

Case 2: Substrate defect creation and deposition on a patterned substrate

Deposition on a patterned substrate



Deposition on a patterned substrate



Film growth studies

- Grain growth
- Shadowing
- GLAD: metal and oxide

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Grain, growth: structure Zone Model - SZM

B. A. Movchan, A. V. Demchishin; J. A. Thornton; P. A. Barna; A. Anders; I. Petrov; …

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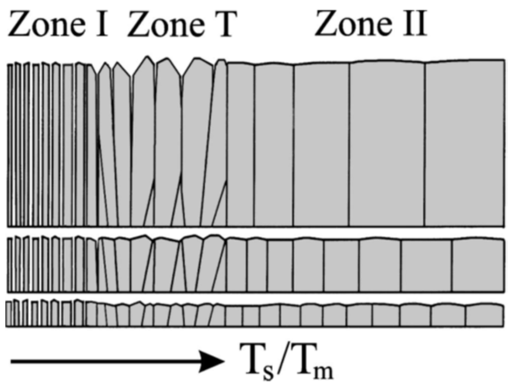
Zone descriptions

(zone numbering changes from author to author)

- Zone I – no atom mobility. Columnar structure, a lot of pores, Ts/Tm<0.2
- Zone T – surface diffusion, no grain boundary mobility. Dense columnar structure, V-shape due to competitive growth , 0.2<Ts/Tm<0.4
- Zone II - surface diffusion, grain boundary mobility. Recrystallization , Ts/Tm>0.4
- Zone III (see the next slide) – impurities at the interfaces



Film growth - stages

- Nucleation: randomly located randomly oriented grains appear
- Growth of individual grains
- Grains touch each other

  Zone I: continuous vertical growth of the grains

  Zone T: competitive growth, grains with orientation providing the fastest vertical growth rate overgrowth others

  Zone II: grain growth by (i) coalescence – recrystallization due to energy minimization; (ii) due to the mobility of the grain boundaries
- Zone III: defects and impurities prevent the mobility of grain boundaries

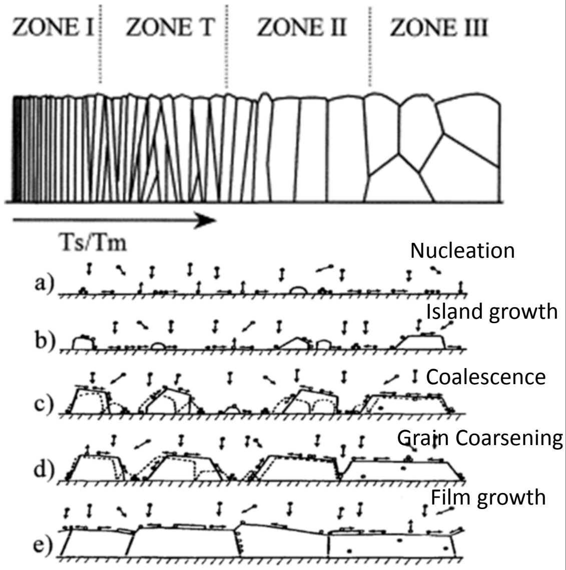


Fig. 1. Growth stages of polycrystalline film formation. *a*: nucleation; *b*: crystal growth; *c*: coalescence; *d*: growth by filling of the channels; *e*: thickness growth of the continuous film. Dark circles mark adatoms; light circles impurity species; crystals before coalescence are marked by dashed line.

From "Growth mechanisms of polycrystalline thin films" by P.Barna and M.Adamik

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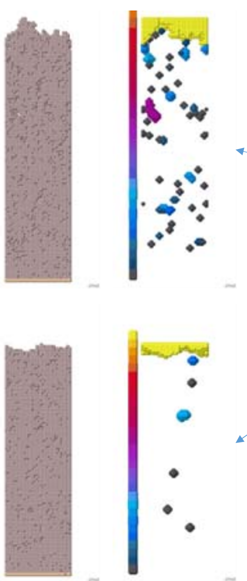
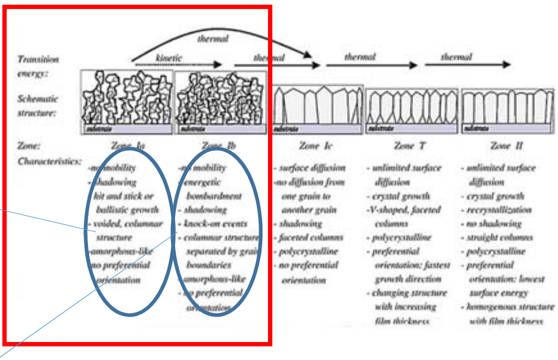
Zone I – low T, no thermal activated mobility

Low energy deposition

High energy deposition



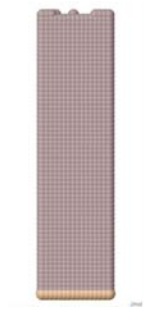


From "Biaxial alignment in sputter deposited thin films" by S. Mahieu, P. Ghekiere, D. Depla, R. De Gryse

S. Lucas, UNamur-Belgium: Plathinium, Antibes, 9/2019

Zone T (transition) – thermally activated surface diffusion

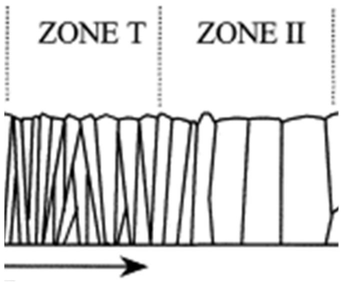
- Grains/crystallites with different orientation grow with different vertical rate because:
- Faces with the higher surface diffusion rate grow slower, as the adatoms migrate from these faces to the faces with lower mobility
- Competitive growth : when different crystallites touch each other during the growth, only crystallites with the highest vertical growth rate survive → V-shapes
- Diameter of the columns is more or less equal to the initial diameter because of no coalescence → narrow columns



Same as above, but at high temperature → no pores (one crystallite)

Zone II – thermally activated bulk diffusion

- Coalescence of the crystallites:
  - To minimize total energy
  - Because of the grain boundary mobility
- Wide columns because of the coalescence



A final structure of the film depends on

- Substrate temperature → thermally activated atom mobility ~exp(-U/kT)
- Energy of deposited particles (depends on material, pressure, voltage etc) → kinetically activated atom mobility, depends on deposited energy per atom (EPA)
- Impurities,
- …

All these factors influence the surface mobility of deposited atoms, grain mobility, bulk mobility

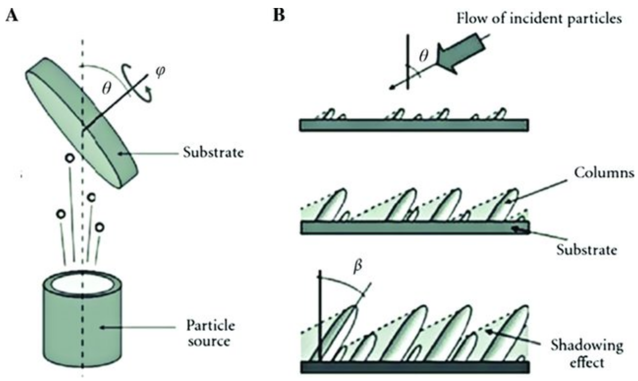
Case 3: GLAD with TiO2

IOP Publishing Journal of Physics D: Applied Physics
J. Phys. D: Appl. Phys. 51 (2018) 195202 (17pp) https://doi.org/10.1088/1361-6463/aabb72

TiO_x deposited by magnetron sputtering: a joint modelling and experimental study

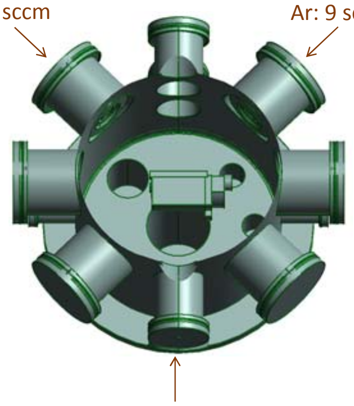
R Tonneau[1], P Moskovkin[1], A Pflug[2] and S Lucas[1]

Glancing Angle Deposition (GLAD)



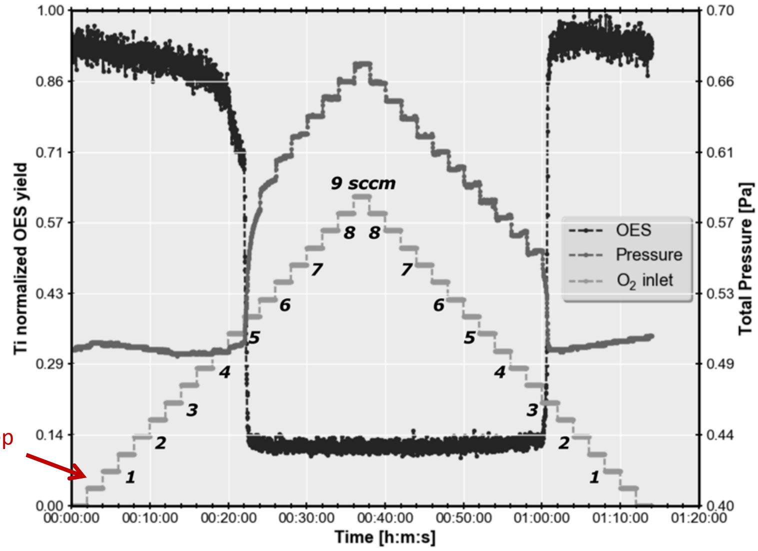
RSD: a well known story…

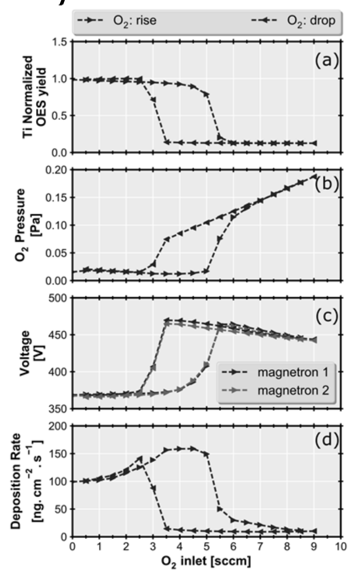
➔ **Let's buy a vacuum chamber with 2 magnetrons and 2 Ti Targets**



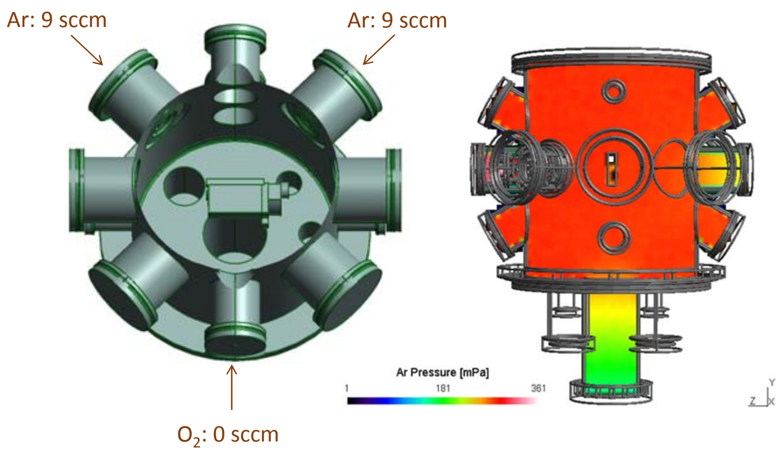
View of Mantis Coater (University of Namur)

RSD: a well known story…





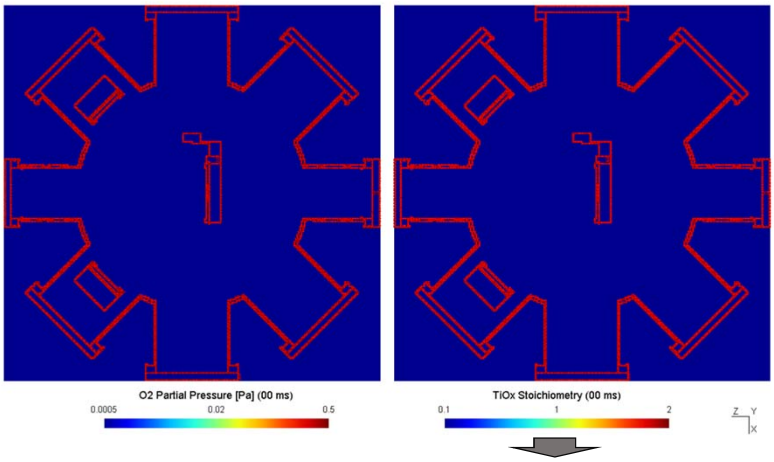
Model definition



Perfect agreement (error less than 5 % on total pressure)

Time evolution of O_2 partial pressure & surface coverage

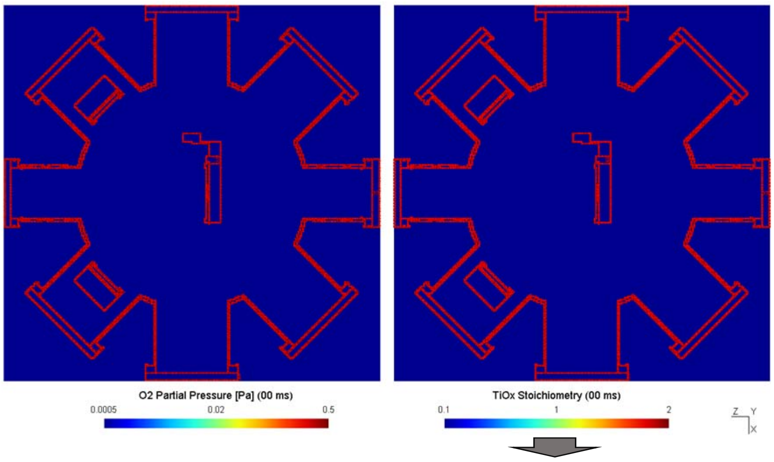
O_2 inlet : *2 sccm* *8 sccm*



Values on walls only

Time evolution of O_2 partial pressure & surface coverage

O_2 inlet : *2 sccm* *8 sccm*



Values on walls only

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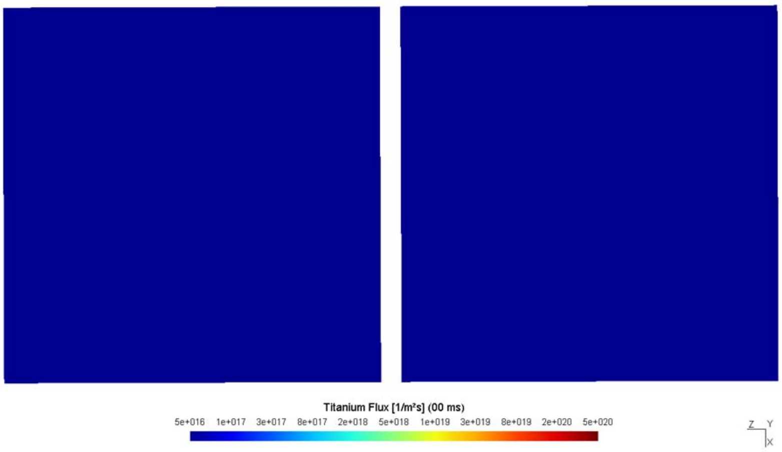
Time evolution of Titanium flux

O_2 inlet : *2 sccm* *8 sccm*



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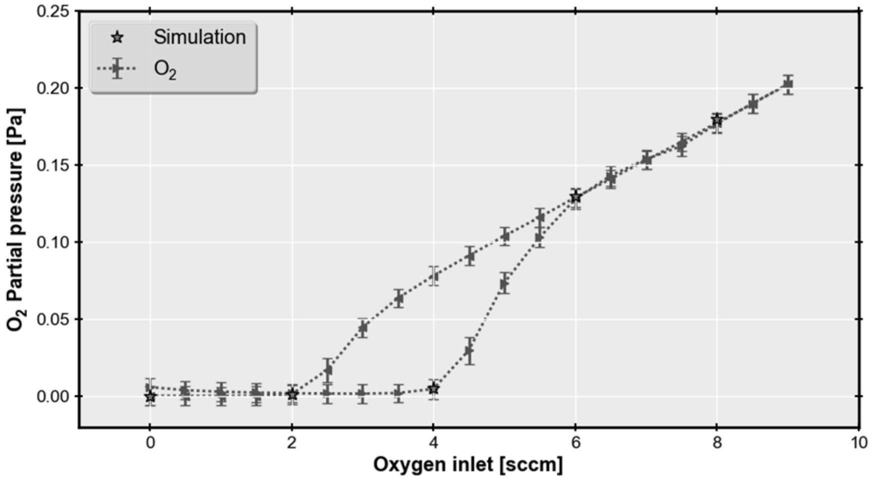
Comparison with experiment



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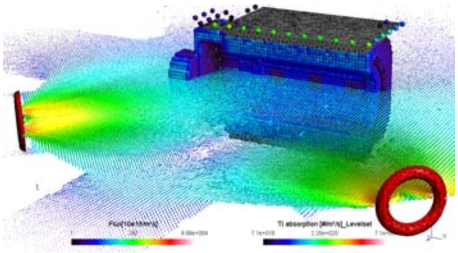
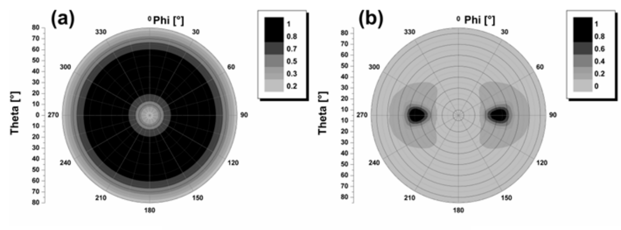
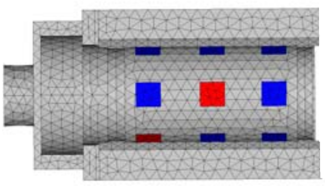
Focus on substrate

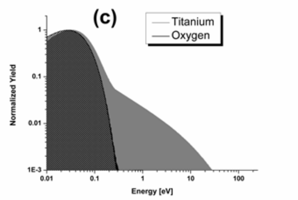
➔ **Angular and energy distributions**



Oxygen ***Titanium***







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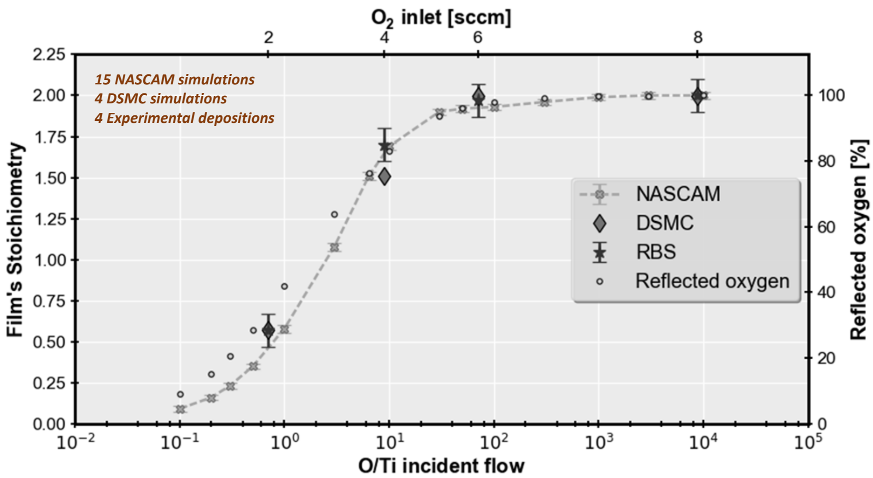
Focus on substrate

➔ **Let's vary flux ratio O/Ti**



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O/Ti order of magnitude in RSD

$$\Gamma = \frac{n\,v}{4}$$

$v = average\ velocity$
$\Gamma = particle\ flux$
$n = particle\ density$

$$\Gamma_{reactive} = \frac{p_{O_2}}{(2\pi mkT)^{1/2}}\ [part.\ s^{-1}\ m^{-2}]$$

$$\Gamma_{metal} = S.t.D_R.\rho_{TiO_2}.M_{TiO_2}{}^{-1}.N_A.(\frac{1}{3})$$

N_A: avogadro number
S: substrate surface
t: deposition time
D_R: depostion rate
M_{TiO_2}: molar mass of titania

$D_R = 0.1$ Å s^{-1}

$\rho_{TiO_2} = 4.23\ g\ cm^{-3}$

$M_{TiO_2} = 79.86\ g\ mol^{-1}$

$p_{O_2} = 0.18\ Pa$

$T = 300\ K$

$\Gamma_{reactive} = 4.843\ 10^{17}$ part. $s^{-1}\ cm^{-2}$

$\Gamma_{metal} = 1.062\ 10^{13}$ part. $s^{-1}\ cm^{-2}$

$$\frac{\Gamma_{reactive}}{\Gamma_{metal}} \cong 10^4$$

At least 2 orders of magnitude difference !

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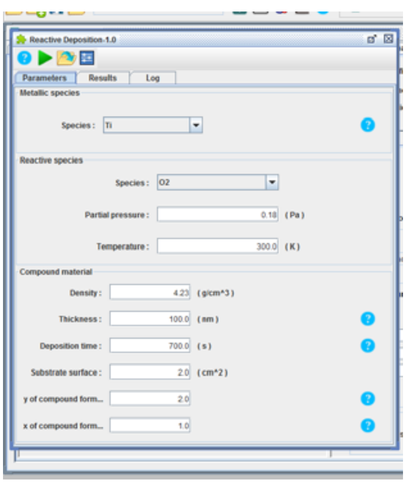
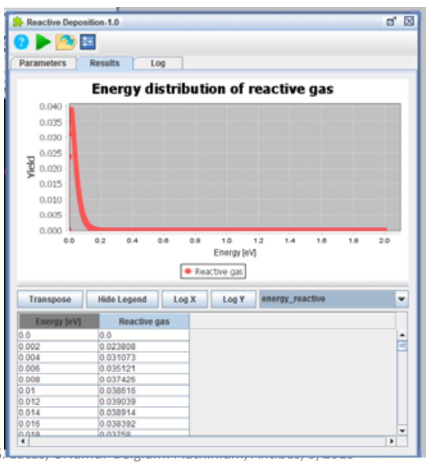
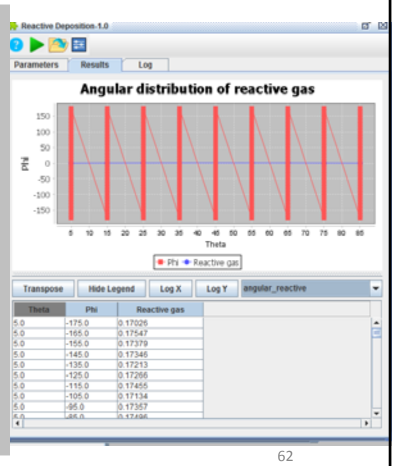
O2 Angular and energy distribution



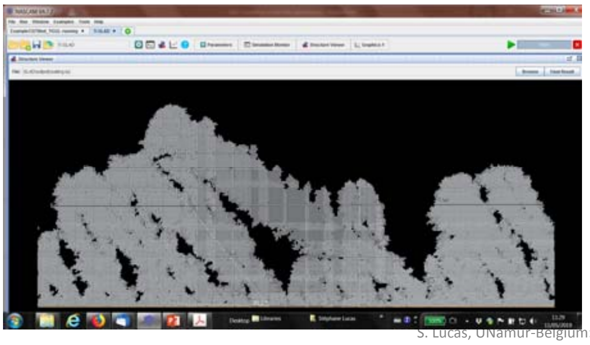


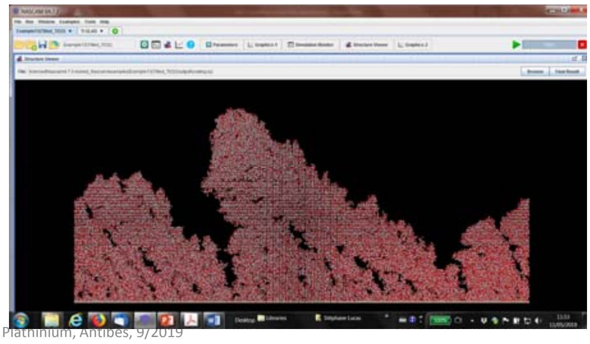


Let’s now simulate film growth

Ti by GLAD versus TiO2 by GLAD

70 °





KMC morphology’s results versus experimental data

J. Phys. D: Appl. Phys. 51 (2018) 195202 R Tonneau et al

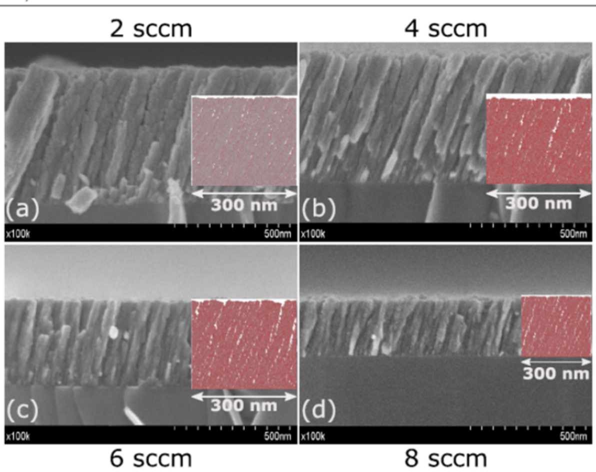
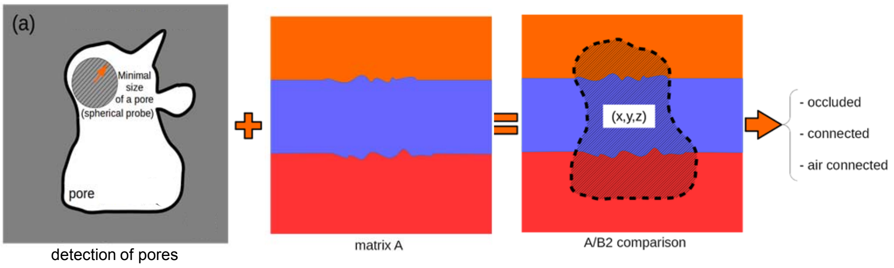
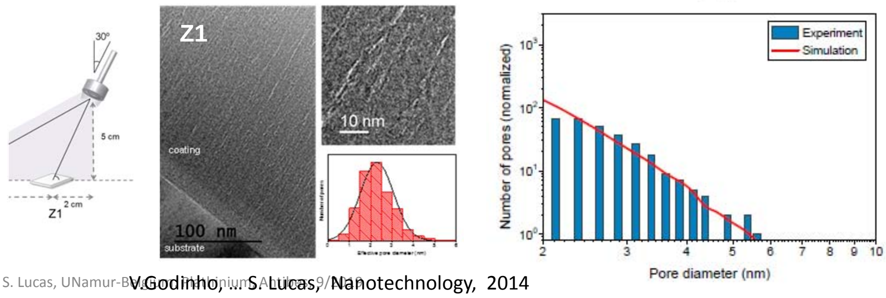


Figure 14. Comparison of the film’s structure between SEM analyses and NASCAM simulations for the corner sample located along the hysteresis curve.

Porosity analysis (J. Müller (and help from CSIC-Sevilla)





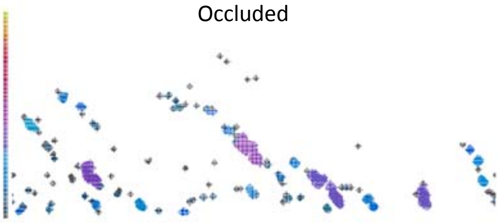
S. Lucas, UNamur-B… V.Godinho, … S. Lucas, Nanotechnology, 2014

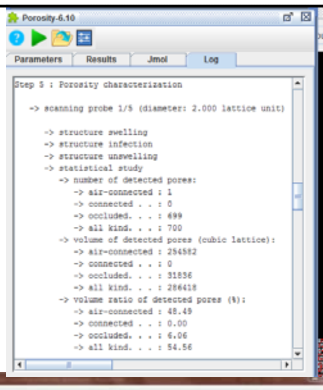
Porosity evaluation

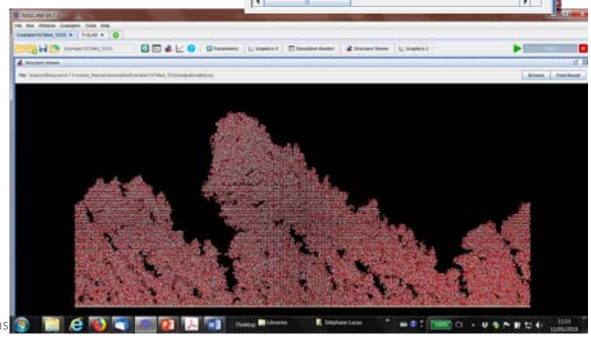
TiO2, size 4

Air connected

Occluded





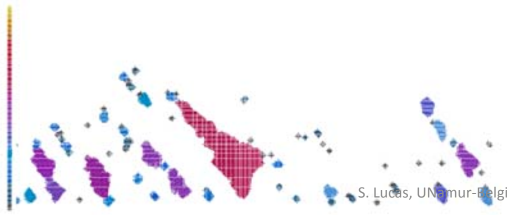


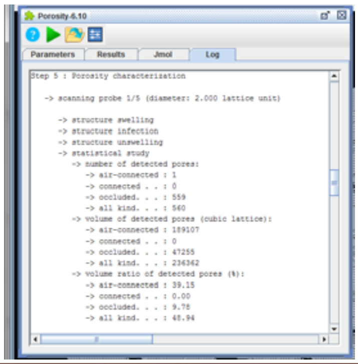
Porosity evaluation

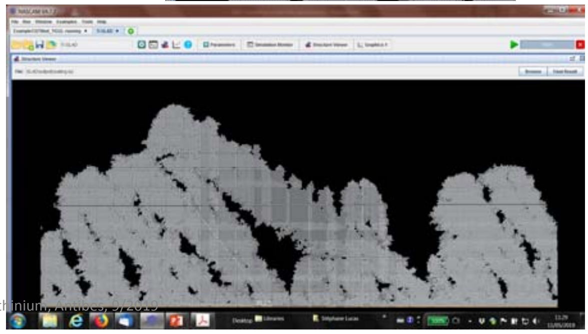
Ti, size 4

Air connected

Occluded







Case 4 (from literature): Heat reflector

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Heat reflector

SCIENTIFIC REPORTS

OPEN

Color tunable low cost transparent heat reflector using copper and titanium oxide for energy saving application

Received: 19 June 2015
Accepted: 23 December 2015
Published: 05 February 2016

Goutam Kumar Dalapati*, Saeid Masudy-Panah*, Sing Teng Chua, Mohit Sharma, Ten It Wong, Hui Ru Tan & Dongzhi Chi

Multilayer coating structure comprising a copper (Cu) layer sandwiched between titanium dioxide (TiO_2) were demonstrated as a transparent heat reflecting (THR) coating on glass for energy-saving window application. The main highlight is the utilization of Cu, a low-cost material, in-lieu of silver which is widely used in current commercial heat reflecting coating on glass. Color tunable transparent heat reflecting coating was realized through the design of multilayer structure and process optimization. The impact of thermal treatment on the overall performance of sputter deposited TiO_2/Cu/TiO_2 multilayer thin film on glass substrate is investigated in detail. Significant enhancement of transmittance in the

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Heat reflector

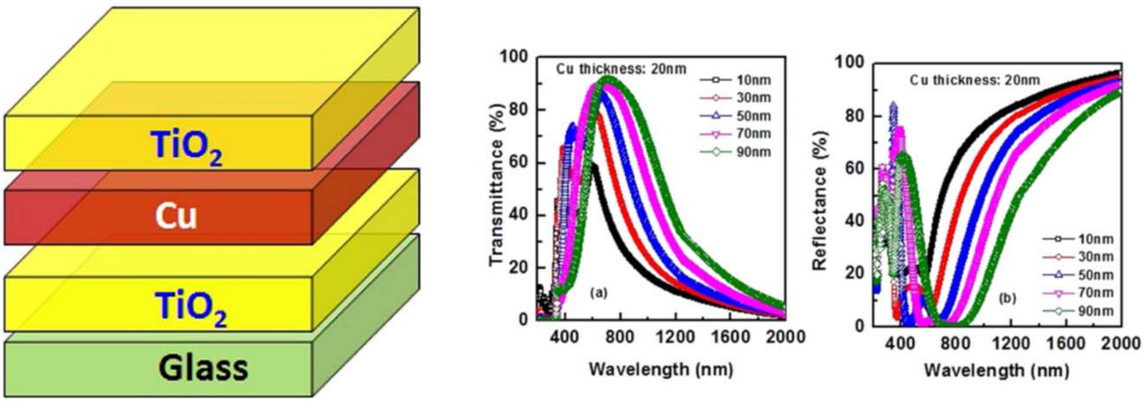
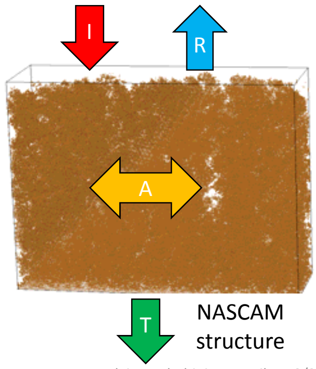


Figure 1. Schematic diagram of transparent heat reflector (THR) using symmetrical dielectric (TiO_2) and identical thickness over and below Cu layer.

Plugin: Optics algorithm within NASCAM (J. Müller)

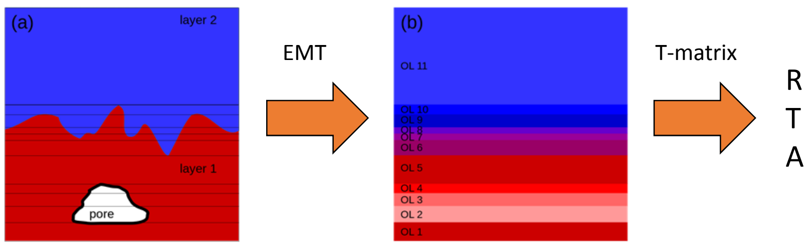
- **Goal**: optical characterization of a nano-structured stack provided by NASCAM.
- **Method**: computation of the absorptance, the reflectance and the transmittance by using the effective medium theory and the T-Matrix method



Plugin: Optics algorithm

Principle of effective medium theory

- conversion of 3D porous structure to 1D uniform optical layers
- the optical layer thickness is based on the volume fraction for each material of the structure.
- computation of an effective optical index for each optical layer and each wavelength (5 effective medium models available)
- calculation of the reflectance, transmittance and absorptance by T-matrix



3D structure

1D simplified stack of optical layers

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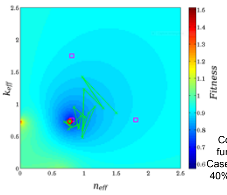
Effective medium theory

Five optical models (for a n-material optical layer) are available:

- the **Maxwell-Garnett method**: $\frac{\epsilon_{eff}-\epsilon_h}{\epsilon_{eff}+\gamma\epsilon_h}=\sum_{i=1}^{n-1} f_i \frac{\epsilon_i-\epsilon_h}{\epsilon_i+\gamma\epsilon_h}$
- the **Lorentz-Lorentz method**: $\frac{\epsilon_{eff}-1}{\epsilon_{eff}+2}=\sum_{i=1}^{n} f_i \frac{\epsilon_i-1}{\epsilon_i+2}$
- the **Volume Average method**: $\epsilon_{eff}=\sum_{i=1}^{n} f_i\epsilon_i$
- the **Bruggeman method**: $\sum_{i=1}^{n} f_i \frac{\epsilon_i-\epsilon_{eff}}{\epsilon_i+2\epsilon_{eff}}=0$

NB: The optimization method used to solve the Bruggemann equation is the bounded Nelder–Mead method (or downhill simplex method)



$\epsilon_{eff}=(n_{eff}+j\cdot k_{eff})^2$

$Fitness=\sum_{i=1}^{3} f_i \frac{\epsilon_i-\epsilon_{eff}}{\epsilon_i+2\epsilon_{eff}}$

Convergence of Bruggeman solution in function of optical indexes (n_{eff} and k_{eff}). Case of a 3 materials domain (air: 20%, Mo: 40%, Si: 40% at the wavelength λ=100nm)

- **hybrid method:** based on the Maxwell-Garnett and the Bruggeman models. The choice of the model is function of the volume ratio of each material in an optical layer

the effective index has to be computed for each optical layer and each wavelength!

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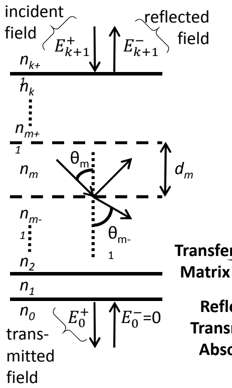
T-Matrix method

- calculation of the reflectance, transmittance and absorptance by T-matrix:



Fresnel coef.

$r^p_m=\frac{n_m\cos\theta_{m-1}-n_{m-1}\cos\theta_m}{n_m\cos\theta_{m-1}+n_{m-1}\cos\theta_m}$ $\quad r^s_m=\frac{n_m\cos\theta_m-n_{m-1}\cos\theta_{m-1}}{n_m\cos\theta_m+n_{m-1}\cos\theta_{m-1}}$

$t^p_m=\frac{2nm\cos\theta_m}{n_m\cos\theta_{m-1}+n_{m-1}\cos\theta_m}$ $\quad t^s_m=\frac{2nm\cos\theta_m}{n_m\cos\theta_m+n_{m-1}\cos\theta_{m-1}}$

complex Snell's law

$n_m\sin\theta_m=n_{m-1}\sin\theta_{m-1} \quad \rightarrow \quad \theta_{m-1}=\ \mathrm{real}\left[\sin^{-1}\left(\frac{n_m}{n_{m-1}}\sin\theta_m\right)\right] -\mathrm{i.\,abs}\left\{\mathrm{im}\left[\sin^{-1}\left(\frac{n_m}{n_{m-1}}\sin\theta_m\right)\right]\right\}$

phase shift factors

$\delta_m=\frac{2\pi}{\lambda}n_m d_m\cos\theta_m$

Transfer Matrix

$M_{m-1}=\frac{1}{t_m}\begin{bmatrix}\exp(\mathrm{i}\delta_{m-1}) & r_m\exp(-\mathrm{i}\delta_{m-1})\\ r_m\exp(\mathrm{i}\delta_{m-1}) & \exp(-\mathrm{i}\delta_{m-1})\end{bmatrix} \quad \rightarrow \quad \begin{bmatrix}E^+_{k+1}\\ E^-_{k+1}\end{bmatrix}=MkM_{k-1}\dots M_2M_1\begin{bmatrix}E^+_0\\ E^-_0\end{bmatrix}$

Reflectance Transmittance Absorbance

$R=\frac{|E^-_{k+1}|^2}{|E^+_{k+1}|^2} \quad T=\frac{n_0\cos\theta_0}{n_{k+1}\cos\theta_{k+1}}\frac{|E^+_0|^2}{|E^+_{k+1}|^2} \quad A=1-R-T$

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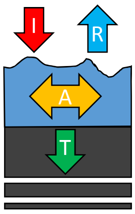
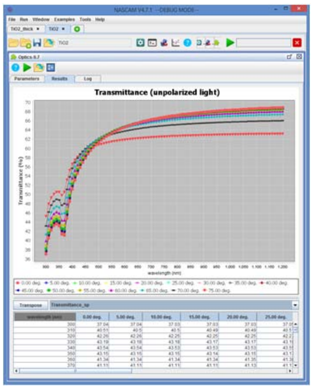
Plugin: Optics algorithm

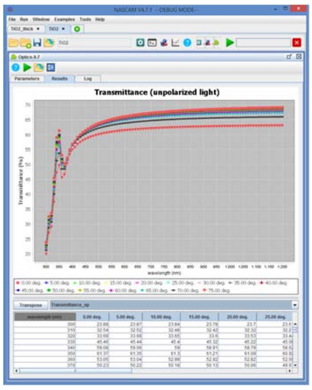
- TiO_2 deposition on c-Si substrate
  - TiO_2 thickness: 0nm, 13.5nm, 48nm
  - transmittance/reflectance calculation



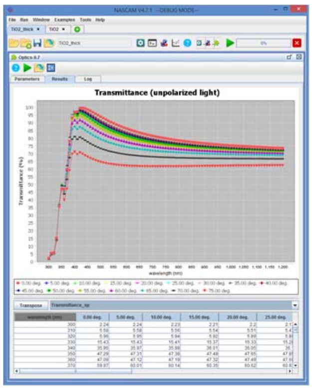
transmittance of TiO2 layer on c-Si substrate



no TiO2



TiO2: 13.5nm



TiO2: 48nm

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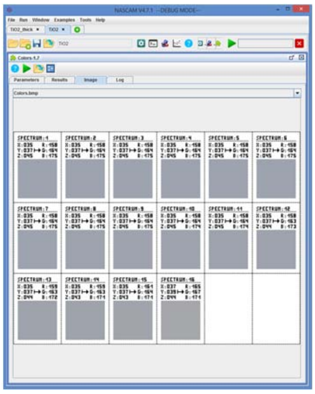
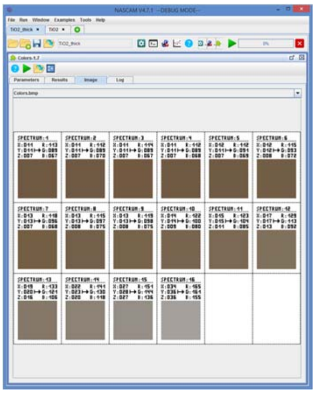
Plugin: Colors algorithm (J. Müller)

Colors simulation

- application to the light reflected by the sample c-Si/TiO_2



RGB color (no TiO2)



RGB color (TiO2: 48nm)

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WP2

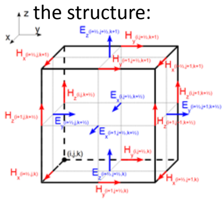
Optics 2.0 → FDTD

- Maxwell equations discretized by finite difference:

$$\nabla\times\mathbf{E}=-\frac{\partial\mathbf{B}}{\partial t}\qquad \nabla\times\mathbf{H}=\mathbf{J}+\frac{\partial\mathbf{D}}{\partial t}$$
$$\nabla\cdot\mathbf{D}=\rho\qquad \nabla\cdot\mathbf{B}=0$$
$$\mathbf{D}=\epsilon\mathbf{E}\qquad \mathbf{B}=\mu\mathbf{H}$$

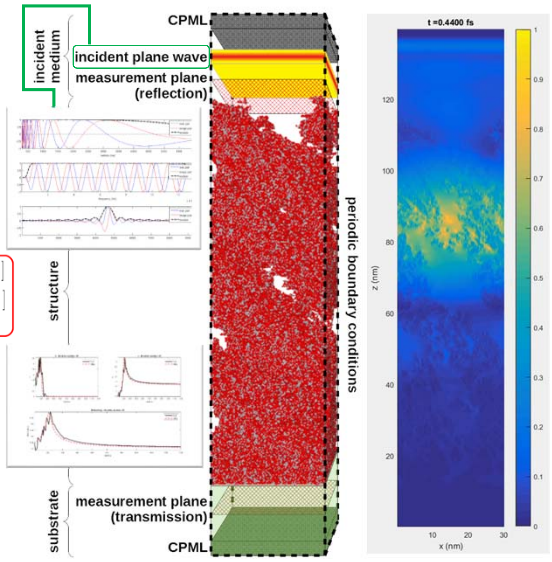
$$\epsilon_{i,j+\frac{1}{2},k+\frac{1}{2}}\left[E_x\Big|^{n+1}_{i,j+\frac{1}{2},k+\frac{1}{2}}-E_x\Big|^{n}_{i,j+\frac{1}{2},k+\frac{1}{2}}\right]=\frac{\Delta t}{\Delta y}\left[H_z\Big|_{i,j+1,k+\frac{1}{2}}-H_z\Big|_{i,j,k+\frac{1}{2}}\right]+\frac{\Delta t}{\Delta z}\left[H_y\Big|_{i,j+\frac{1}{2},k}-H_y\Big|_{i,j+\frac{1}{2},k+1}\right]-\Delta t J_x\Big|_{i,j+\frac{1}{2},k+\frac{1}{2}}$$

- Yee cell used to discretize the structure:



Incident light spectrum in the frequency and time domains

TiO2 optical index fitted by 2 modified Lorentz



cost: 10GB and 7 hours! BUT it's possible to reduce that! With a space step 2 times bigger → 1.25GB and 25 min.

S. Lucas, UNamur-Belgium: Plathinium, Antibes, 9/2019

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Some info for this case

50 nm TiO2:

- $D_{average}$ = 2.5 A = 0.25 nm.
- -> 50 nm = 200 layers roughly.
- 200 x 20x20 = 80.000 atoms to be deposited if fully stacked.
- If 80 % density, roughly 65000 atoms to be deposited

Cu:

- Interplanar spacing of {110} planes: $D_{average}$ = 2.55 A

(b) $d_{hkl} = \frac{a}{\sqrt{h^2+k^2+l^2}}$

$$d_{110} = \frac{3.61\times10^{-10}}{\sqrt{2}} = 2.55\times10^{-1}$$

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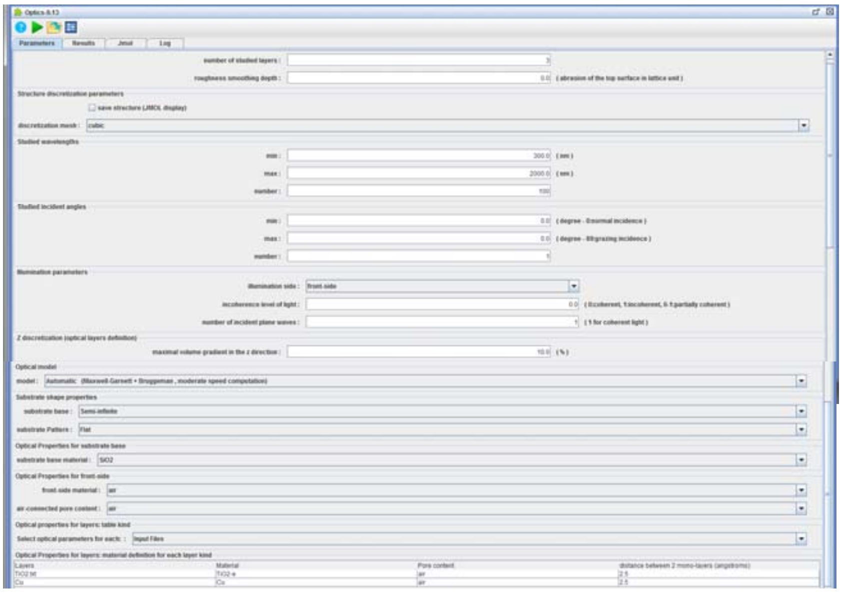

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Heat reflector as simulated with by KMC (NASCAM)

SCIENTIFIC REPORTS

OPEN **Color tunable low cost transparent heat reflector using copper and titanium oxide for energy saving application**

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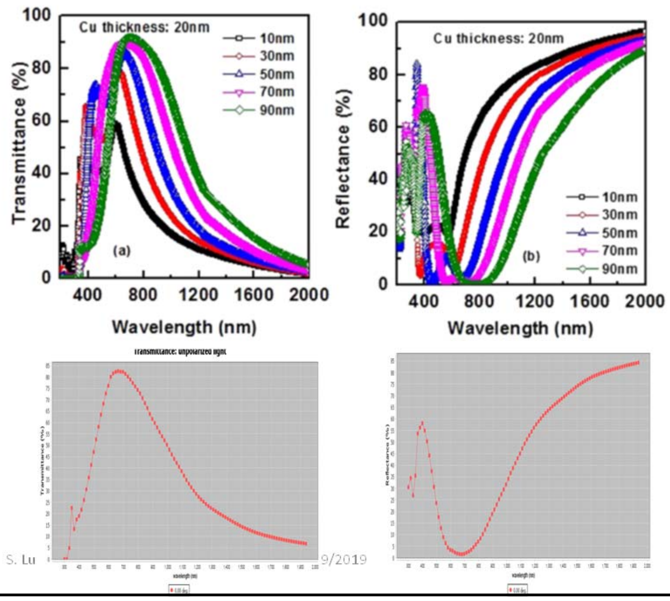

50 nm Cu

End for 2019