Plasma-Material Interaction Research for Space Propulsion and Fusion Energy

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And
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Presentation Outline

UCLA Engineering Research Interests

- Ann Karagozian (MAE): Simulations of Non-equilibrium reactive and plasma flows for EP &laser-plasma interactions (LPI).
- Richard Wirz (MAE): Space Electric Propulsion, PMI, edge plasma flows.
- Dan Goebel (MAE): PMI, Pulsed power, Space Electric propulsion.
- Jaime Marian (MSE): Atomistic computer simulations, sputtering & defect physics.
- Nasr Ghoniem (MAE): PMI, Space Electric Propulsion, Pulsed Power, Defect Physics.

1. Karagozian Research on Reactive Gases & Plasmas.
2. Wirz/ Goebel Research on Electric Propulsion.
3. Experimental Facilities.
4. Commonality between PMI for fusion & EP applications.
5. Thermomechanics in Severe Pulsed Plasma Environment.
6. Surface Stability.

Modeling of Nonequilibrium Reactive Gases and Plasmas: Fluid Models and Beyond

Richard Abrantes, Hai P. Le, and Ann R. Karagozian
UCLA Department of Mechanical and Aerospace Engineering

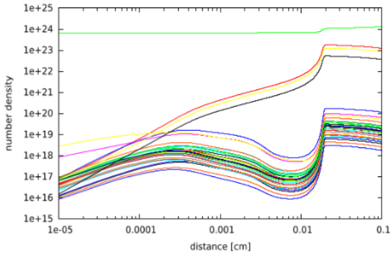
- Our computational research focuses on simulating non-equilibrium processes in reactive and plasma flows, using:
  - Collisional-Radiative (CR) kinetics
  - Single-Fluid (SF) Magnetohydrodynamics
  - Multi-Fluid (MF) Modeling
- Applications of interest include:
  - Electric propulsion for spacecraft systems
  - Plasma-Assisted Combustion Systems (PACS), including
    - Plasma ignition processes
    - Pulse Detonation Rocket Induced MHD Ejector (PDRIME)
  - Laser-Plasma Interactions (LPI), including
    - High Energy Density Physics (HEDP)
    - Laser-Induced Breakdown Spectroscopy (LIBS)

Collisional-Radiative (CR) Modeling

- Detailed state-to-state approach in determining temporal evolution of the system's average charge state, relaxation timescales, and other transient phenomena
- Rates for all processes associated with each plasma state are summed to a highly stiff system of ordinary differential equations and propagated in time to evolve the system.

Elementary processes:

- Collisional excitation:
  $A_i^{Z+} + M \leftrightarrow A_j^{Z+} + M$
- Collisional ionization:
  $A_i^{Z+} + M \leftrightarrow A_j^{(Z+1)+} + e + M$
- Bound-Bound radiation:
  $A_i^{Z+} + h\nu \leftrightarrow A_j^{Z+}$
- Photoionization:
  $A_i^{Z+} + h\nu \leftrightarrow A_j^{(Z+1)+} + e$

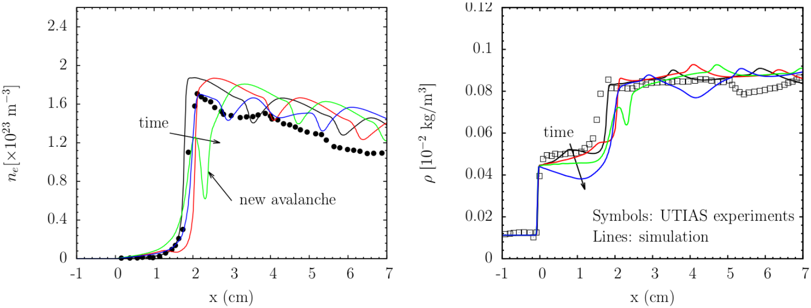


Many states: O(N)

Temporal evolution of plasma is accurate, but costs memory

Single-Fluid Modeling

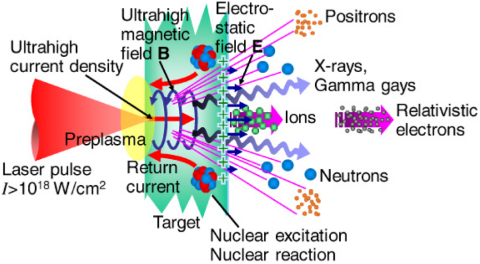
- Embeds relevant species into continuity equation for solving the Euler equations
- Coupling of the species and Euler equations helps elucidate the effect changes in the atomic scale have on large scale motions



Comparison of electron number and total mass densities for ionizing shocks in Argon with UTIAS experiments. Note the change in induction length as a function of time.

Multi-Fluid (MF) Modeling

- Extends Single-Fluid model by including another set of Euler equations for other species, such as the electron fluid
- Aim of increasing number of fluid equations is to capture events/processes that are unresolved by low order approximations, such as those observed in HEDP



Various processes associated with HEDP

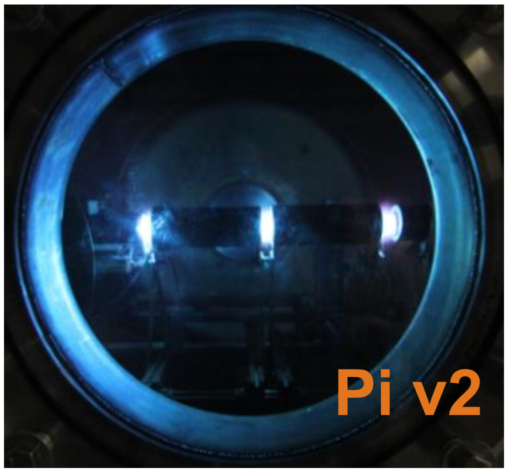
Work being explored:

- **Radiation Transport** coupling into the fluid equations
- **Grouping**[1] to reduce the size of system due to plasma states
- **Coupling** continuity of plasma states with MF solver

[1] Le et al. Physics of Plasmas, 2013

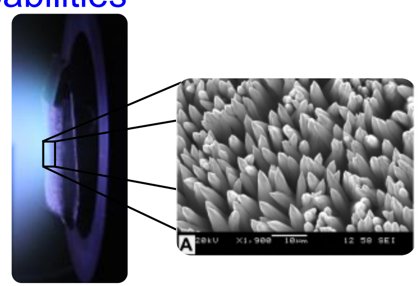
UCLA Facilities: Pi (Erosion) and HEFTY (Thermo-mechanics) : Wirz/Goebel/Ghoniem

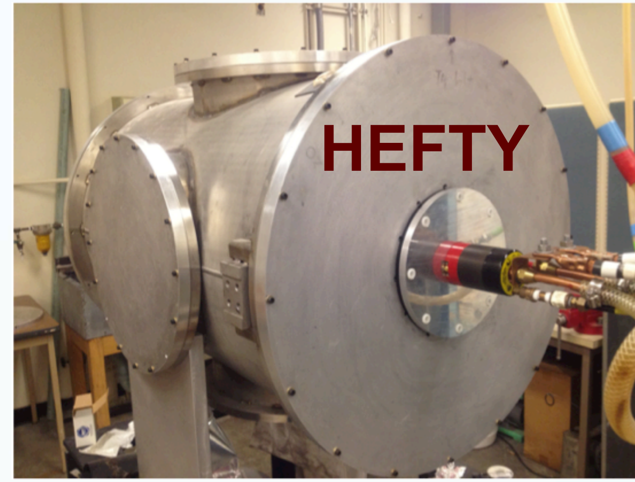
Pi v2 (Enhanced with in-Situ Diagnostics)

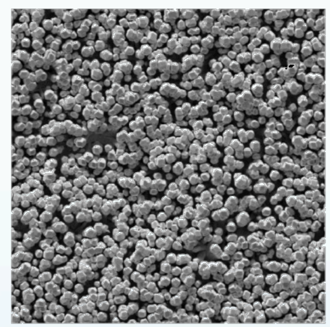


1) In-situ plasma and material analyses
2) Non-intrusive plasma diagnostics
3) Ion energies, 50 – 300 eV
4) Plasma pulsing capabilities

Crossatron Plasma-Switch







Thermo-mechanical material testing experiments can be performed through pulsed operation of the system allowing for evaluation of materials in a more realistic operating environment.

DURIP: In Situ Precision Diagnostic Facility for Studies of Materials and Processes Far From Equilibrium (Wirz, Ghoniem, Kodambaka; UCLA)

Pi v2

World-class diagnostic suite for in-situ plasma-material analysis

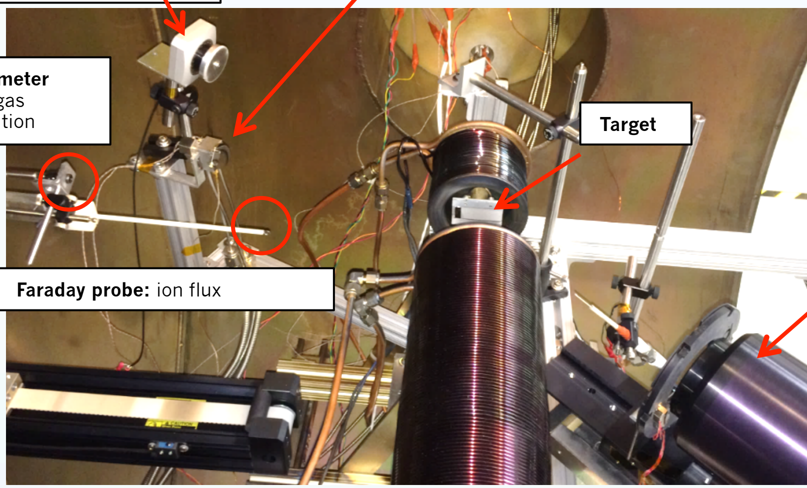
Rotating witness plate: time-resolved sputter composition

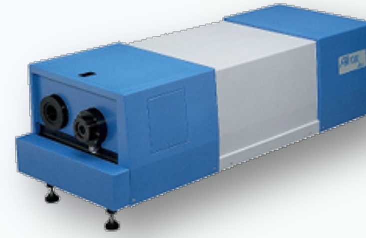
QCM: sputter rate

Spectrometer optics: gas composition

Target

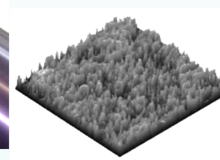
Faraday probe: ion flux



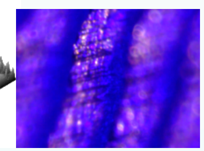


Long focal length spectrometer w/ CCD and PMT detection (Horiba FHR1000)

Long distance microscope: *in-situ* topology evolution (Questar QM100)

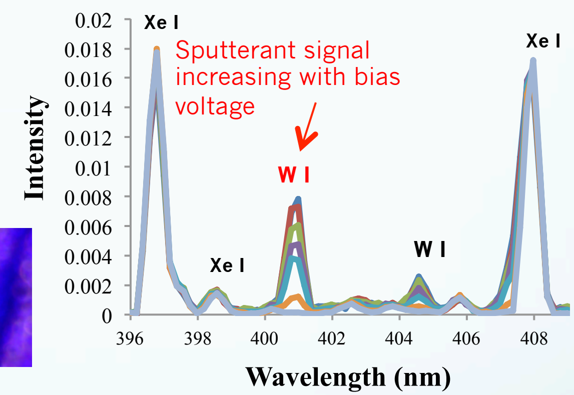


3D profilometry



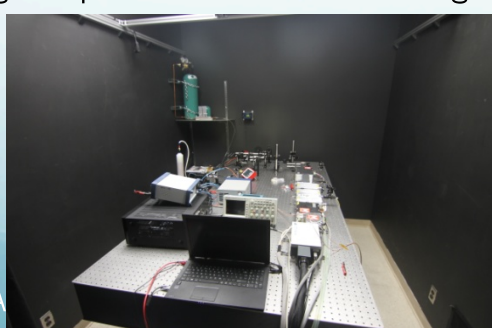
In-situ image

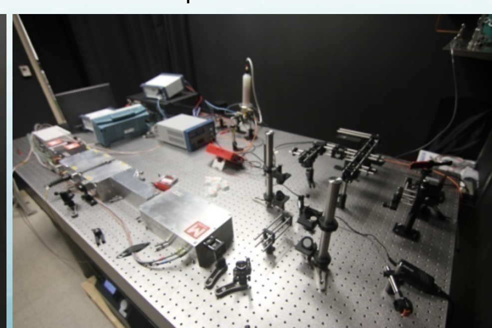
Spectrometer Results for Flat W with Xe

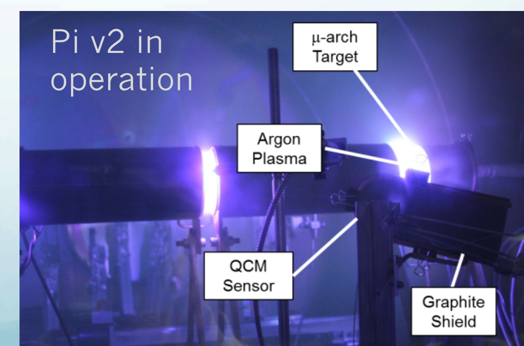


Tunable, Narrow Linewidth Laser System

(Enables wide range of plasma and material diagnostic techniques

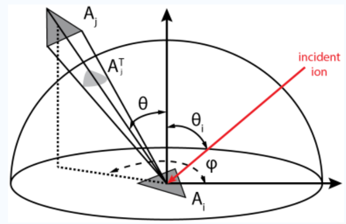


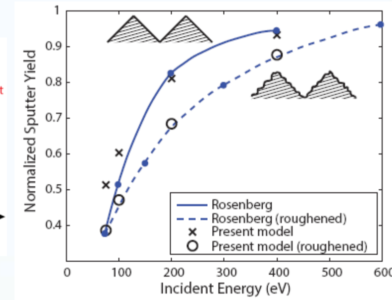


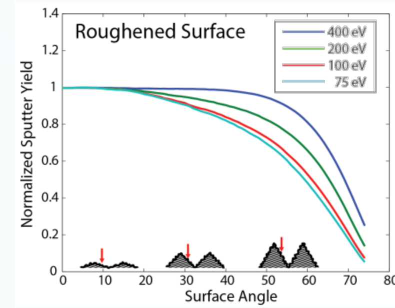


Experiments & View Factor Modeling for Sputtering/Deposition of Micro-architectured Surfaces

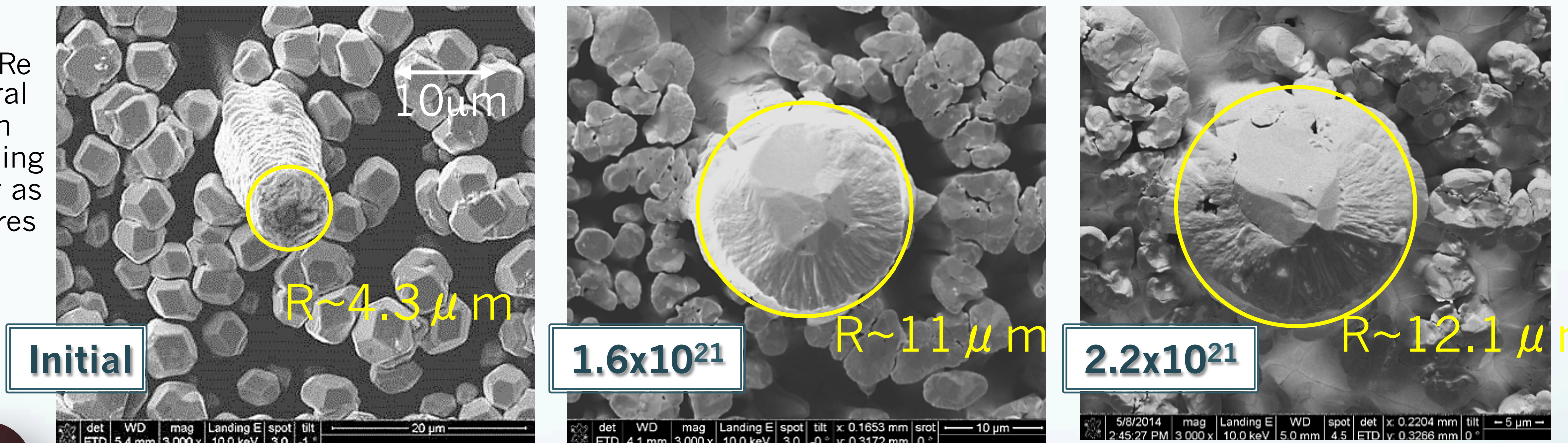
- Ballistic sputter deposition rates
  - Semi-empirical sputter models
  - View factor
  - Shadowing
- Study net erosion v. features[1]





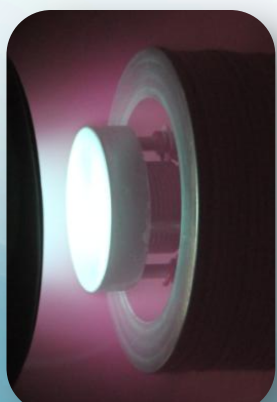


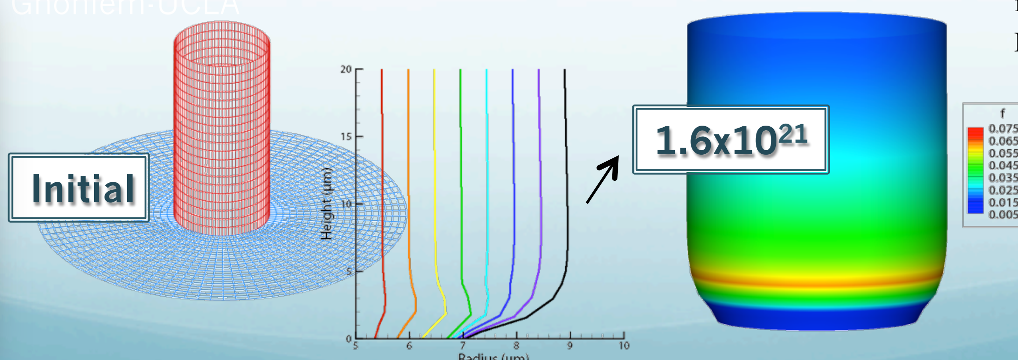
Images of Mo on Re dendrites at several levels of total ion dose. Shows widening of overgrown pillar as surrounding features erode.



Ghoniem-UCLA

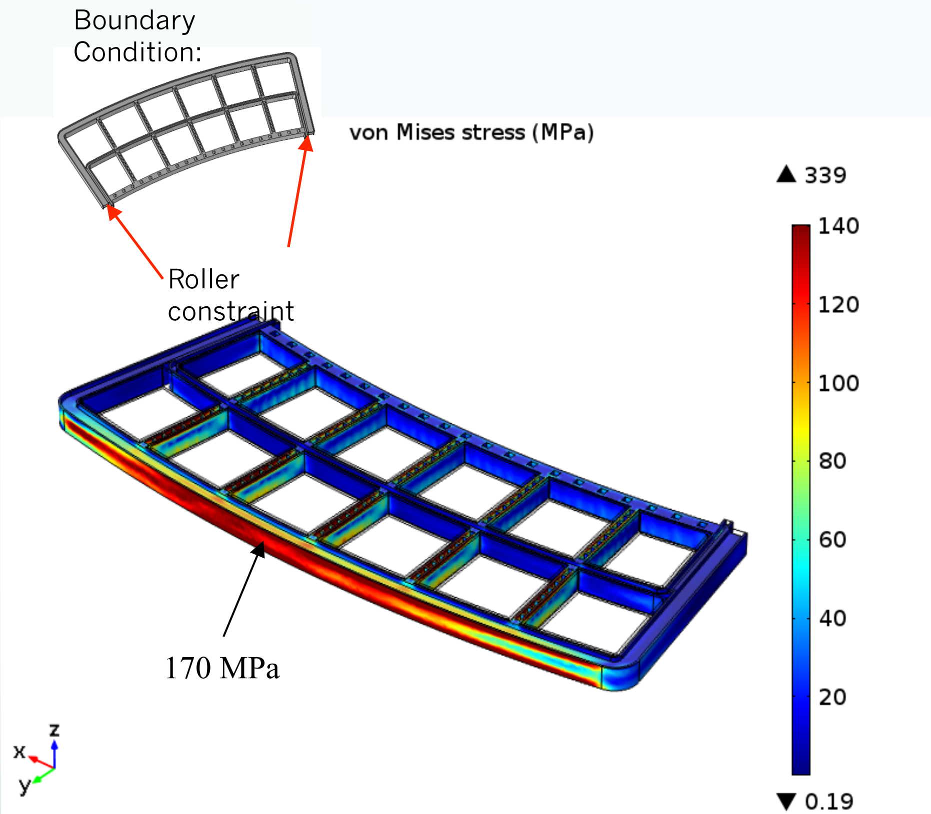
[1]Huerta, Matlock & Wirz, Journal of Applied Phsyics, submitted (2015)



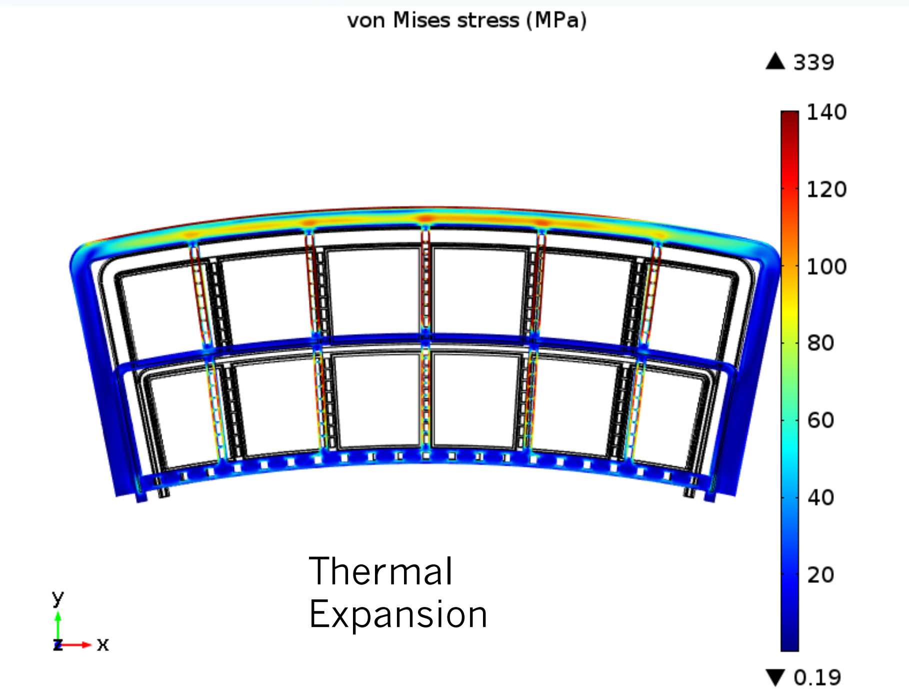


View factor model applied to single Mo pillar on a plane showing pillar widening due to sputter deposition

Common Science & Engineering Issues between Space EP & Fusion PMI

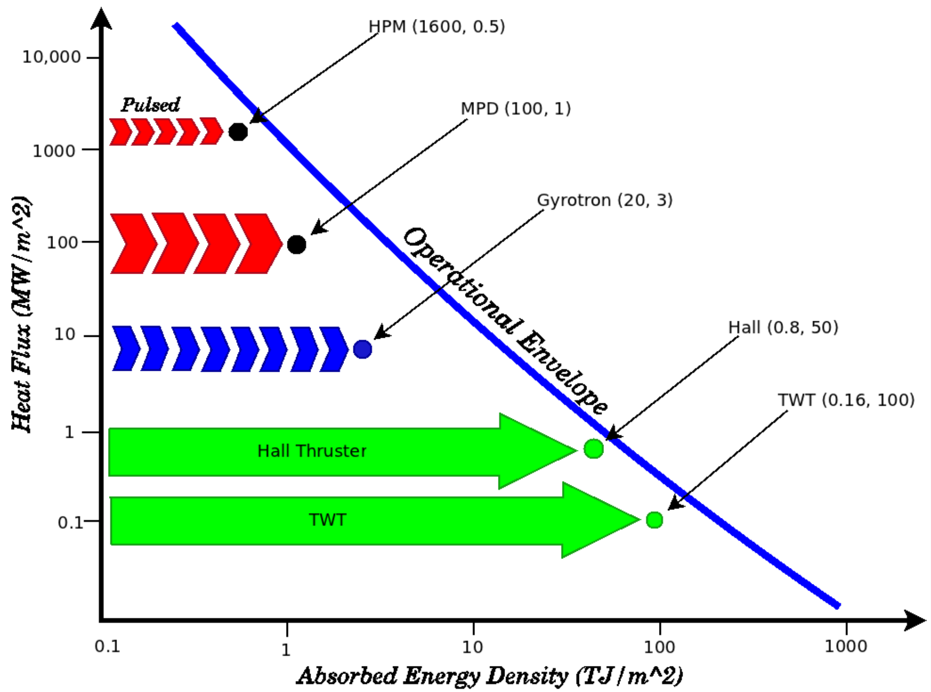


Global thermal stress distribution
– Undeformed configuration

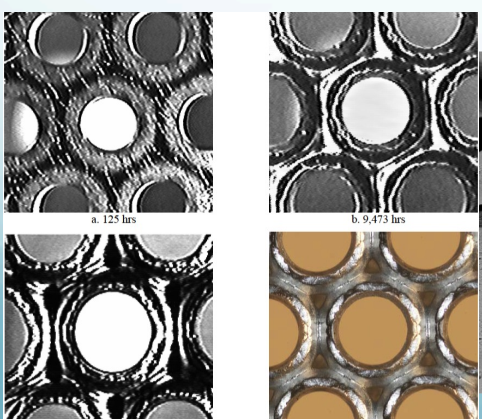


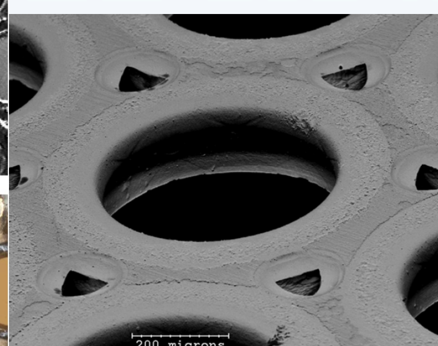
Global thermal stress distribution
–Deformed configuration

Lifetime and Performance of EP & PP Devices are Determined by the Physics of Plasma-Material Interaction



Device	Particle Flux (#/m^2/s)	Particle Energy (eV)	Heat Flux (MW/m²)	Pulse Duration (s)	Ion/Photon Type	Material	Lifetime (yrs)
Hall thrusters - ions - electrons	 $1x10^{21}$ $5x10^{22}$	 50 – 400 30 - 100	 $5x10^{-3}$ $5x10^{-1}$	 CW CW	 xenon electron	 Boron nitride	 1 - 2
Ion thruster - screen grid - accel grid - cathode	 $3x10^{20}$ $6x10^{18}$ $6x10^{21}$	 25- 50 250-500 25-50	 $2.5x10^{-3}$ $5x10^{-4}$ $5x10^{2}$	 CW CW CW	 Xenon	 Moly Moly Mo/W	 3 - 5
Field Emission thruster	$5x10^{17}$	1000-5000	4e-4	CW	Colloid	Ti SiO_2	0.2
MPD thrusters - electrons - ions	 $1x10^{24}$ $2x10^{23}$	 50 – 100 50 – 100	 80.0 1.6	 10^{-3}- CW	Ar,H, electron	 Copper	 0.1 -2
Gyrotrons (collector)	$2x10^{21}$	≈100kV	20	10^{-3}- CW	Electron	Copper	1-5
HPM sources	$1x10^{22}$	0.1-1MV	1600	10^{-7}-10^{-5}	Electron	Copper, moly, W	1
Traveling Wave Tubes (collector)	$1x10^{20}$	1 – 10 kV	0.16	10^{-3}- CW	electron	Copper, moly, graphite	25





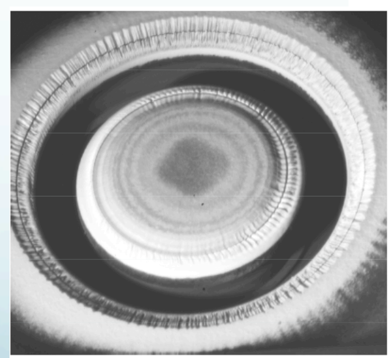
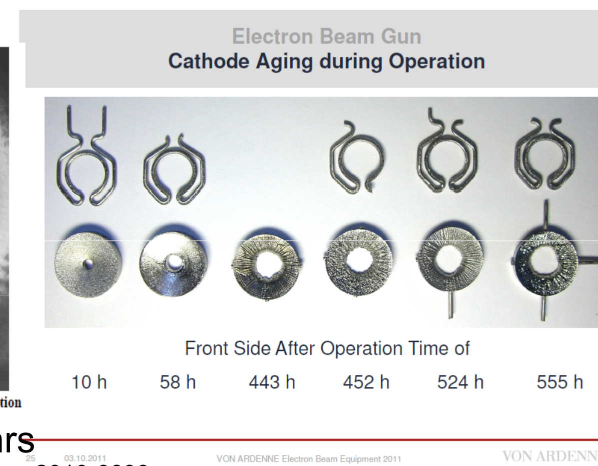


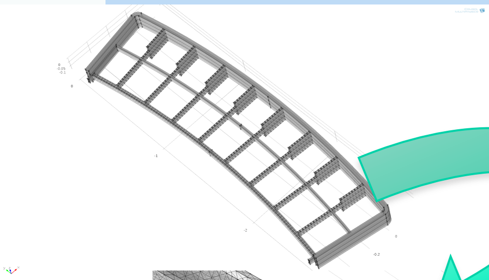
Figure 10 - In-Situ Photograph of Thruster at 10,400 hrs of Operation



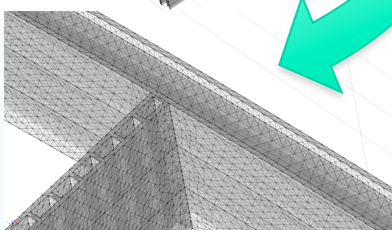
BPT-4000, 10,400 hrs

De Grys, K. H., et al., AIAA Paper 2010-6698

Heterogeneous Multiscale Multiphysics Mechanical (HMMM) Design of Fusion Components

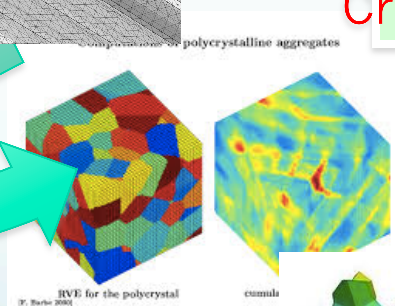


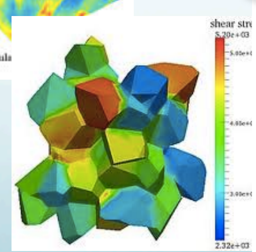
Elastic Analysis & Shape Optimization: ~2-5 MDOF

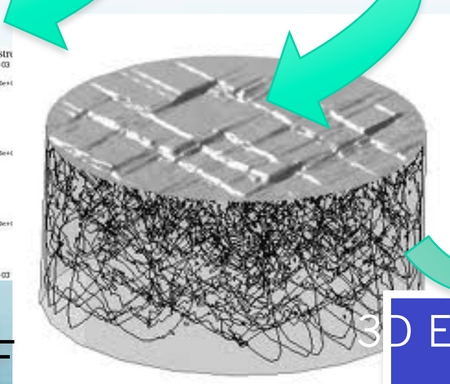


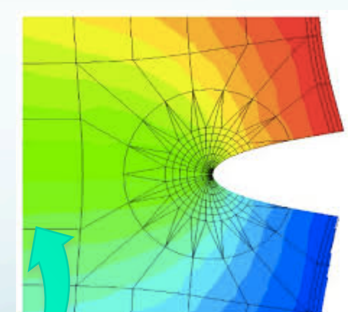
Visco-plastic Model of Critical Region (CR) ~ 0.5 MDOF

Crystal Plasticity of Macro-RVE ~ 0.1 MDOF









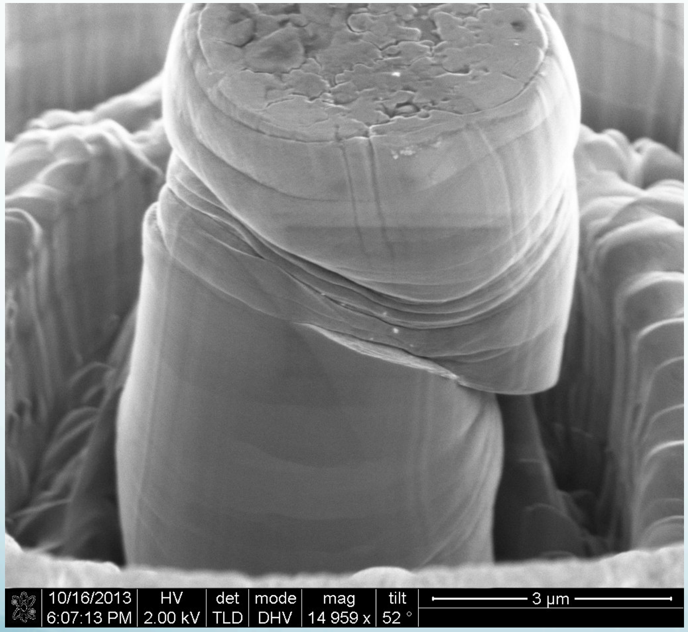
DD Simulation of Micro-RVE~ 10K DOF

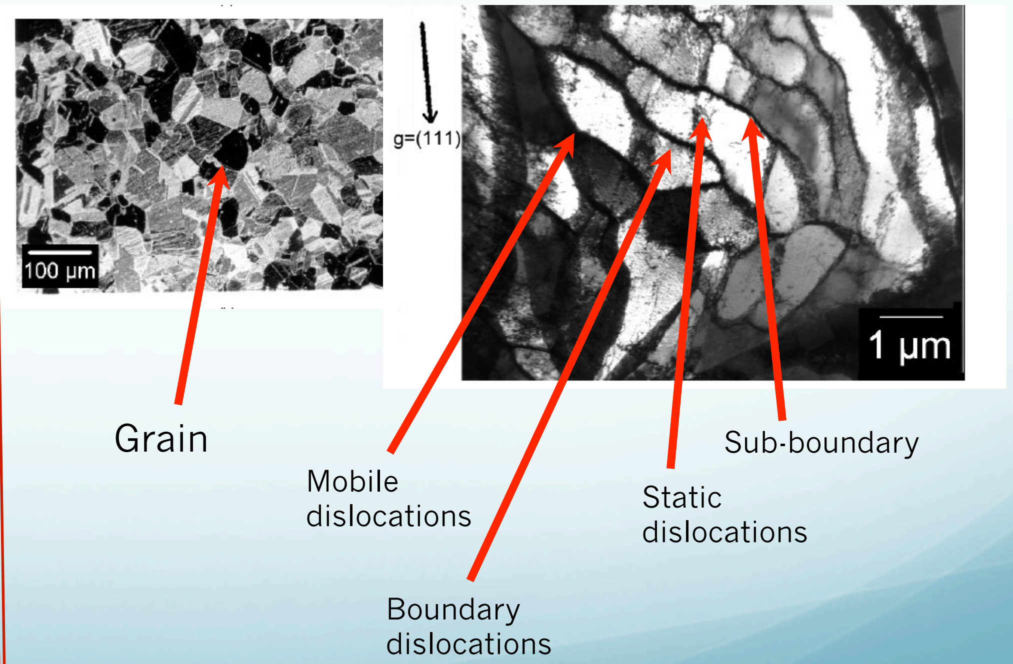
3D Elasto-plastic Fracture Mechan
of Critical Flaw

The Heterogeneous Multiscale Method (HMM) for Thermo-Mechanics

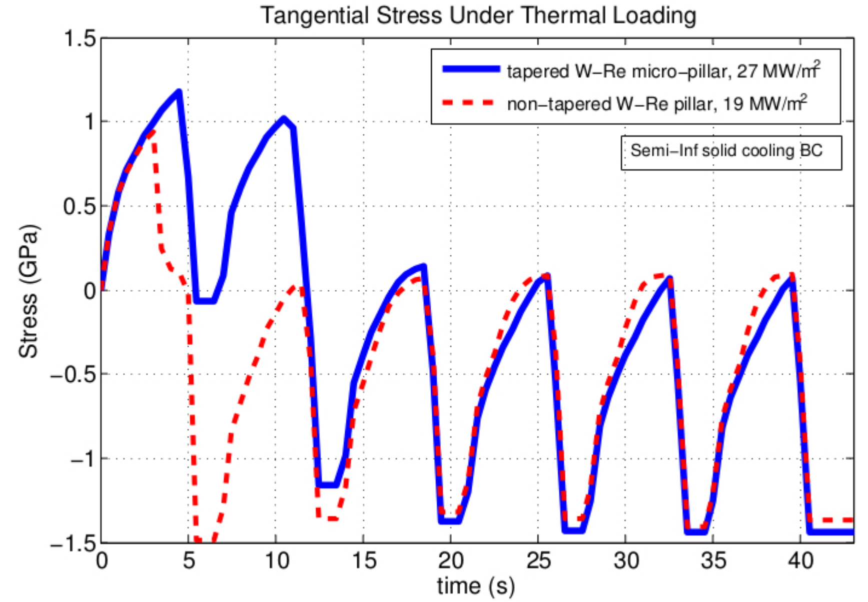
The Microscale is Based on the MODEL Code (Mechanics Of Defect Evolution Library) Developed by Po, Ghoniem et al. (JMPS 66:103-116, 2014.)

The Macroscale is Based on the Ghoniem-Matthews-Amodeo (GMA) Viscoplasticity Model – (Res Mechanica 29, 197 (1990) -updated 2015)

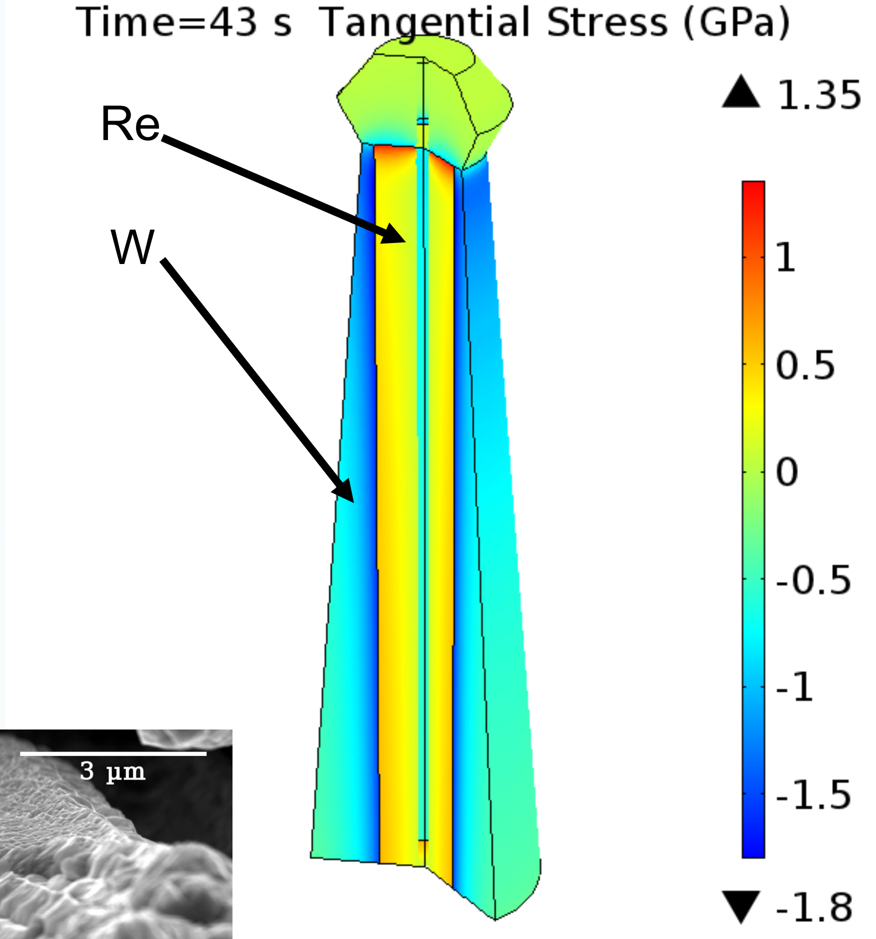




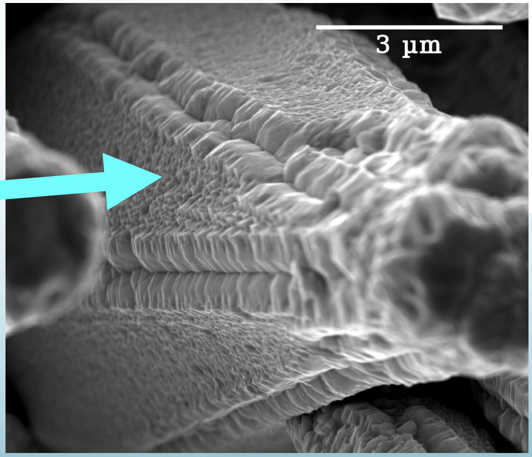
GMA Model Applied to Micro-pillars



Tangential stress in W coating for a tapered and un-tapered micropillar, similar stress response even though the tapered pillar is undergoing a greater heat flux

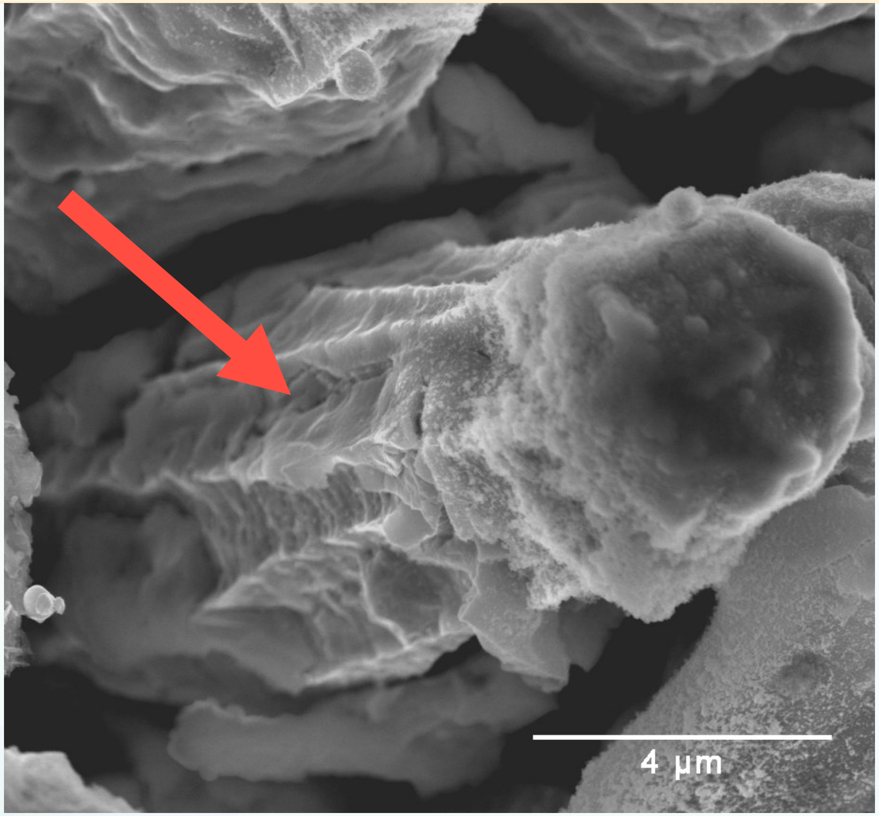


- FE simulation was conducted to investigate the stress response of the pillars during thermal pulsing
- Geometric features such as tapering of the pillars appear to play a significant role in the stress response
- Model consists of a Re core undergoing elastic deformation and a W casing allowed to deform plastically

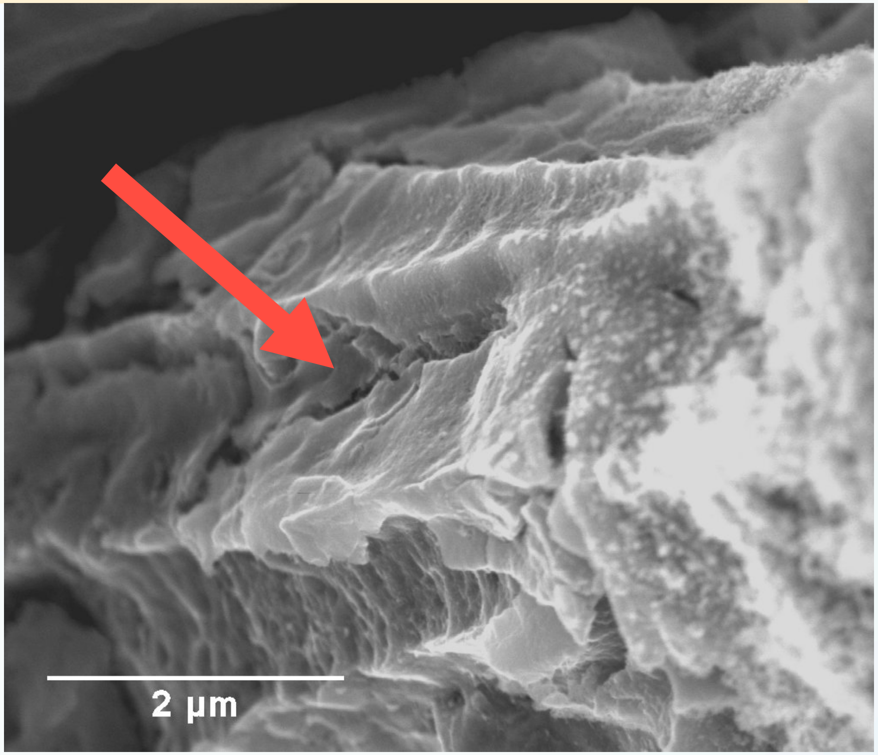


FEA results showing residual tangential stress in a micropillar after 6 cycles of 27 MW/m^2 heat flux exposure, semi-infinite solid BC applied at base of pillar

Micro-Architected Materials



W-Re micro-pillar after thermo-mechanical testing



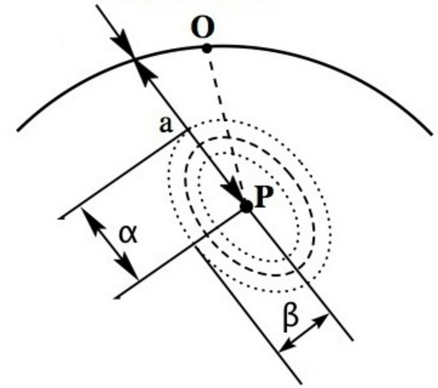
W-Re micro-pillar after thermo-mechanical testing, showing evidence of cracking along the surface

- Under pulsed plasma transients, pillars show fracture behavior dependent upon size and coating thickness
- Opens the possibility to establish design criteria for micro-architected materials, in essence, geometry plays a key role in the thermo-mechanical response and can be optimized to yield an ideal materials system

Erosion Velocity

Sigmund's theory of sputtering, the average energy deposited by by an ion:

$$E(r) = \frac{\epsilon}{(2\pi)^{3/2}\alpha\beta^2}\exp\left\{-\frac{Z'^2}{2\alpha^2} - \frac{X'^2+Y'^2}{2\beta^2}\right\}$$



The normal erosion velocity:

$$v_n = p\int_{\mathcal{R}} d\boldsymbol{r}\Phi(\boldsymbol{r})E(\boldsymbol{r})$$

The velocity equation evaluates to:

$$v_n(\varphi, R) = \frac{J}{n}Y_0(\varphi)\left[\cos\varphi - \Gamma_X(\varphi)a/R_X - \Gamma_Y(\varphi)a/R_Y\right]$$

The Γ functions are dependent on φ and the parameters a, α, β

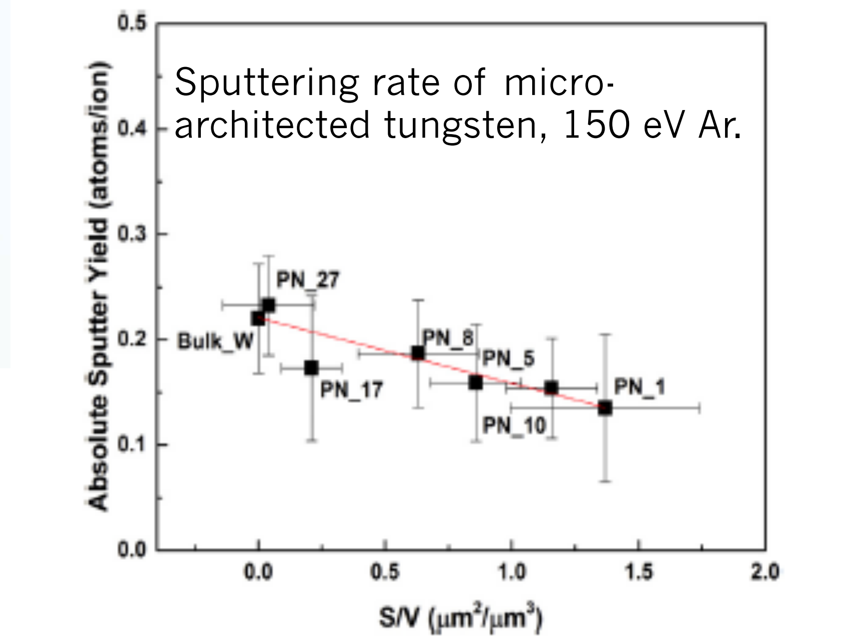
Projecting the normal velocity along the vertical h-axis, and adding a term for surface diffusion results in the following height equation:

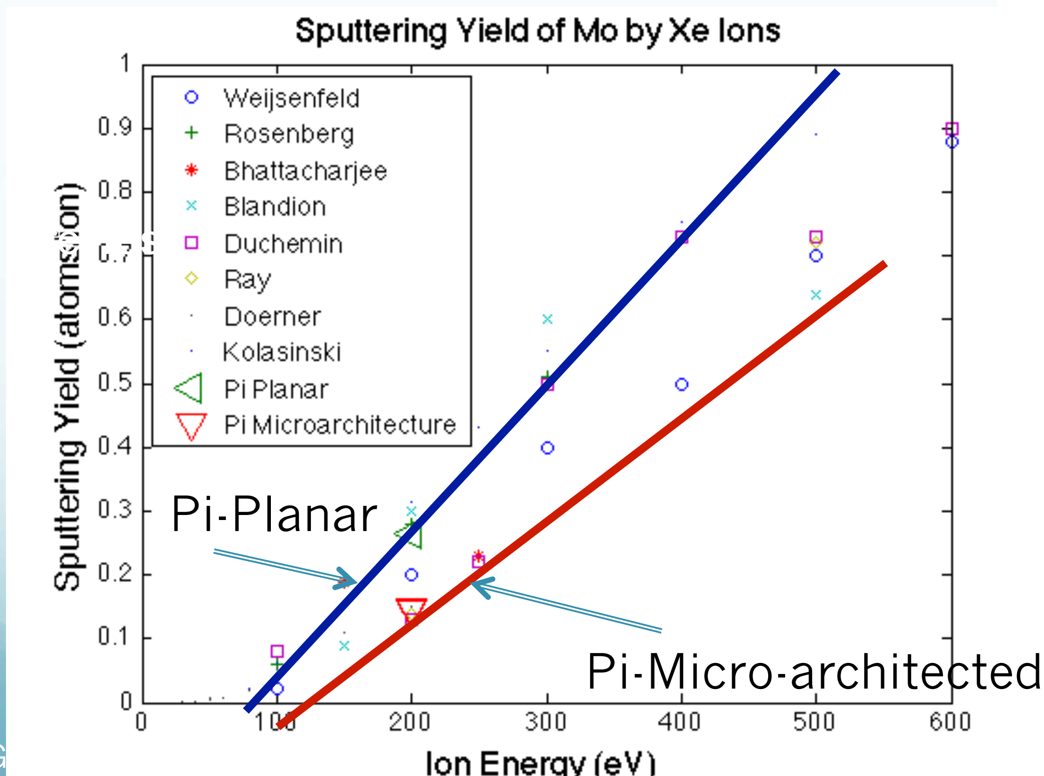
$$\frac{\partial h}{\partial t} = -v_0 - \frac{J\epsilon p a_\alpha^2 e^{-a_\alpha^2/2}}{2(2\pi)^{1/2}}\left[\frac{a}{2}\nabla^2\bar{h} + \frac{a_\alpha^2}{2}(\nabla\bar{h})^2\right] - K\nabla^4\bar{h}$$

Symbol	Parameter	Unit
J	Ion flux	$m^{-2}s^{-1}$
Φ	corrected flux	$m^{-2}s^{-1}$
ϵ	Ion energy	eV
p	relates binding energy velocity of erosion	m/eV
n	surface density	m^{-2}
α, β	Dimensions of collision cascade	m
a	Depth of ion penetration	m
a_α	a/α	N/A
R_X, R_Y	radius of curvature	m

Micro-architected Molybdenum & Tungsten Response to Continuous Plasma Exposure Show a reduction in of Erosion Rate by 30% (Mo) and ~100% (W).

- 2 hour bombardment by 200 eV xenon ions (50 kW/m²)
- Evidence of Mo being removed, exposing Re scaffolding underneath



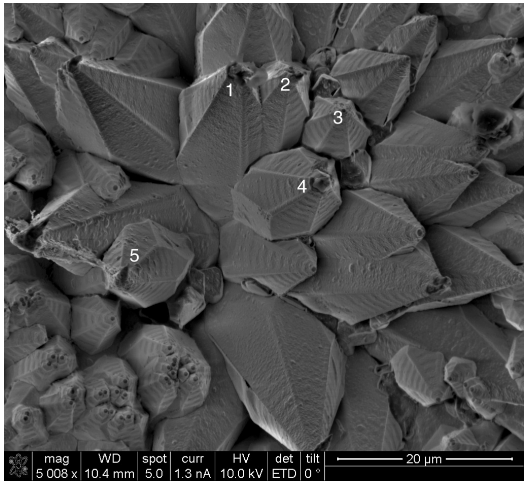


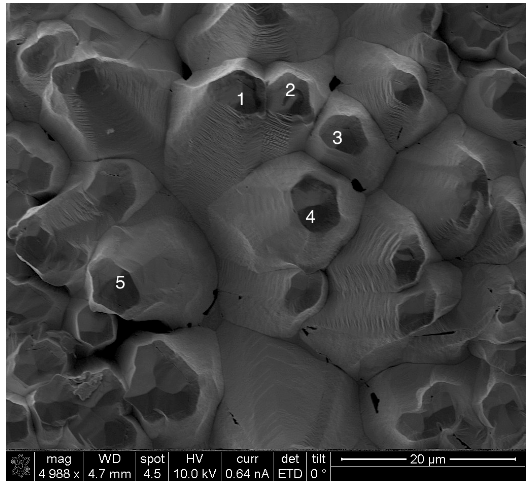
Ghoniem et al., Applied Surface Science 331 (2015) 299–308

Wirz R.E., Ghoniem N.M., "Reconfigurable Long-Life Plasma Systems," UCLA Invention Report 2015

Deposition and Re-deposition Processes

Surface feature before and after 5th fluence exposure of 1x10^{23} m^{-2}:





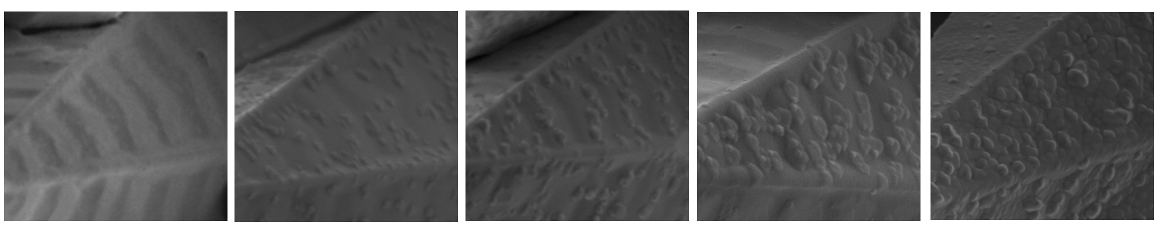
Self-healing of materials

Process 1: Sputter deposition

- Direct deposition onto adjacent surfaces
- Achieved by material design

Process 2: Re-deposition

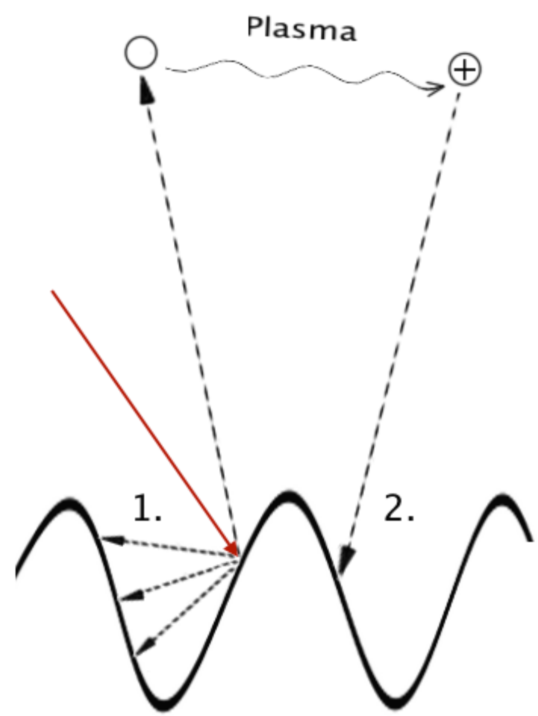
- Deposition after interaction with plasma
- Achieved by device design



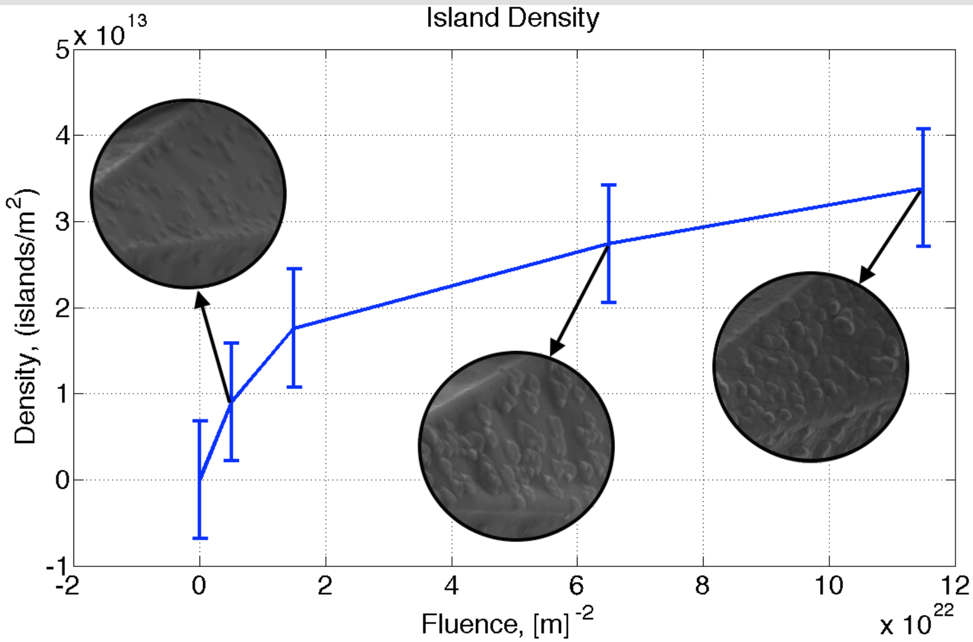
Unexposed | 5x10^{21} m^{-2} | 1.5x10^{22} m^{-2} | 6.5x10^{22} m^{-2} | 1.15x10^{23} m^{-2}

- Sputter deposition has been observed experimentally on micro-architectured samples
- Current model does not account for deposition

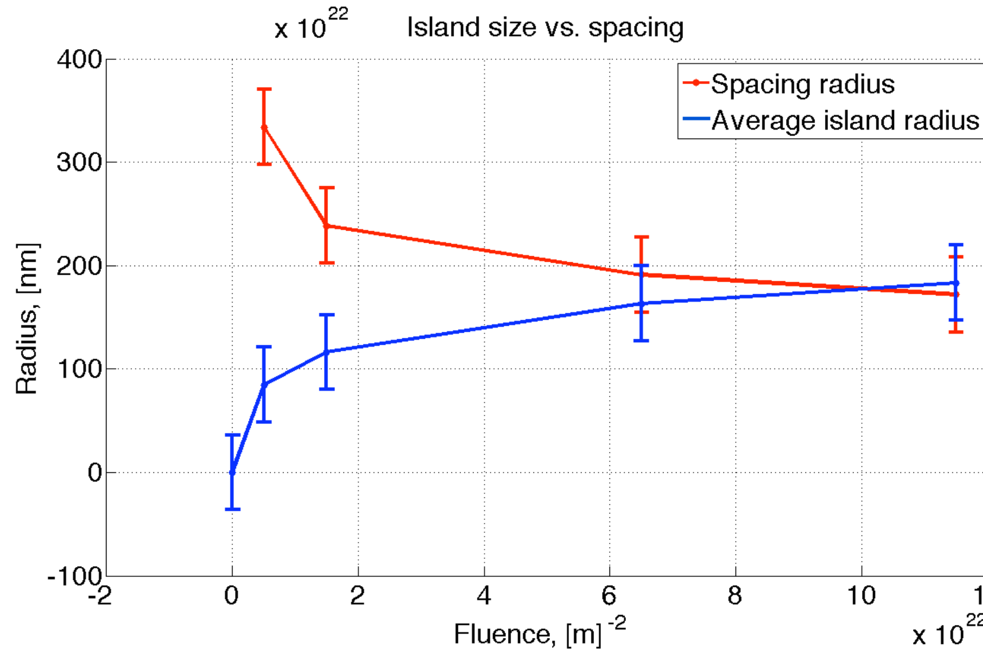
GOAL: Expand BH equation model to include deposition term



Island Formation Measurements



- Analysis performed in SEM images provides island density information on dendrite faces
- Density of island formation increases as a function of fluence
- Rate of island formation levels off at higher fluences



- Radius of spacing between islands compared to the radius of islands themselves
- Coalescence point occurs where lines intersect at ~10^{23} m^{-2}, when island size is larger than spacing between them.
- Fluence corresponds to: 1 s (MPD), 1 min (Hall), 3 hrs (Ion Grid).