Virtual Sputter Chamber - Multiphysics Simulation of Magnetron Sputter & Deposition

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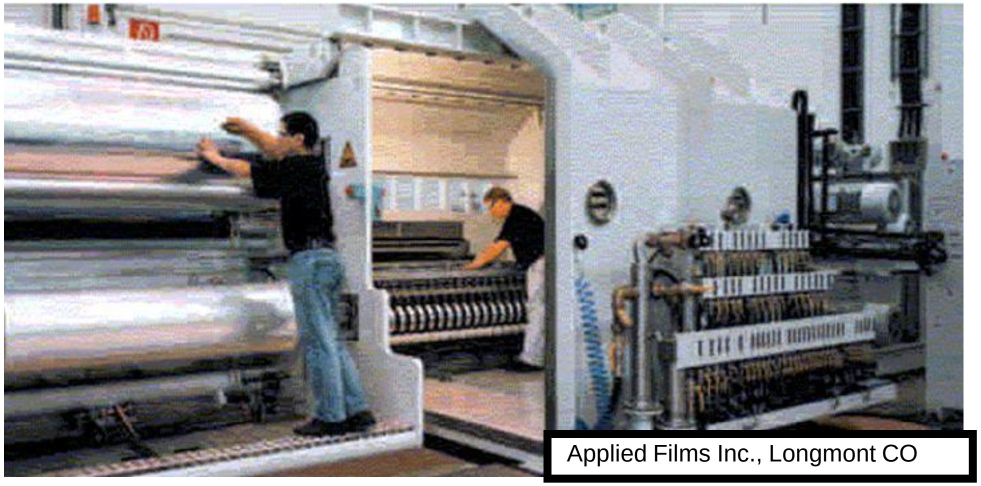
Outline

1) Magnetron sputter in 4 easy pieces – our approach, and current status
2) Side topic: modeling ion-beam deposition for ultra-clean coatings
3) Future work – 3D
4) Conclusions

Magnetron Sputter Deposition is a big economic activity, but a great deal is unknown about the physics

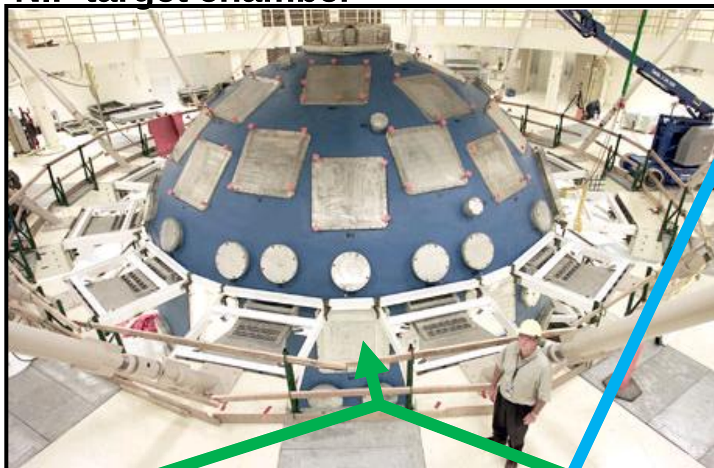
- Annual sales for *sputter targets alone*: $3B projected for 2010
- There is no accepted process model for low-pressure MSD to predict:
  - Thickness uniformity
  - Bombardment energies at substrate
  - Angular distributions of arriving atoms
- Existing process simulations depend on assumptions of continuum fluid behavior and Maxwellian energy distributions
  - limited accuracy at low pressures
  - no atomistic information

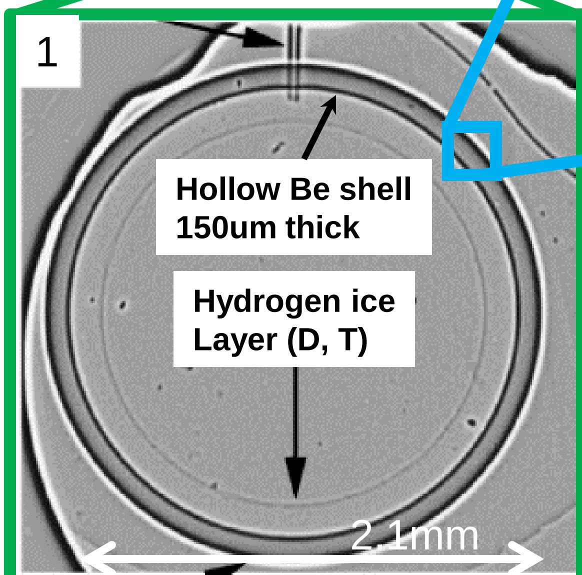


Applied Films Inc., Longmont CO

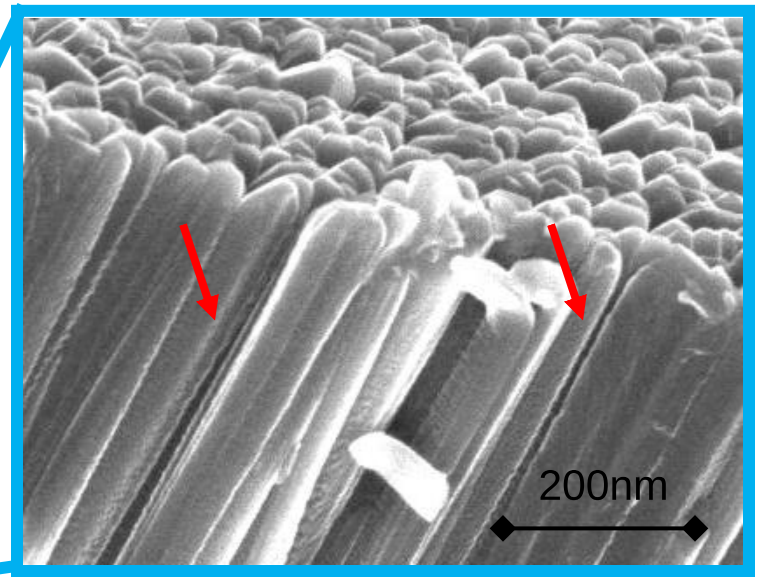
LLNL needs hollow Be spheres as laser fusion targets (National Ignition Facility, NIF)

NIF target chamber



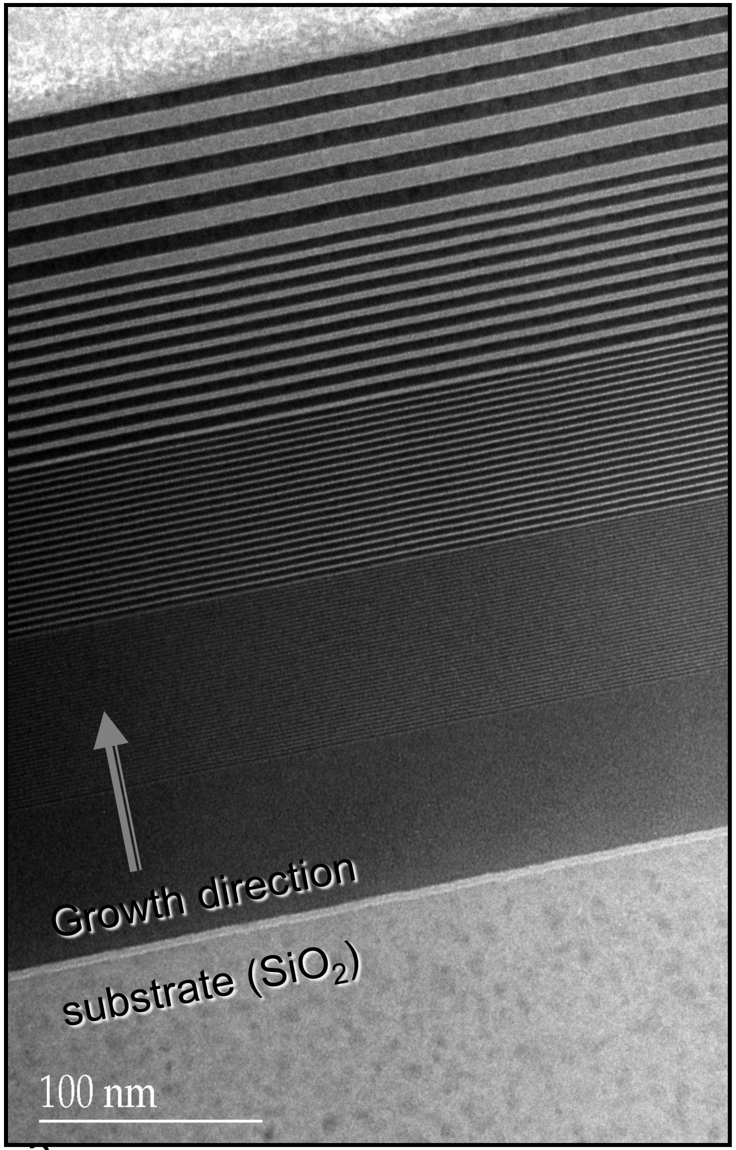


Microstructure of shell (SEM of fracture cross-section, courtesy of A. Detor):



[1]B. J. Kozioziemski, J. D. Sater, J. D. Moody, et al., Journal of Applied Physics **98**, 103105 (2005).

LLNL has a long-standing interest in thin-film optics



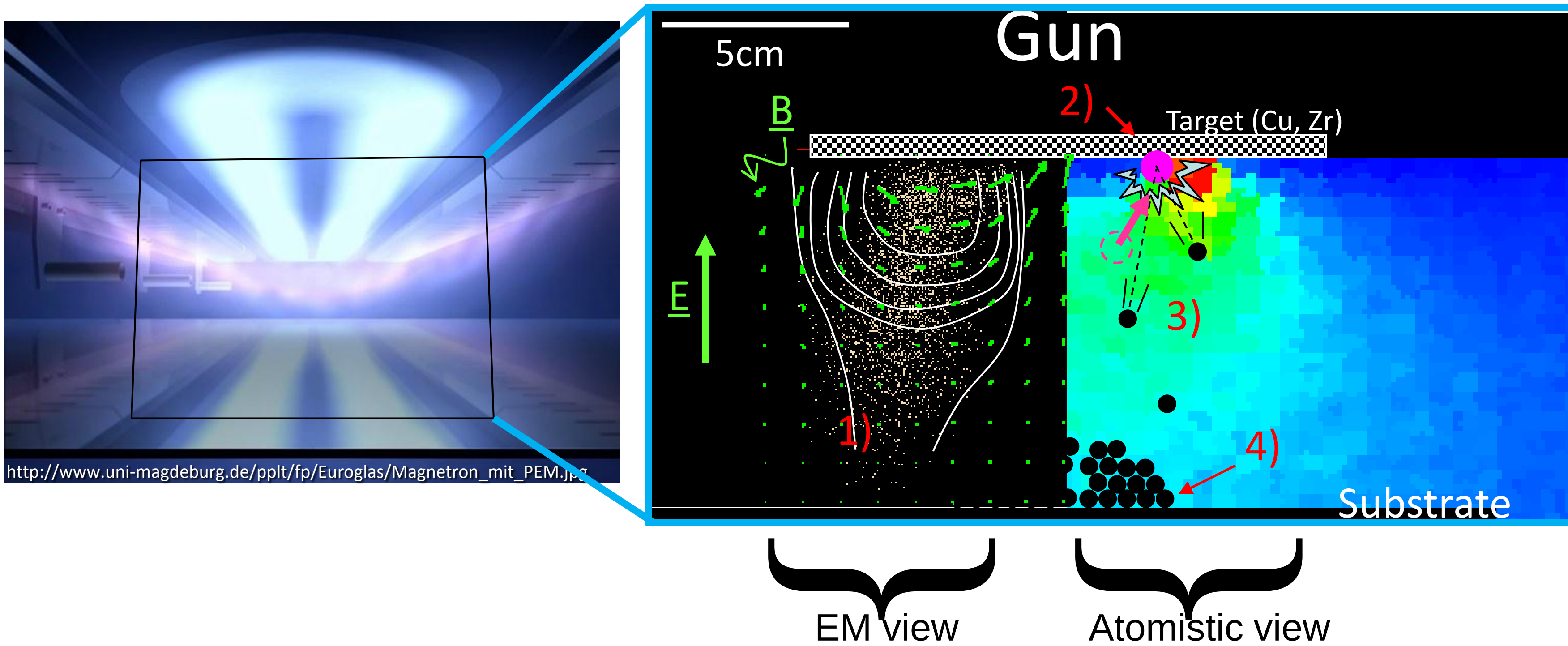
Work by Vernon, Stearns, Barbee, Mirkarimi, Soufli, Jankowski…

Applications: telescope mirrors, fusion diagnostics, and of course EUVL

⇐ Example case of Zr/C multi-band optical coating (TEM cross-section)

- Individual layers range from 0.4nm to 8nm
- Five different layer pitches superimposed
- Thicknesses controlled to ~0.1% accuracy and uniformity across the part

We are building a model of the full process, divided into 4 physics steps



Magnetron Sputter Deposition in 4 physics steps:

1. Plasma dynamics .... Particle-In-Cell (PIC)
2. Impact at target & sputter .... Molecular Dynamics (MD)
3. Transport to substrate .... Direct Simulation Monte Carlo (DSMC)
4. Film growth .... Kinetic Monte Carlo (KMC)

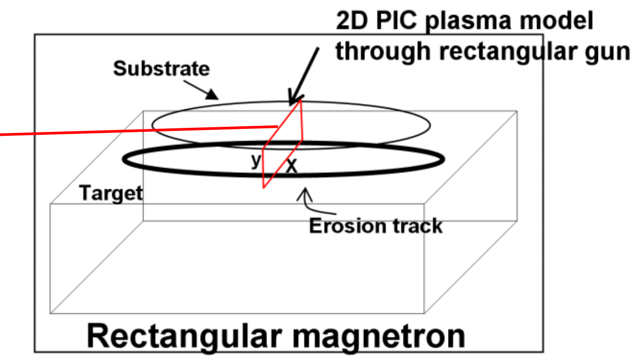
>> Credit due to Dr. Jacques Kools for proposing this work (J. C. S. Kools, in *SVC - 47th Annual Technical Conference Proceedings* (Society of Vacuum Coaters, 2004), p. 31.) ☺

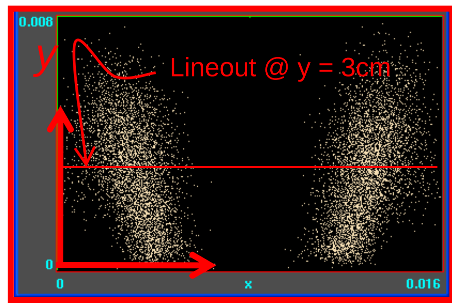
Step 1 (Plasma)VALIDATION: we validated against published Langmuir-probe plasma measurements

Particle-In-Cell method:

1) Divide domain in cells containing simulated particles (about 1e6 ratio of real/simulated)
2) Solve equation of motion iteratively, with self-consistent E and B: interpolate Q and I source terms, calculate fields on mesh points, interpolate fields at particle positions, move, REPEAT
3) XOOPIC code managed at UC Berkeley[1]

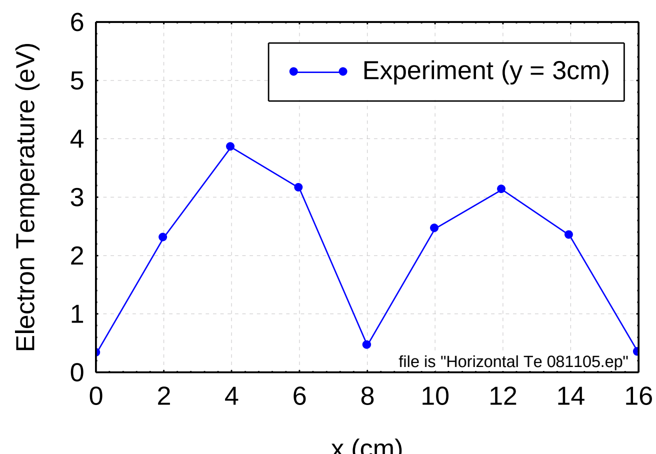
We benchmarked the simulation against published measurements[2]:

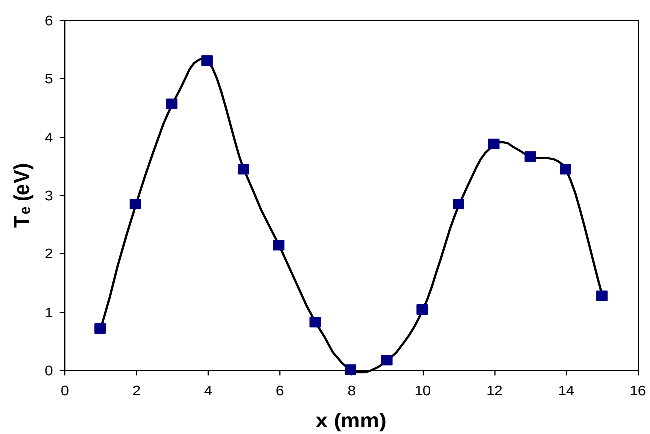




Experiment (Field at al.[2])

Simulation (0.1X scale)



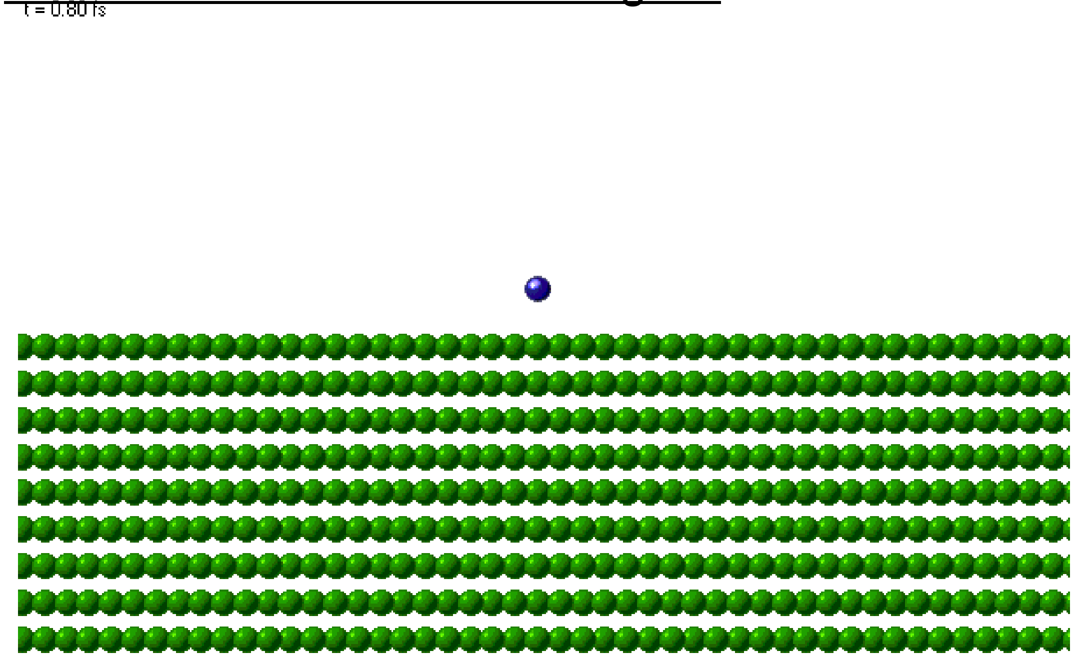


[1]J.P. Verboncoeur, A.B. Langdon and N.T. Gladd, "An Object-Oriented Electromagnetic PIC Code", Comp. Phys. Comm., 87, May11, 1995, pp. 199-211.

[2]D. J. Field, S. K. Dew, and R. E. Burrell, Journal of Vacuum Science & Technology A **20**, 2032 (2002).

Step 2: (Impact at target and sputter): Molecular Dynamics is well-established for problems like this one

MD simulation: 1keV Ar hitting Cu

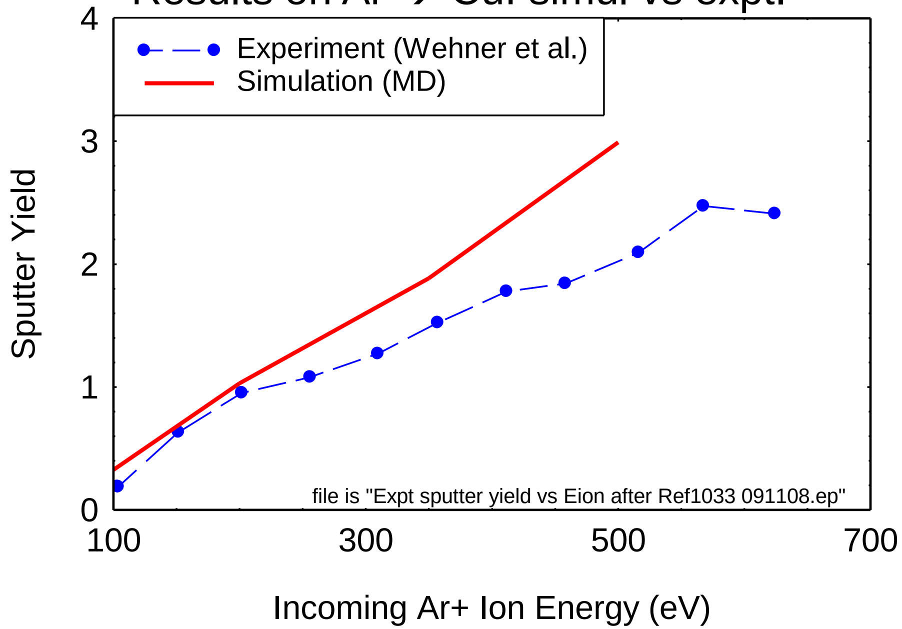


We use Kalypso MD code.[1]

[1]Karolewski, M.A., *Kalypso: a software package for molecular dynamics simulation of atomic collisions at surfaces.* Nucl. Instrum. & Methods B **230**(1-4) 402-5. (2005)

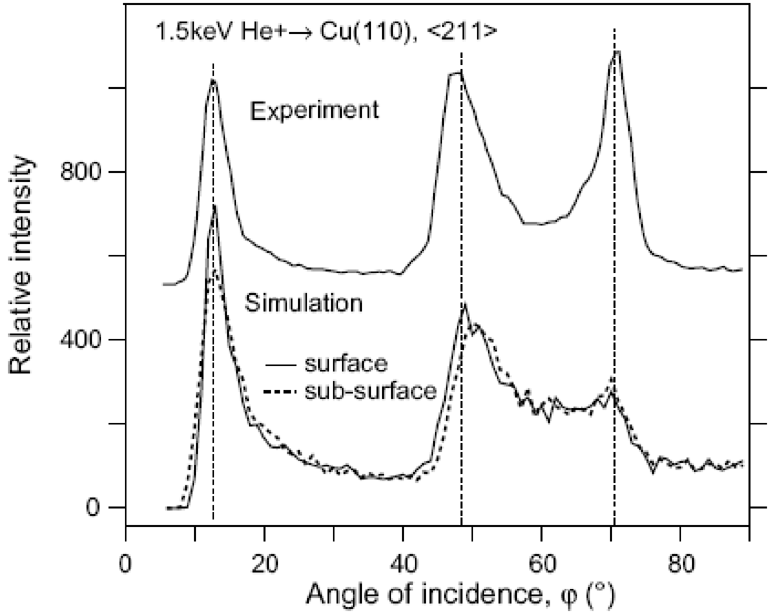
Step 2: - Impact at target and sputter - VALIDATION: MD reproduces experiment well for sputter yield and sputtered-atom angular distribution

Results on Ar → Cu: simul vs expt.



Experimental curve: Wehner, G. K. J. Appl. Phys. **31** 1392 (1960)

Results on He → Cu: simul vs expt.



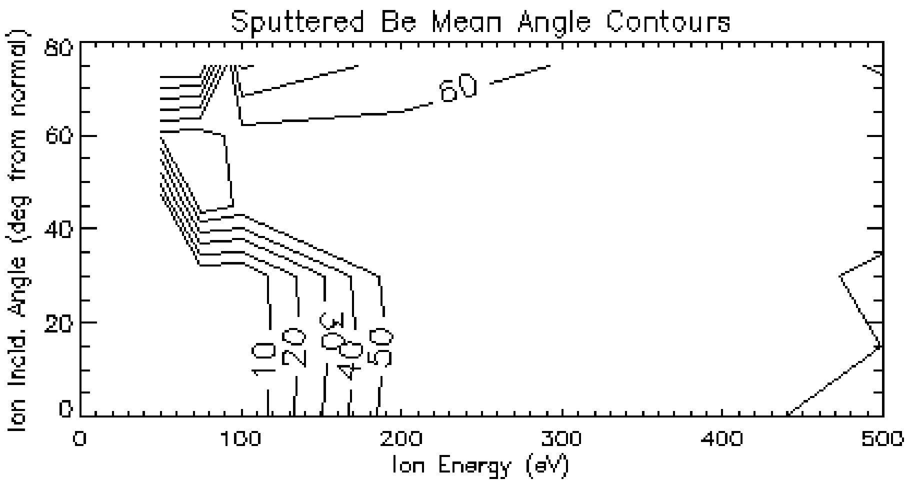
Karolewski, M. A. *ibid.*

Step 2 – sputter - RESULTS: Angle distributions of Be and reflected Ar are very different: Be is approximately cosine, while Ar leaves at nearly normal incidence

<u>Surface: mean angle vs incoming E, θ</u>

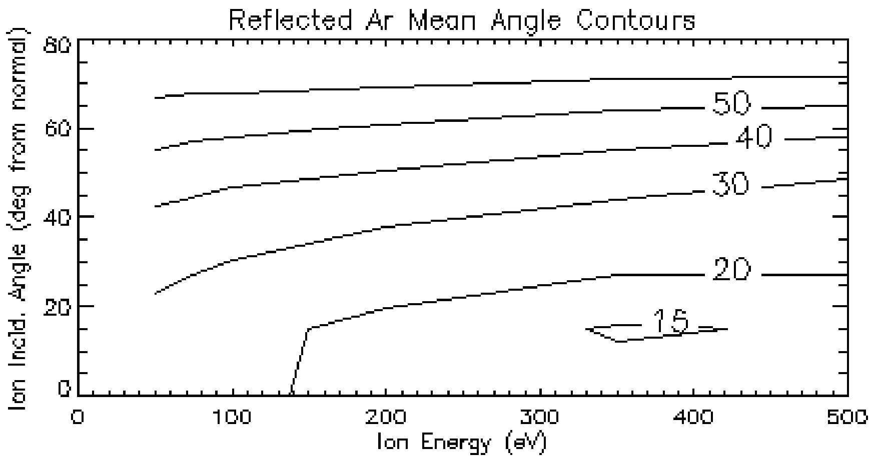
<u>Example of difference between Ar and Be: mean and σ of angle</u>
(for 300eV Ar+ at $\perp$ incidence)

Sputtered Be



$50° \pm 15°$ (1σ)

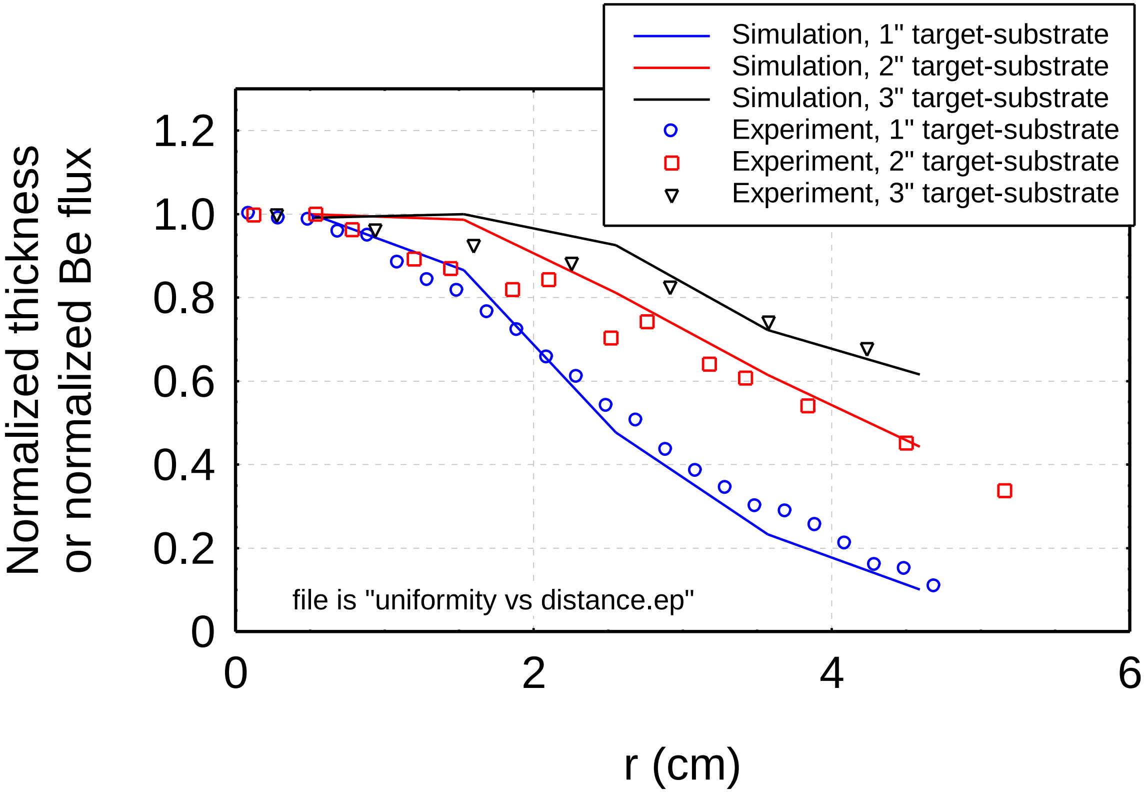
Reflected Ar



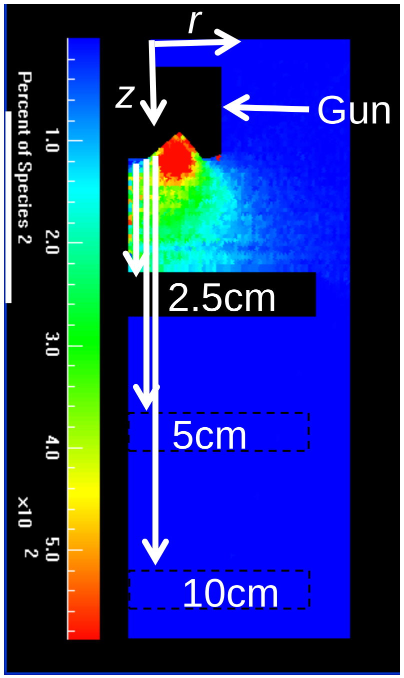
$15° \pm 9°$ (1σ)

3rd step - transport to substrate – VALIDATION: Simulation reproduces thickness profiles to within ~10%

Studying film thickness profiles vs distance:



Map of percent Cu in gas



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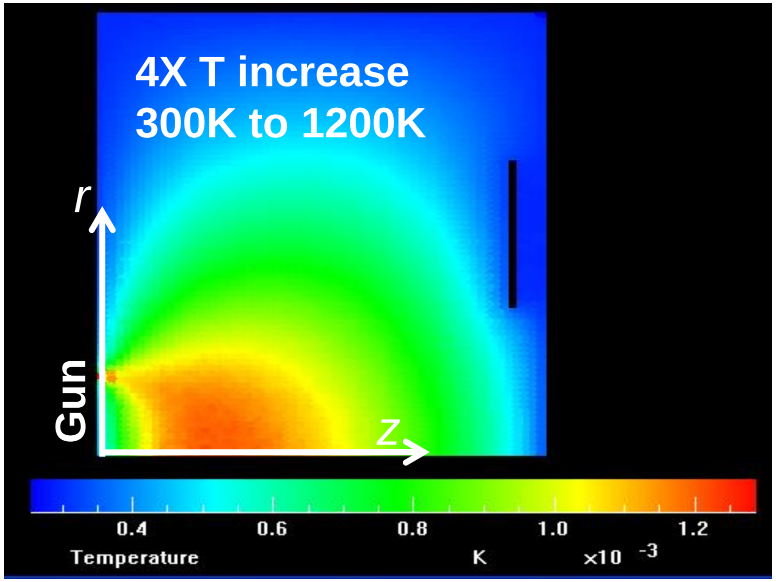
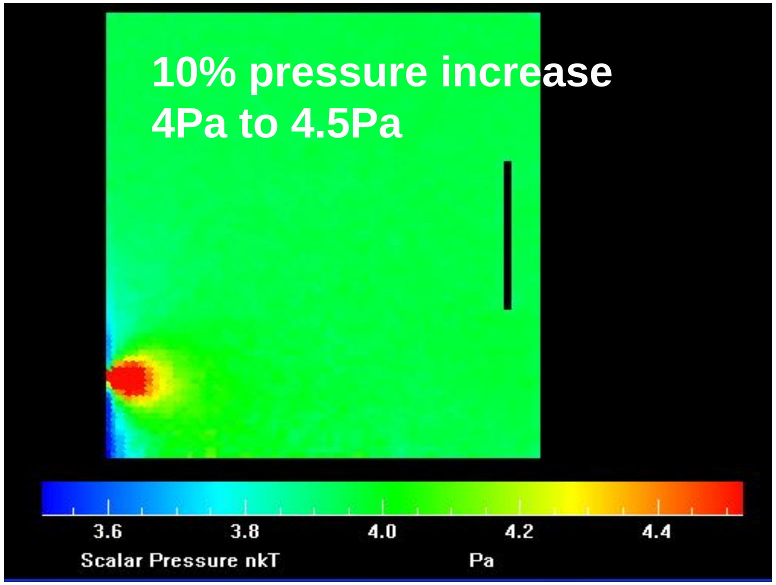
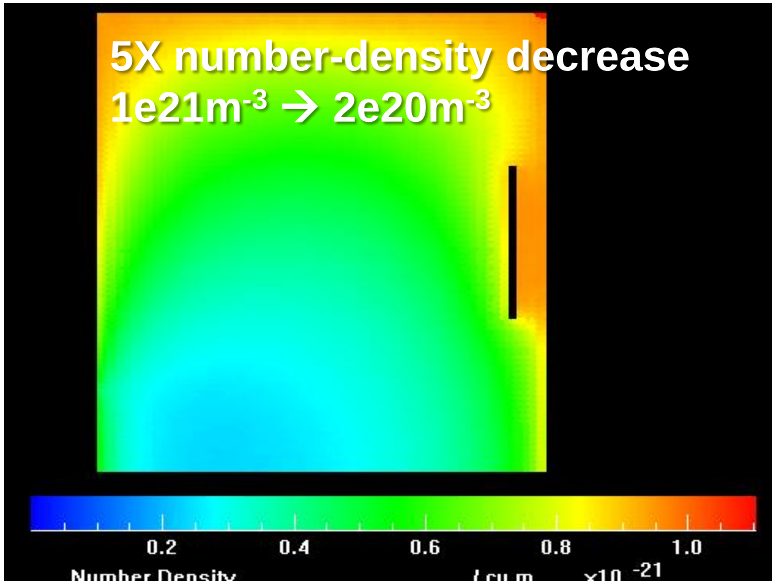
3rd step - transport to substrate – SIDE POINT OF INTEREST: When run at high power, there is significant (1.1 to 2X) heating, pressurization, and rarefaction of gas in front of a magnetron







Conditions:

- 6-inch circular magnetron @ P = 2kW
- sputtering Cu in Ar
- P = 4Pa

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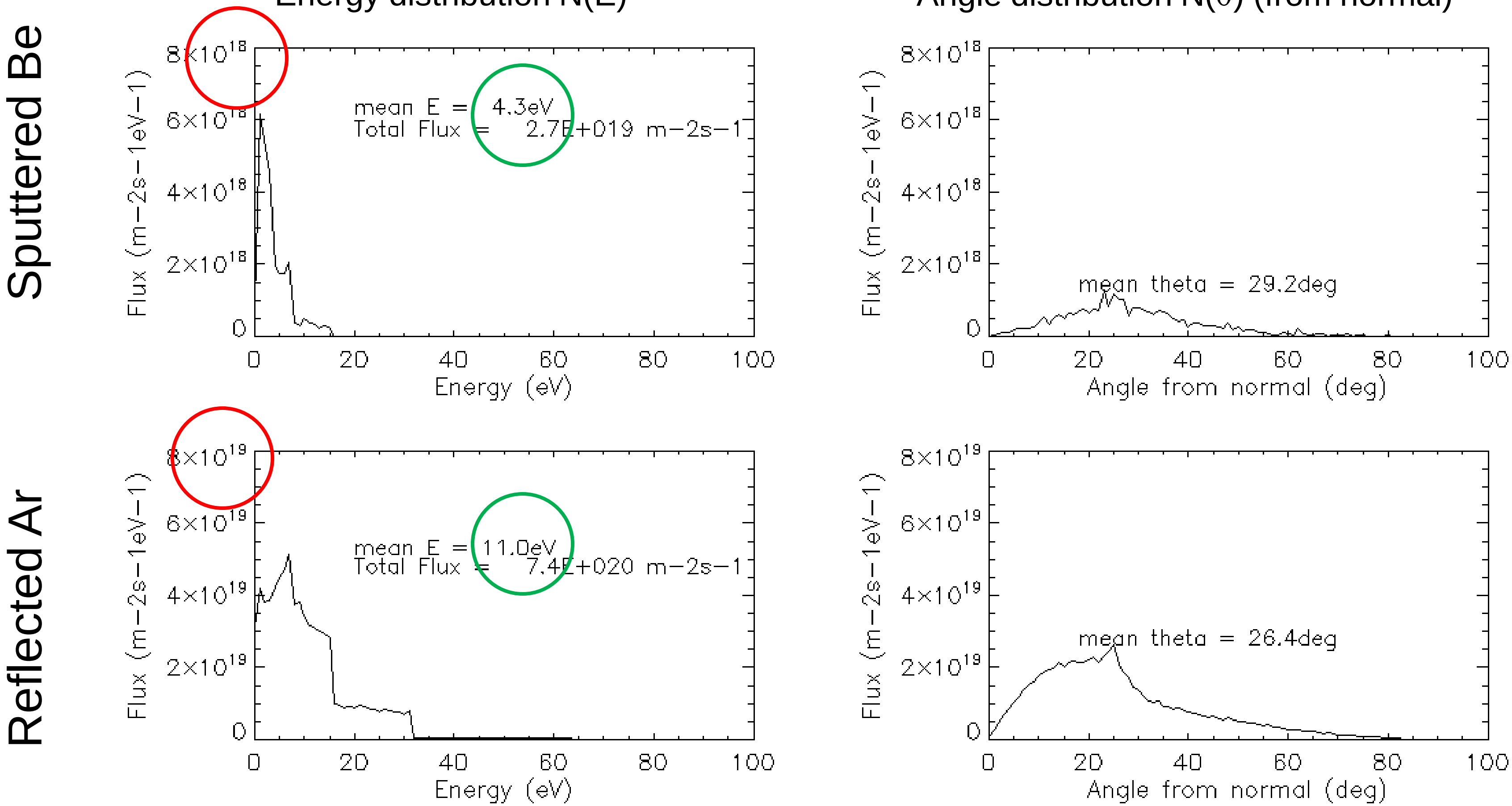
Steps 1-3 RESULTS: At substrate, target-reflected Ar has more energy than the sputtered Be atoms

Energy distribution N(E) | Angle distribution N(θ) (from normal)



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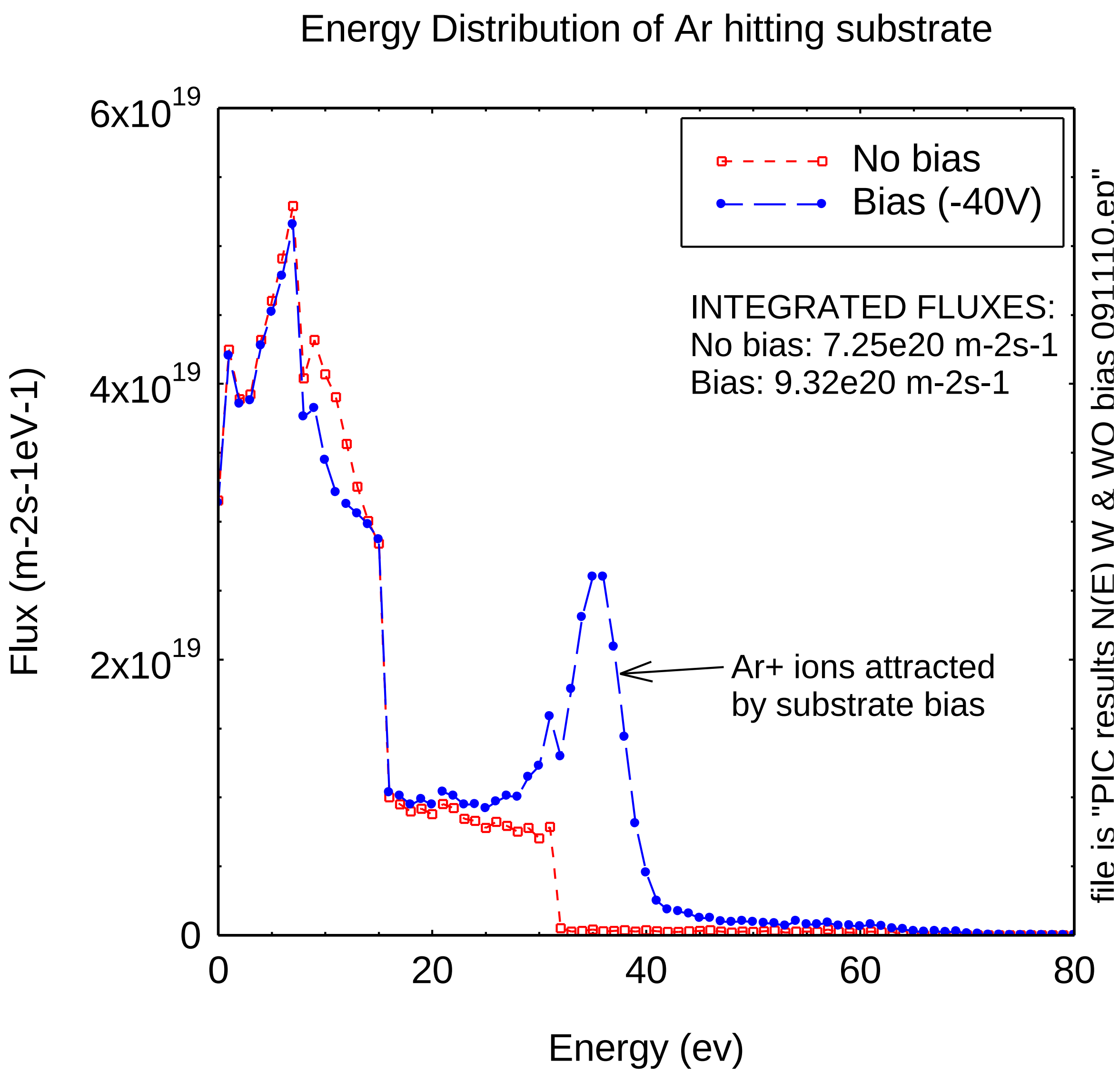
Steps 1-3 RESULTS

If substrate is biased negative, Ar^+ ions hit the substrate at high energy



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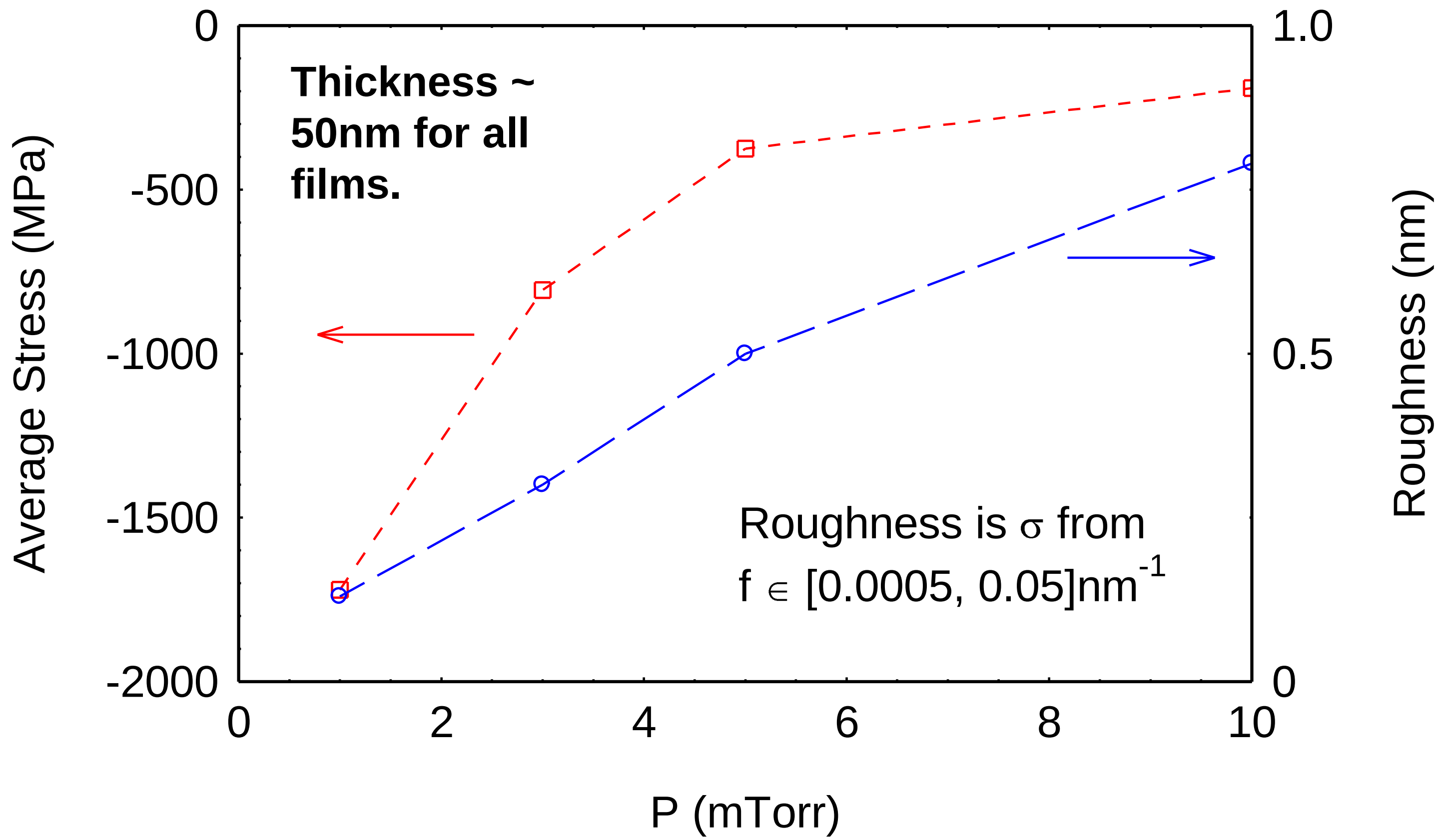
Application to SiC films: can we improve on roughness/stress tradeoff?

With increased sputter pressure, compressive stress is greatly reduced, but at the expense of roughness:

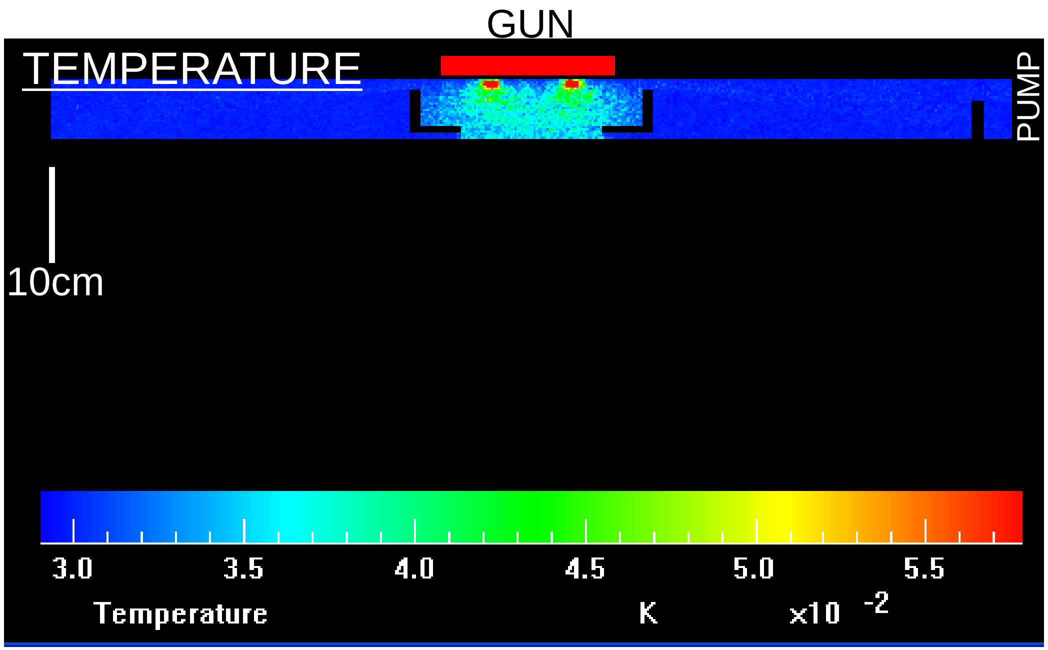


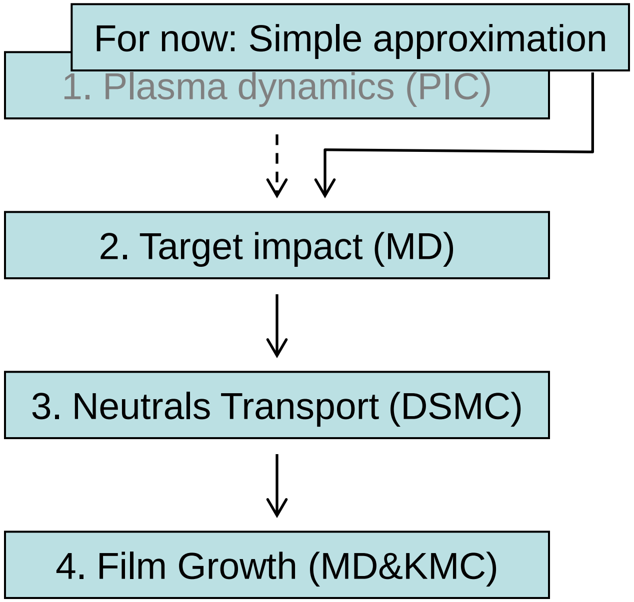
Can we model these results with rational physical processes, and better understand what drives roughness evolution?

Application to SiC: We have used the 3 working model components together for the first time (target impact, neutral transport, film growth).

Simulate sputter, transport and growth of SiC, with varying pressure.

<u>Stretch goal</u>: reproduce increase of roughness with pressure. (Not shooting for stress yet!)





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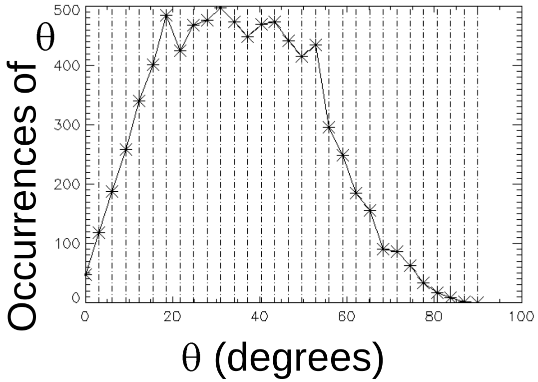
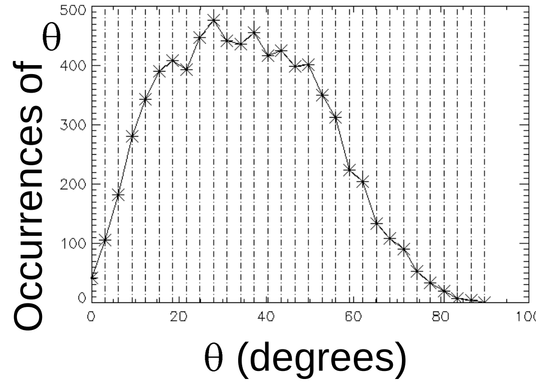
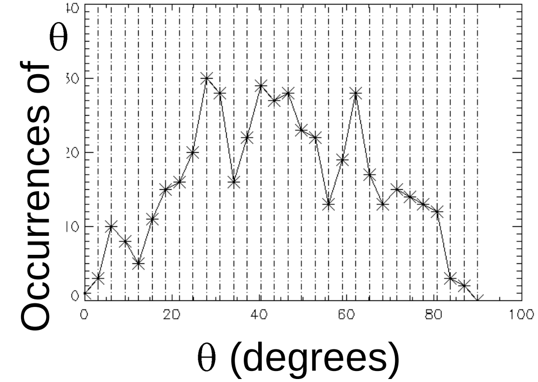
Application to SiC: we obtain angle and energy distributions of all species leaving the target

Carbon | **Silicon** | **Argon**

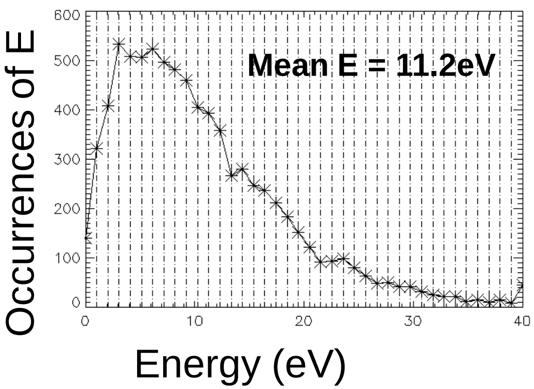
Angle distribution

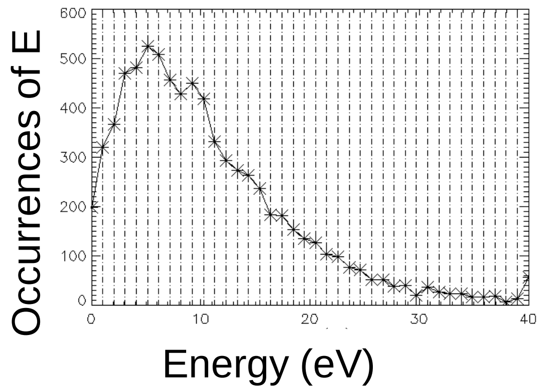


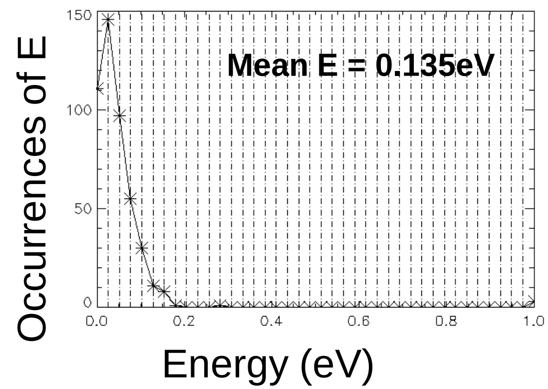




Energy distribution





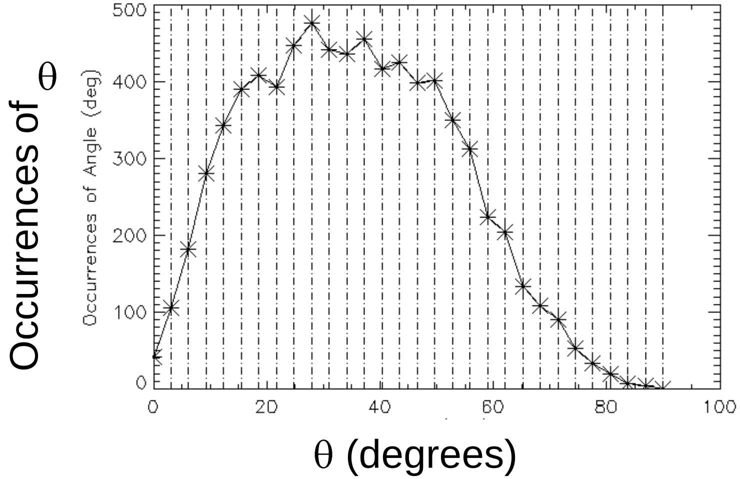


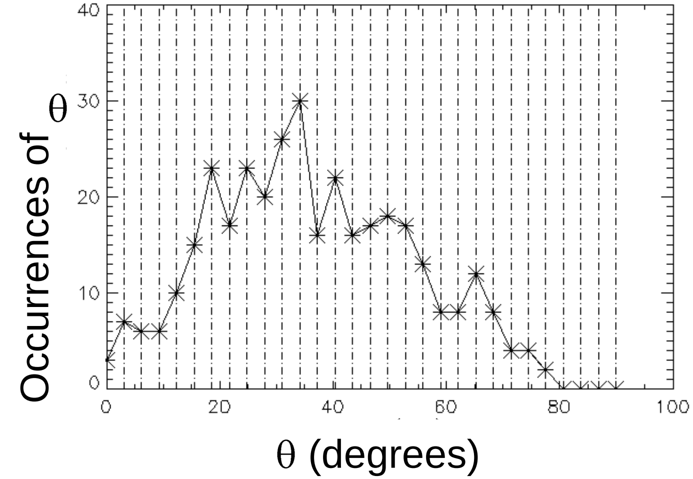
Ar: dominated by low-T "thermal" background – improved sampling needed to capture high-energy tail.

Application to SiC: … and also angle and energy distributions of all species at the substrate

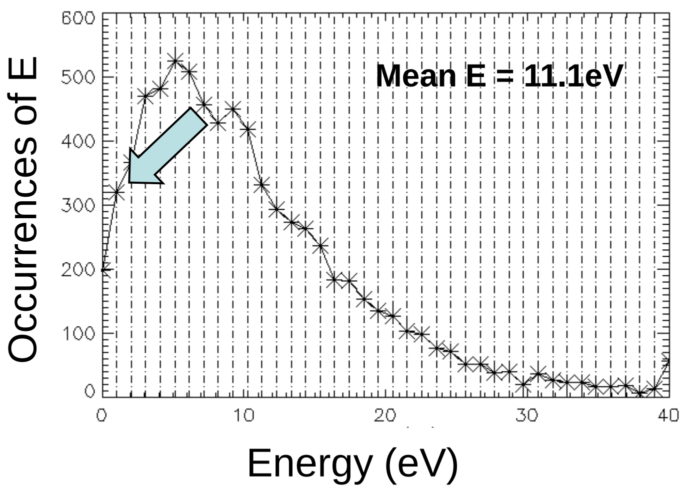
Silicon at pressure 1mTorr | Silicon at pressure 10mTorr

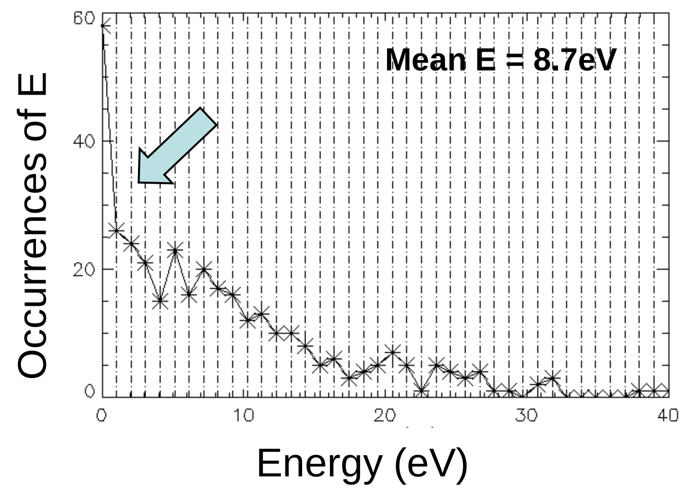
Angle distribution





Energy distribution





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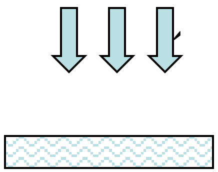
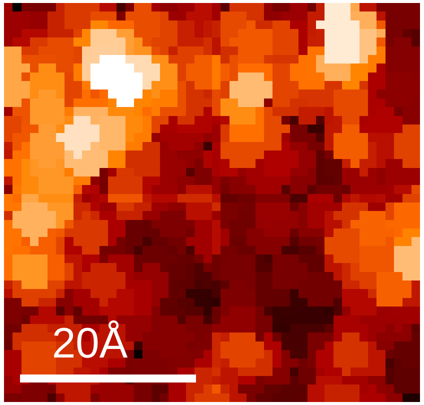
Application to SiC: Pressure effect could not yet be simulated – simulated effect of angular distribution as analog

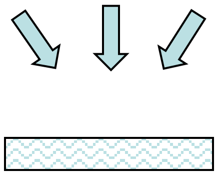
Roughness of simulated SiC films (using very rough analogs for pressure)

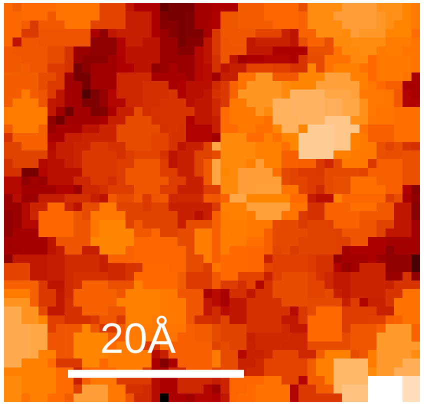
Collimated Flux:



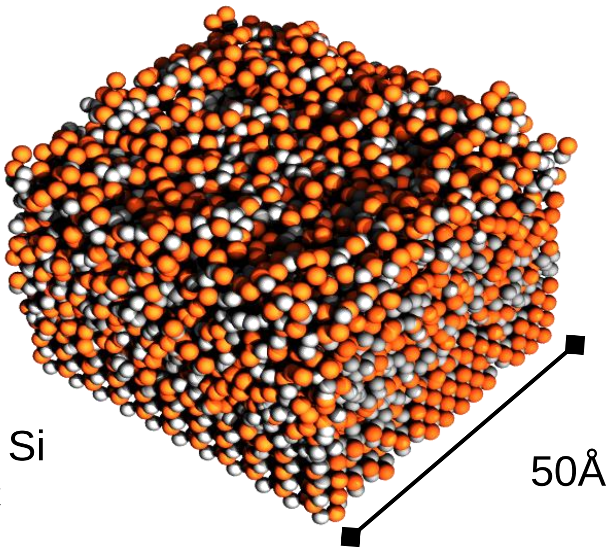


~ Cosine Flux:

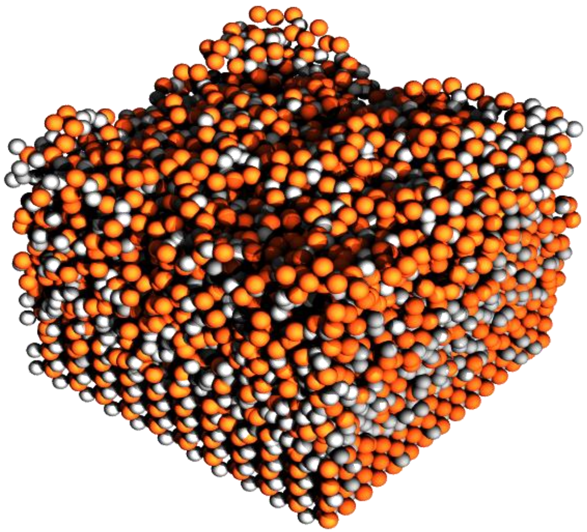




Images and PSDs produced by TOPO code (D. L. Windt)



Orange: Si
Silver: C



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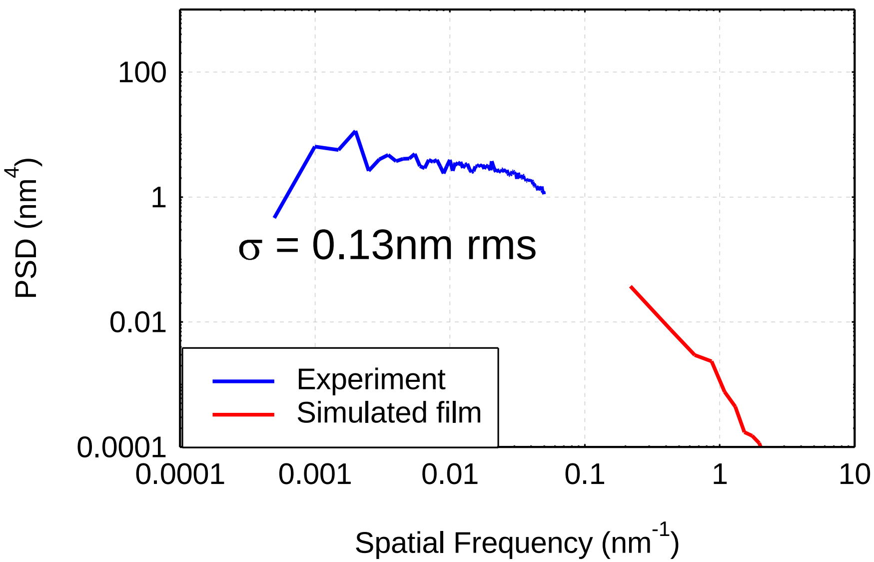
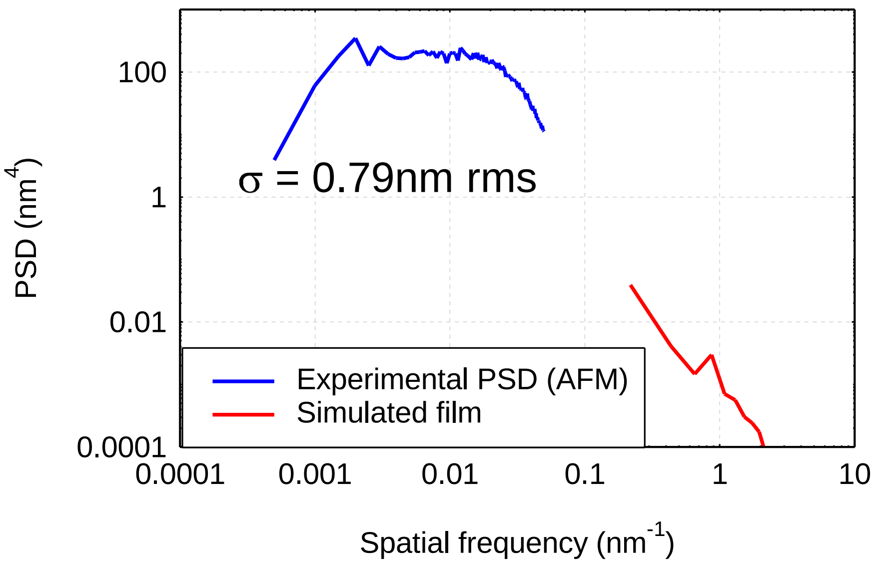
Roughness of simulated film shows very preliminary resemblance to experimental results

PSDs of experimental and simulated films:

P = 1mTorr



P = 10mTorr

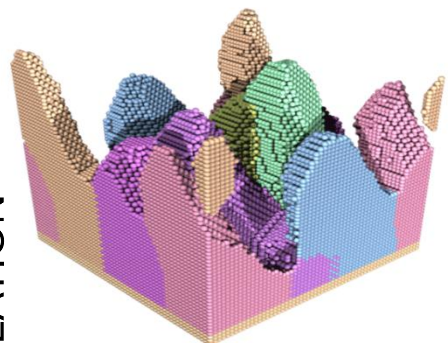


Experimental results by Regina Soufli (LLNL)

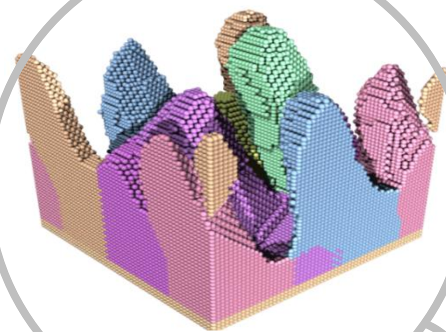
Application to Be films: Increased Ar bombardment (for example from bias) causes decreased roughness

Simulated sputtered Be films, about 20nm thick, with varying energy of bombarding Ar:

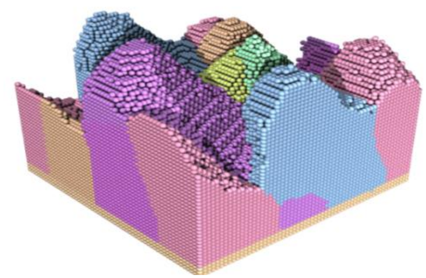
SIMULATION



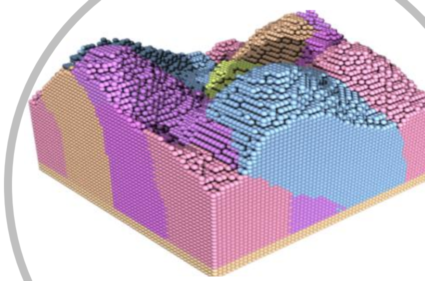
E_{Ar+} = 2.5eV



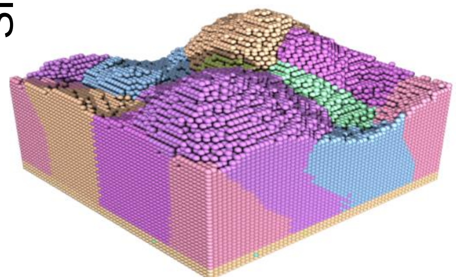
E_{Ar+} =10eV



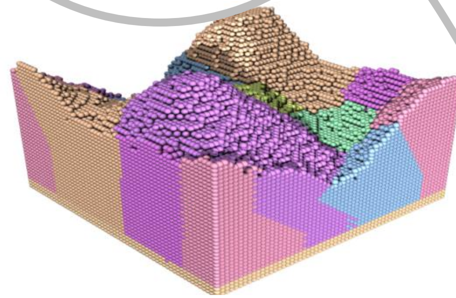
E_{Ar+} = 20eV



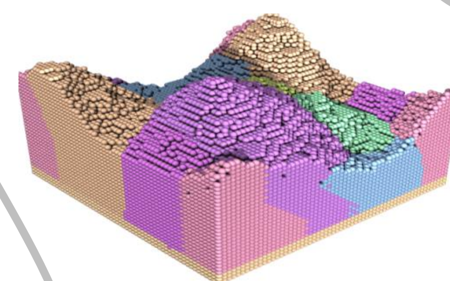
E_{Ar+} = 30eV



E_{Ar+} = 40eV



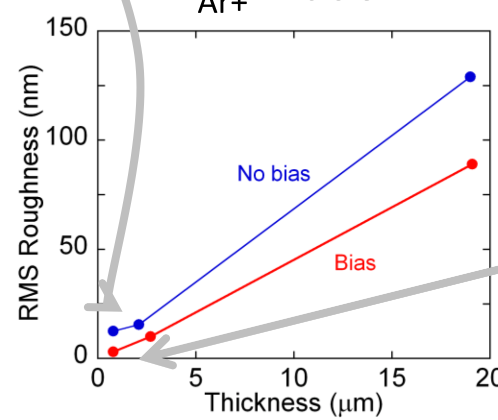
E_{Ar+} =50eV



E_{Ar+} = 60eV

EXPERIMENT

Experimental roughness shows roughness cut about 3X by -80V substrate bias. Corresponding simulated cases also show big reduction (not yet quantified!)

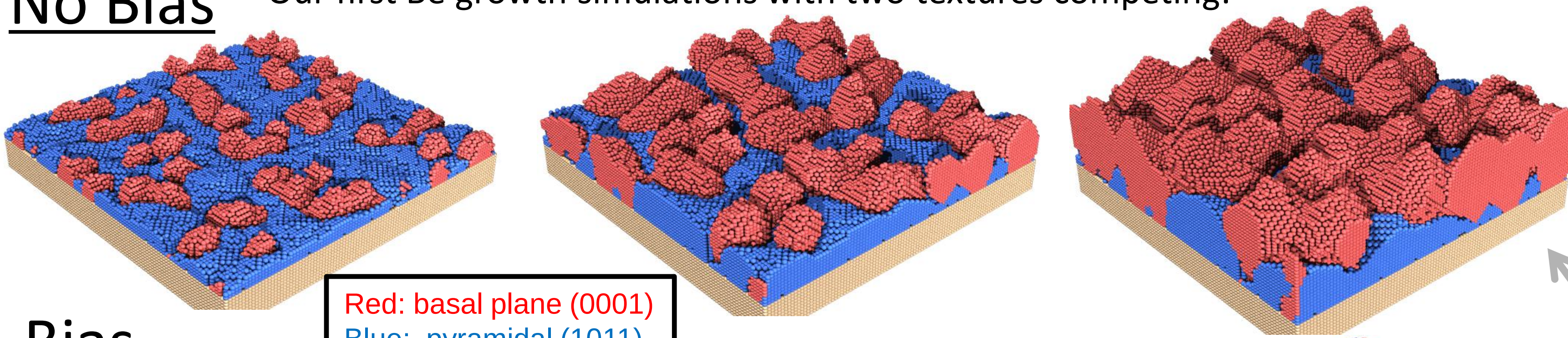


Application to Be films: Simulations show bias favoring (101) film texture, consistent with experiment

SIMULATION

No Bias

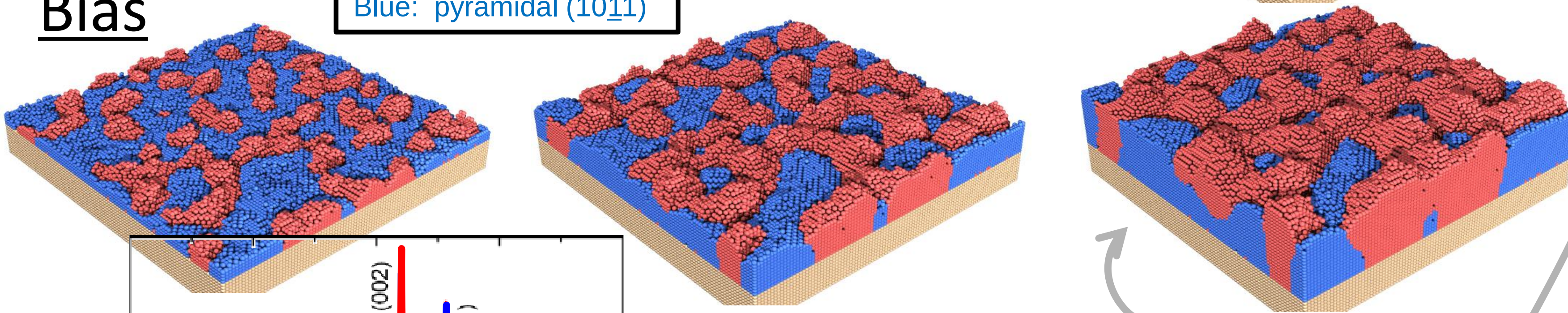
Our first Be growth simulations with two textures competing:



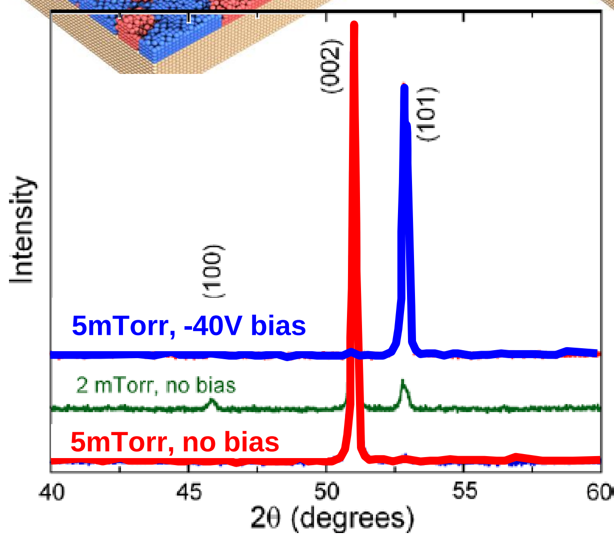
Red: basal plane (0001)
Blue: pyramidal $(10\bar{1}1)$

SIMULATION

Bias



EXPERIMENT



With bias: Closer texture competition

Without bias: Basal plane texture beginning to dominate early

☞Bias pushes texture competition toward $(10\bar{1}1)$, consistent with experiment.

We are beginning to study stress-producing mechanisms directly using these tools. First mechanism is compressive stress from Ar implantation:

Simulation:

-40V substrate bias

⇒ Ar+ ions hit substrate at 30eV

(from plasma simulations)

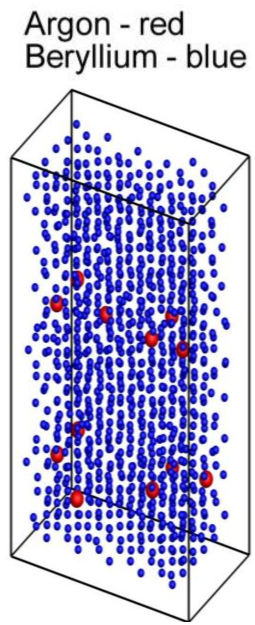
30eV ion energy ⇒ 0.5at% Ar in the film

(from MD implantation studies)

0.5 at% Ar ⇒ 200MPa stress change

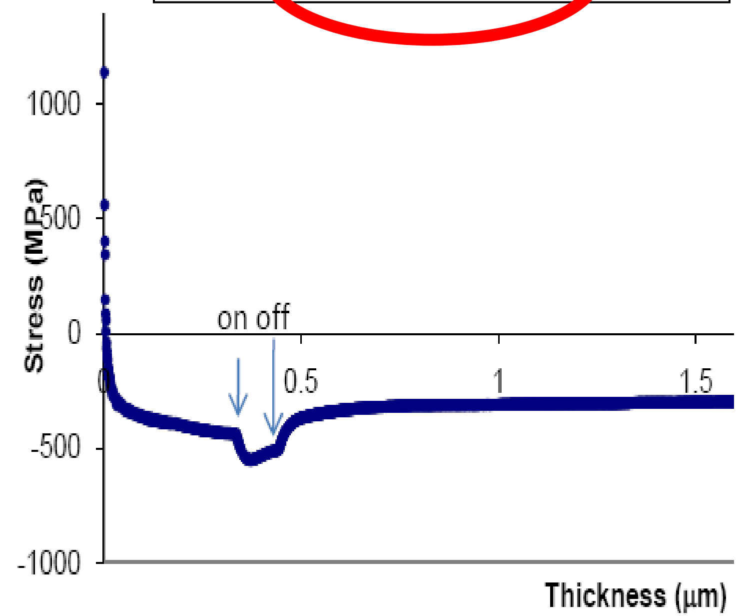
(from MD stress tests)

Method: implant Ar into Be crystal in MD simulation; extract stress in lattice:



Experiment:

Toggling -40V bias changes stress about 150MPa



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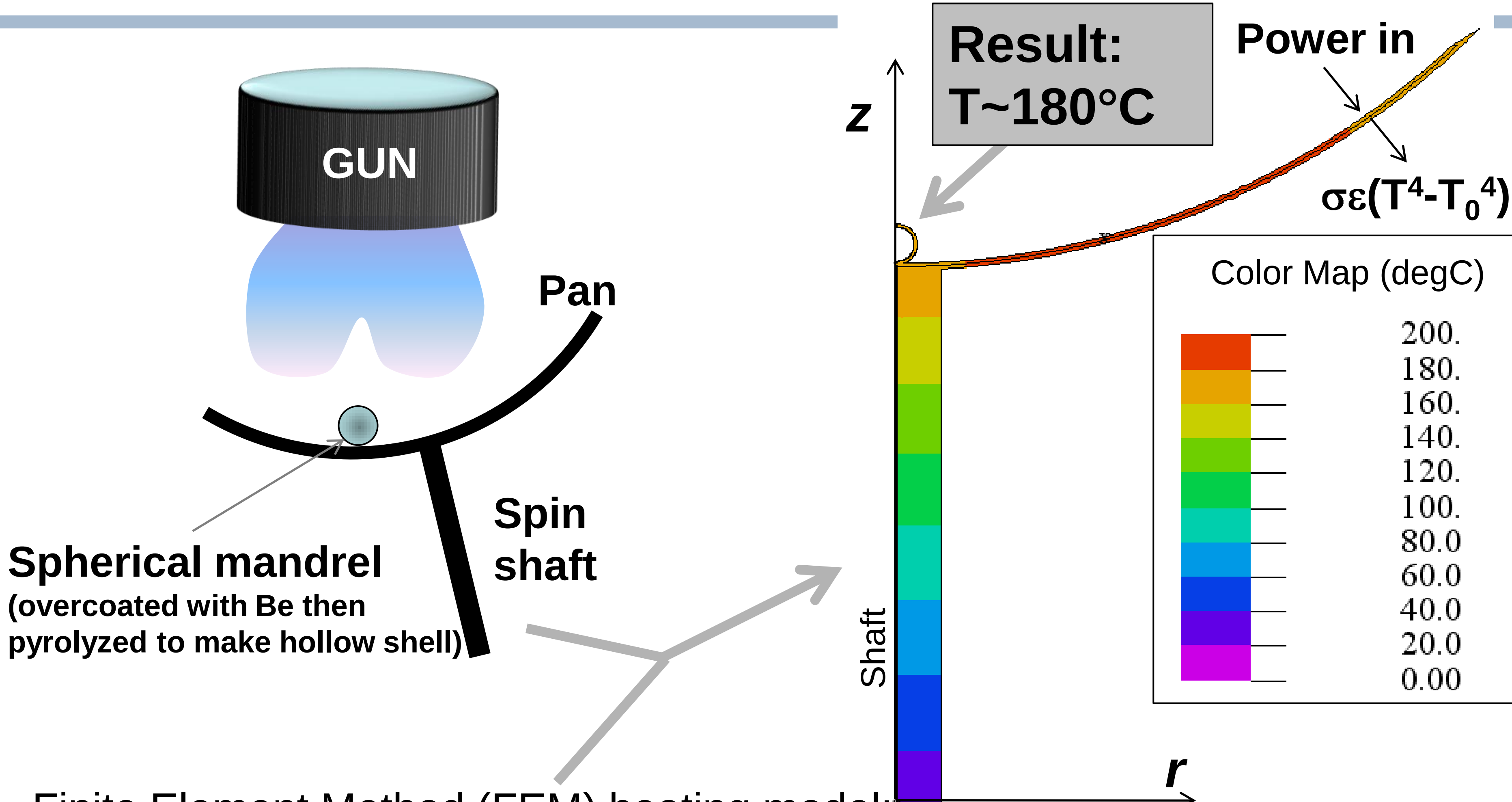
All the calculated energies can be input to a thermal model of substrate and fixturing



Finite Element Method (FEM) heating model:

1) Use 2D (r,z) coordinates
2) Conduction down shaft + radiant heat transfer only
3) Power in= $\Delta H_{condens\text{-}Be} + KE_{Be} + KE_{reflected\text{-}Ar} \approx 50+70+350 \approx$ 470W/m^2

Going parallel: we expect to have new plasma code (3D and parallel) online this summer

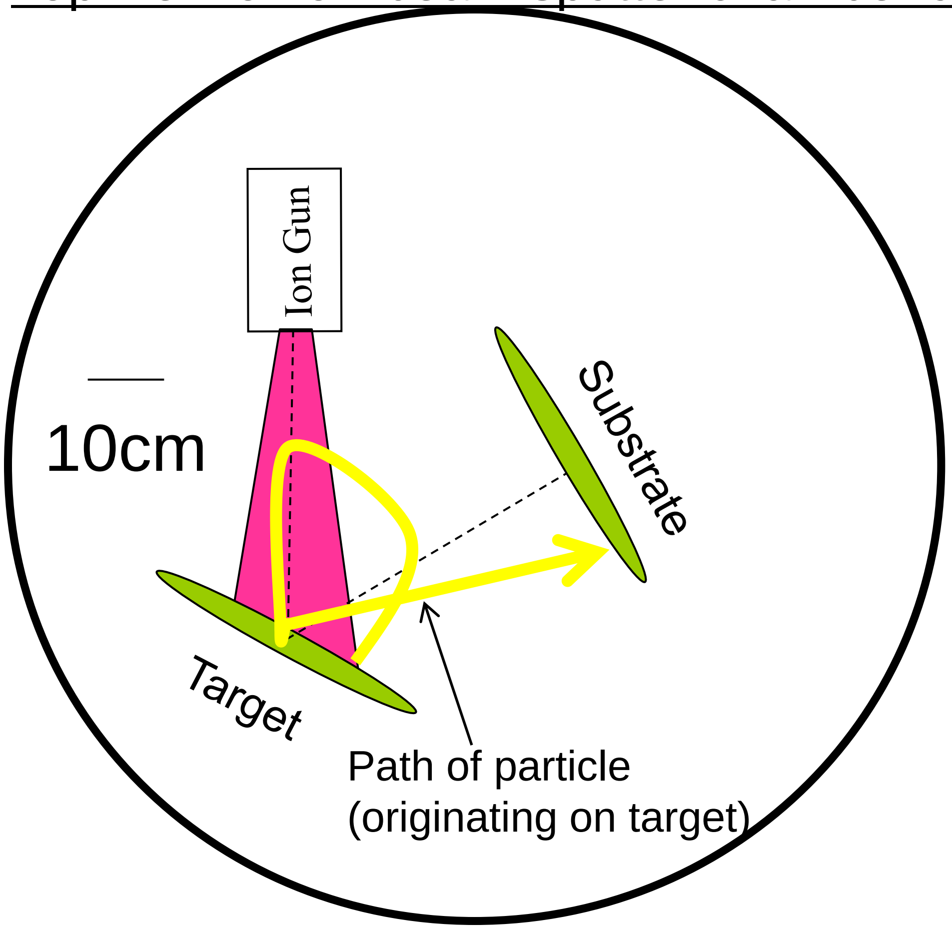
VORPAL code (Tech-X Corp., Boulder, CO)

Summer student Venkattraman Ayyaswamy to work on VORPAL magnetron:

1) Validate against experiments used to validate 2D model
2) Examine 2D/3D agreement
3) Examine effects of target wear (in experiments voltage changes 20% as target wears, and critical [Ar] in the film drops 2X – why?)

Side topic in EUVL: Plasma modeling could be used strengthen previous model used in EUVL: particle transport in ion-beam sputter chamber

Top view of ion-beam sputter chamber used for LLNL mask blanks work:



Model was developed for particle transport:

- Forces on particle: ion drag in beam, gravity, bounce from walls, electrostatic force
- Conducted experiments to verify mechanisms
- Evidence found in experiments that electrostatic forces dominant for small particles
- Electrostatic force in model derived from Langmuir probe measurements on Albany Veeco tool, but results never satisfactory
- >>> could now improve this using PIC plasma model for charging and local electrostatic force

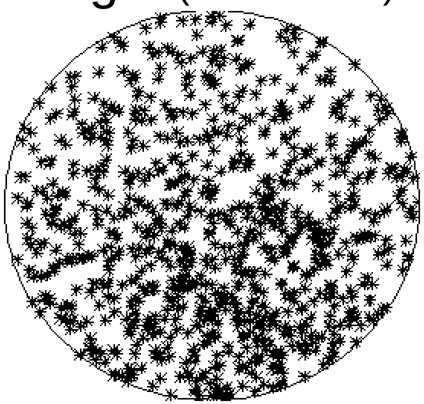
Walton, C.C., Kearney, P.A., Folta, J.A., Sweeney, D.L., Mirkarimi P.B. *Understanding particle defect transport in an ultra-clean sputter coating process.* Proceedings of SPIE - the International Society for Optical Engineering, 2003. **5037**: p. 470.

Side topic in EUVL: the particle transport model reproduced general trend of density of particles deposited in different locations

<u>Maps of particles collected on witness wafers at 3 locations in chamber:</u>

Simulation:

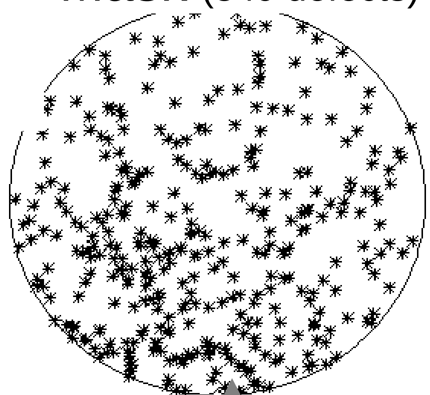
Target (867 defects)



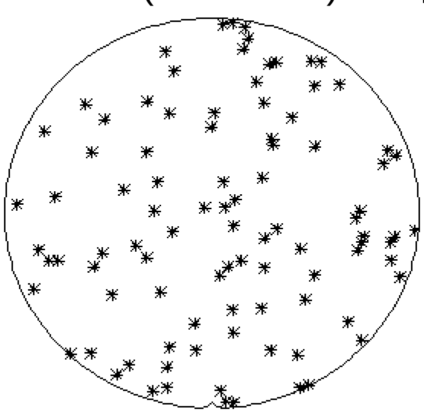
Scenario modeled:

- Particles originate at target
- V_0 = 300m/s,
- Cosine direction distribution

Mask (349 defects)

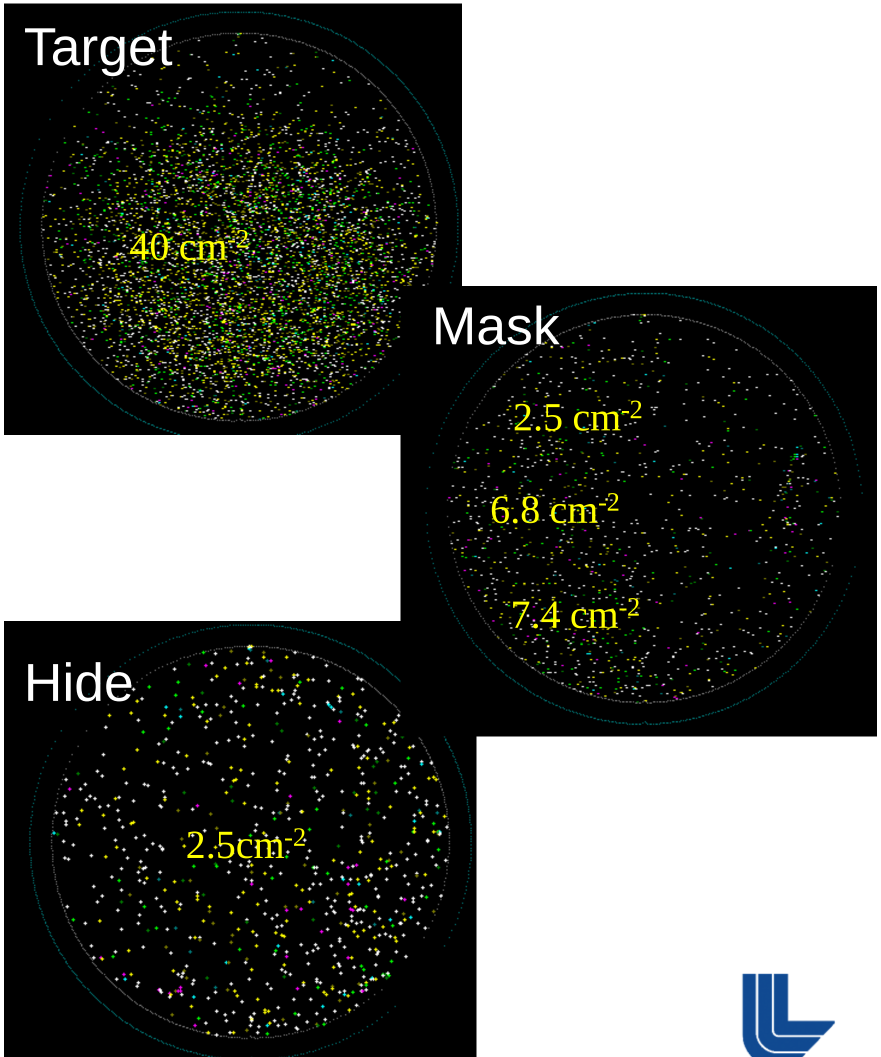


Hide (94 defects)



Model did not have “shadowing” wafer in front: no shadowing expected. Gravity bias reproduced by model.

Experiment:



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Summary

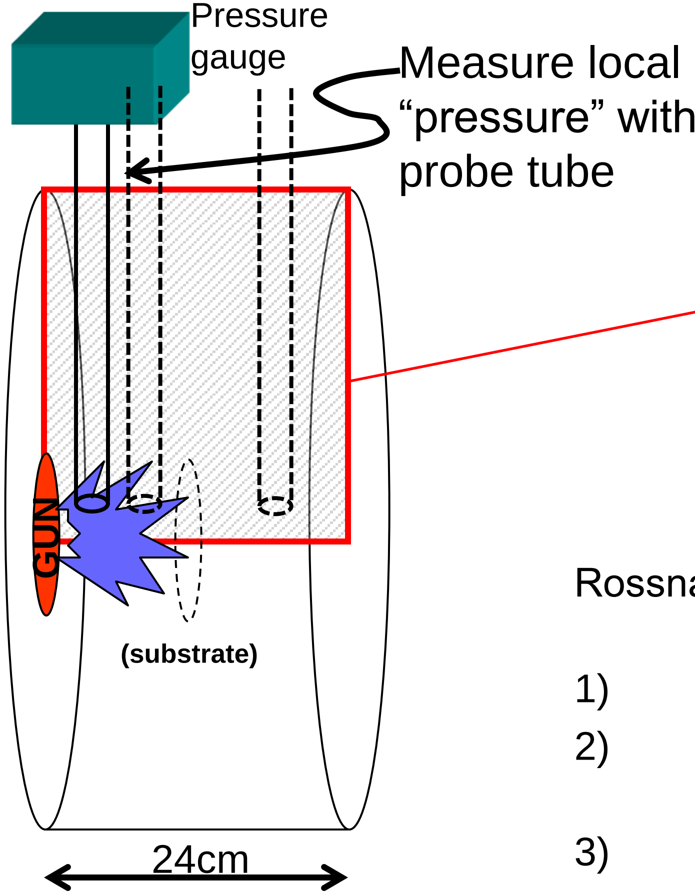
1) We are building a multi-physics simulation of magnetron sputter deposition, breaking down to 4 steps
2) Some validation achieved of each step independently
3) Largest limitation for now is computation speed and model validation for plasma dynamics
4) Now using all 4 parts of simulation together
5) Promising but lots of work still to do!

THANK YOU!

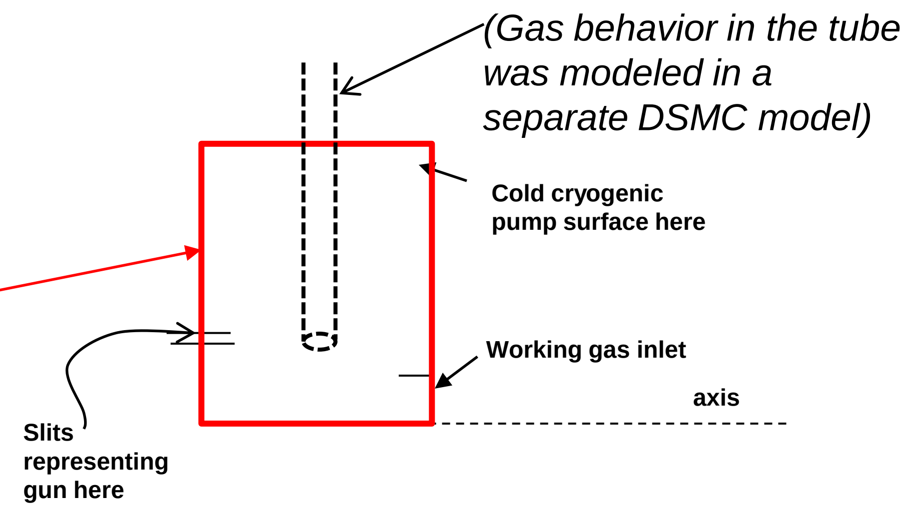
BACKUP SLIDES

Step 3 – Transport - VALIDATION:
We compared DSMC results to published published pressure vs position

Rossnagel[1] coating chamber:



Simulation as 2D axial system



Rossnagel's work includes typical sputter conditions of interest to us:

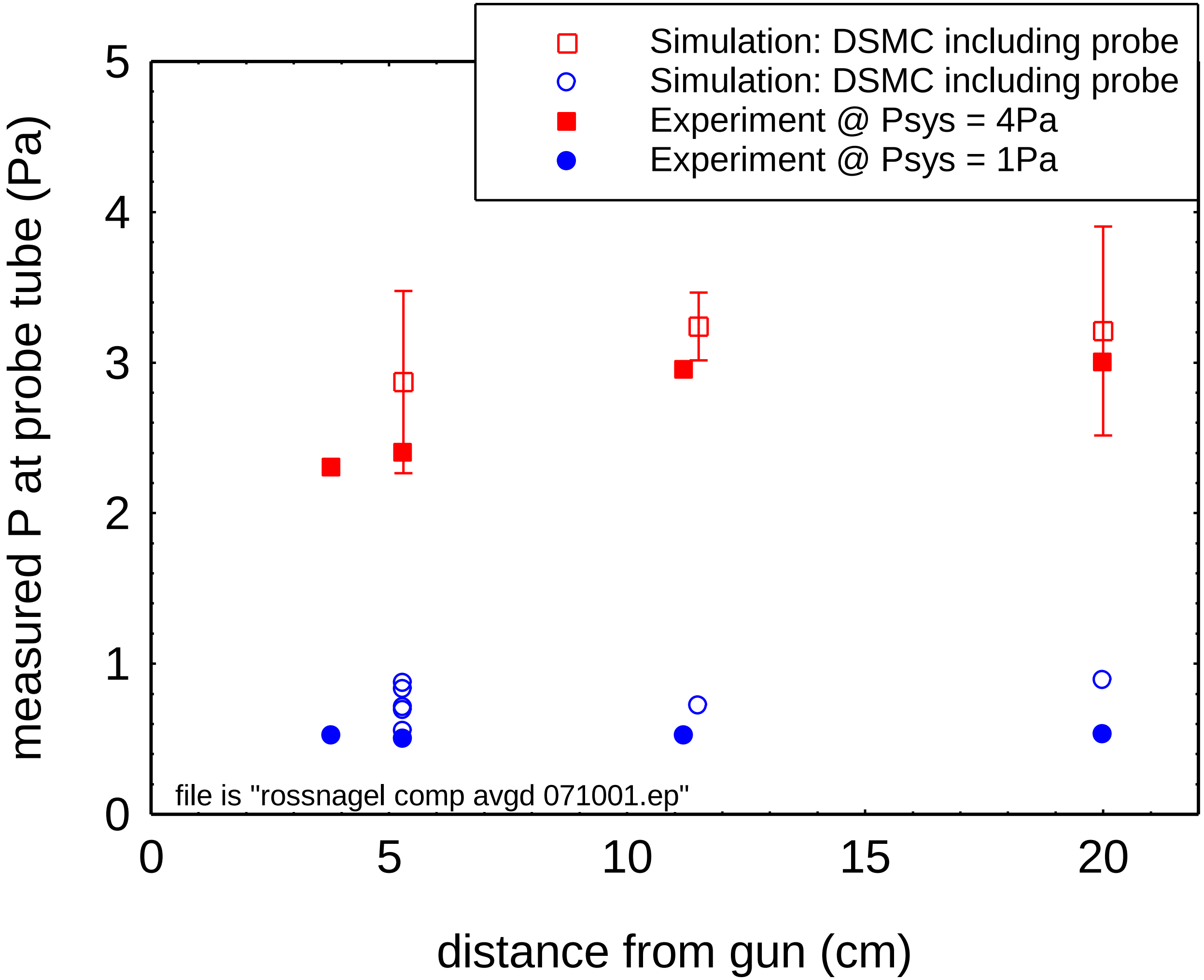
1) Pressure 1-10mTorr
2) DC magnetron deposition at target-substrate distances 10-15cm
3) Sputtering metals with Ar working gas

These results approximate: used Ar^+ energy equal to estimated gun voltage. Gun too large to calculate E_{Ar+} with PIC.

[1]S. M. Rossnagel, Journal of Vacuum Science & Technology A-Vacuum Surfaces & Films 6(1) 19 (1988)

3rd step - transport to substrate – VALIDATION: simulated pressure vs position captures magnitude and trend of experiment, but substantial scatter

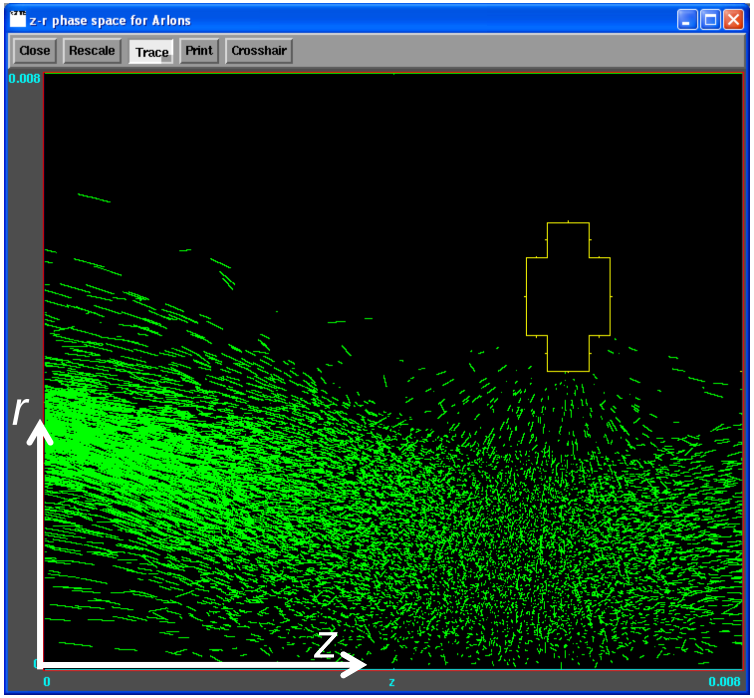
Comparison of simulated local gas pressure to Rossnagel experiment:



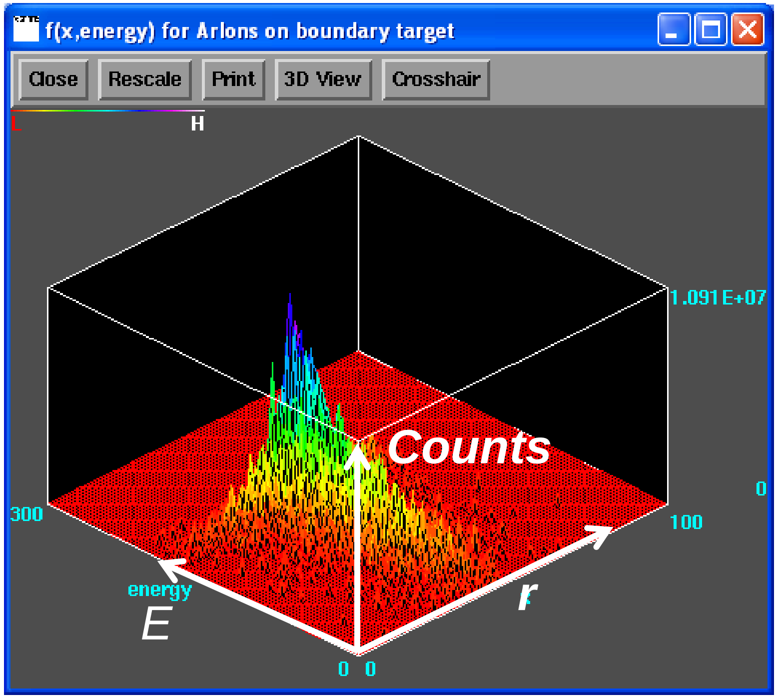
Scatter in simulation results comes from instability in simulated pressure inside the measurement tube – working on whether this is an artifact of radial weighting.

Step 1 (Plasma) RESULTS: we calculated energy and spatial distributions of Ar^+ hitting the target

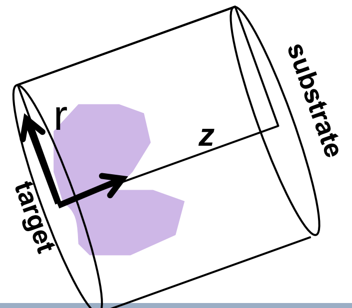
Snapshot of electron paths



Resulting impact distribution at target: N(r, E)



<u>Modeling a circular magnetron:</u>



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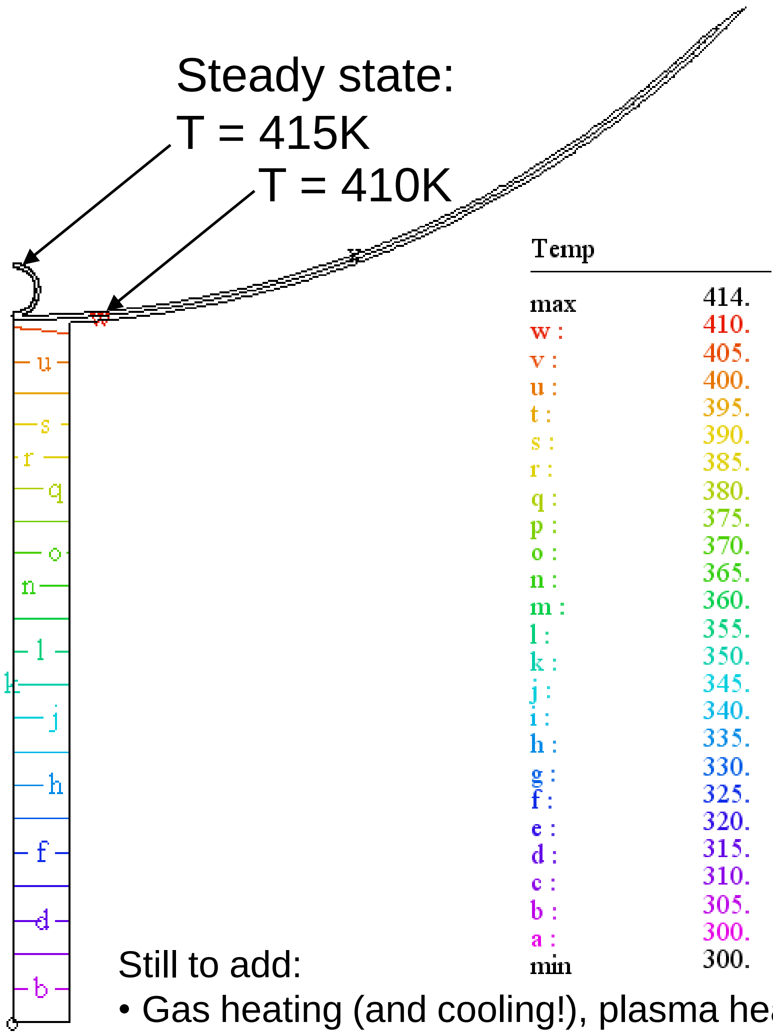
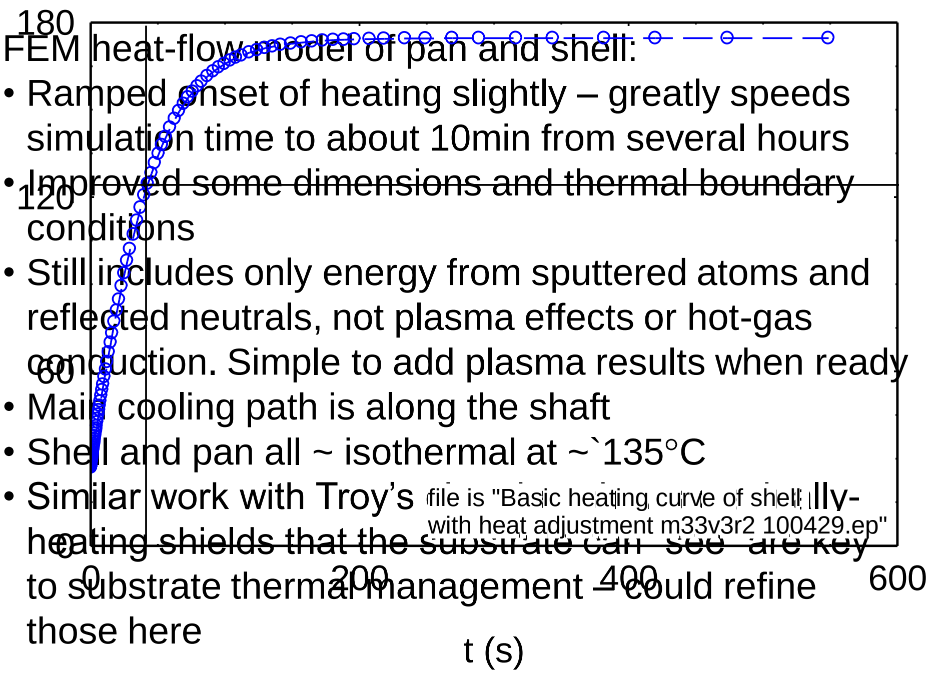
Thermal model of pan improved in geometries and emissivities; results need further examination

Temperature map of 2D axial model, single shell in center of pan:





FEM heat-flow model of pan and shell:

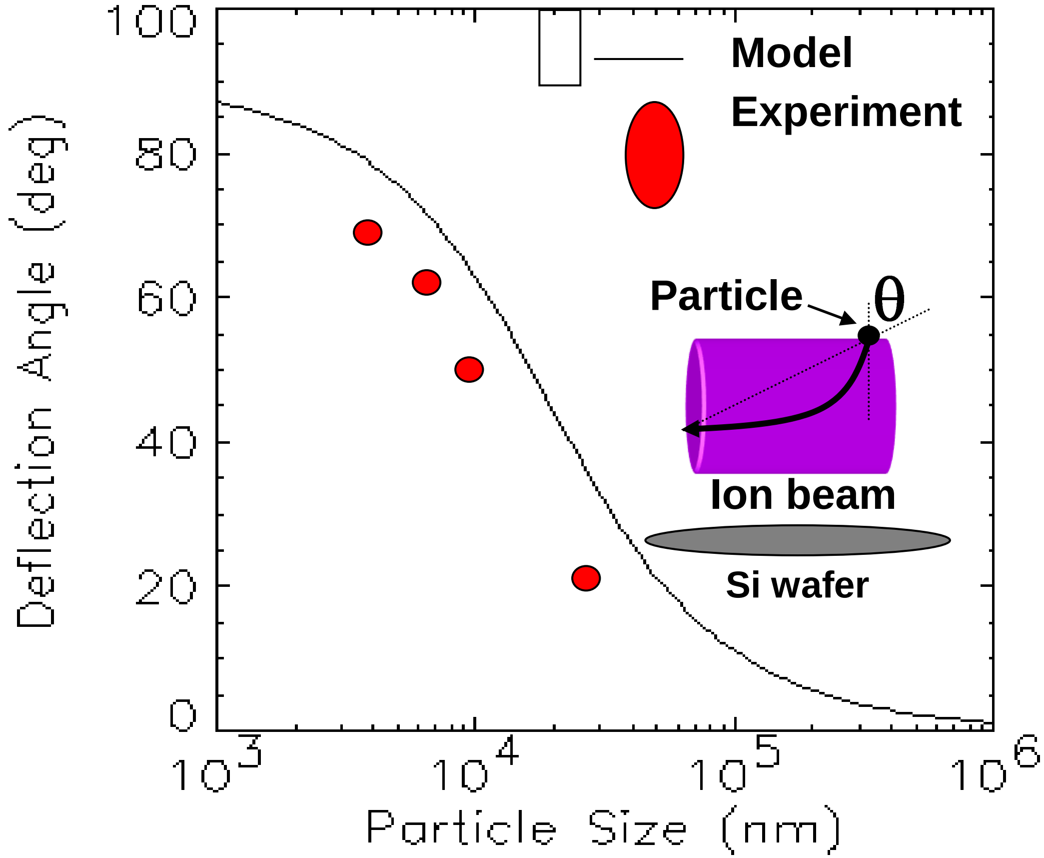
- Ramped onset of heating slightly – greatly speeds simulation time to about 10min from several hours
- Improved some dimensions and thermal boundary conditions
- Still includes only energy from sputtered atoms and reflected neutrals, not plasma effects or hot-gas conduction. Simple to add plasma results when ready
- Main cooling path is along the shaft
- Shell and pan all ~ isothermal at ~`135°C
- Similar work with Troy's [illegible]lly-heating shields that the substrate can "see" are key to substrate thermal management – could refine those here

Discussion: what would be useful results to you from this model?

Still to add:

- Gas heating (and cooling!), plasma heating (ion and electron bombardment)
- Possibly add shield and wall below pan – what is geometry?
- Emissivity of rough Be surface on pan unknown – study sensitivity to this. <u>Interested in any experimental temperatures LLNL or GA has</u>.

Result: clusters of test particles were strongly deflected by the ion beam



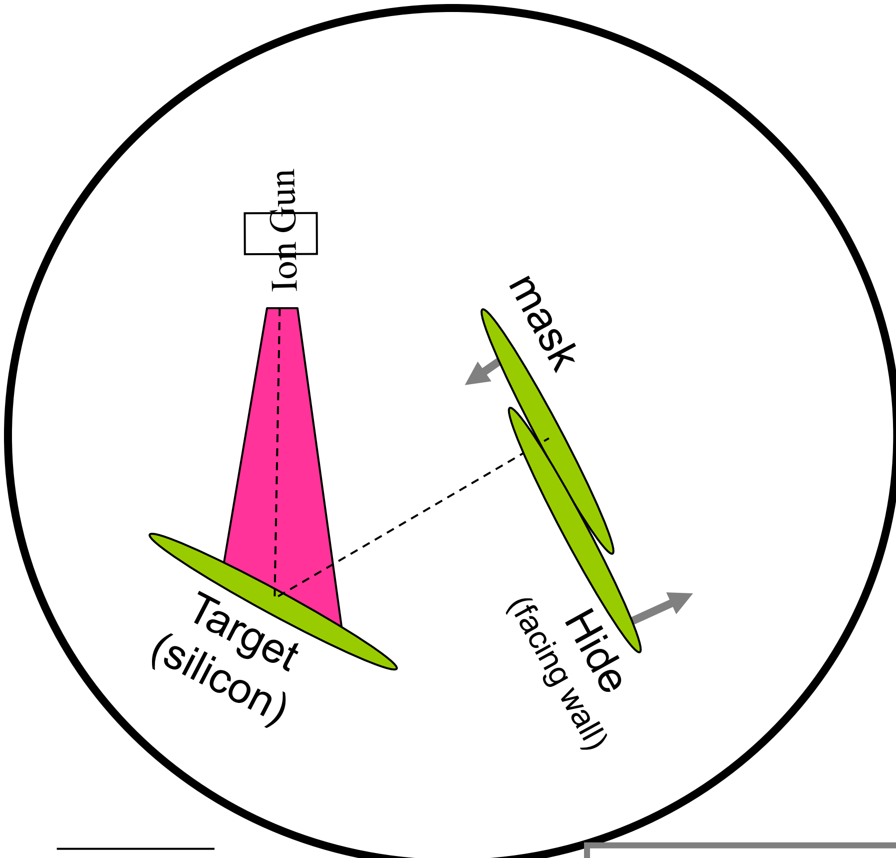
Message:

a) We have some understanding of particle transport by beam

b) Beam can accelerate micron-size particles to 10-30m/s

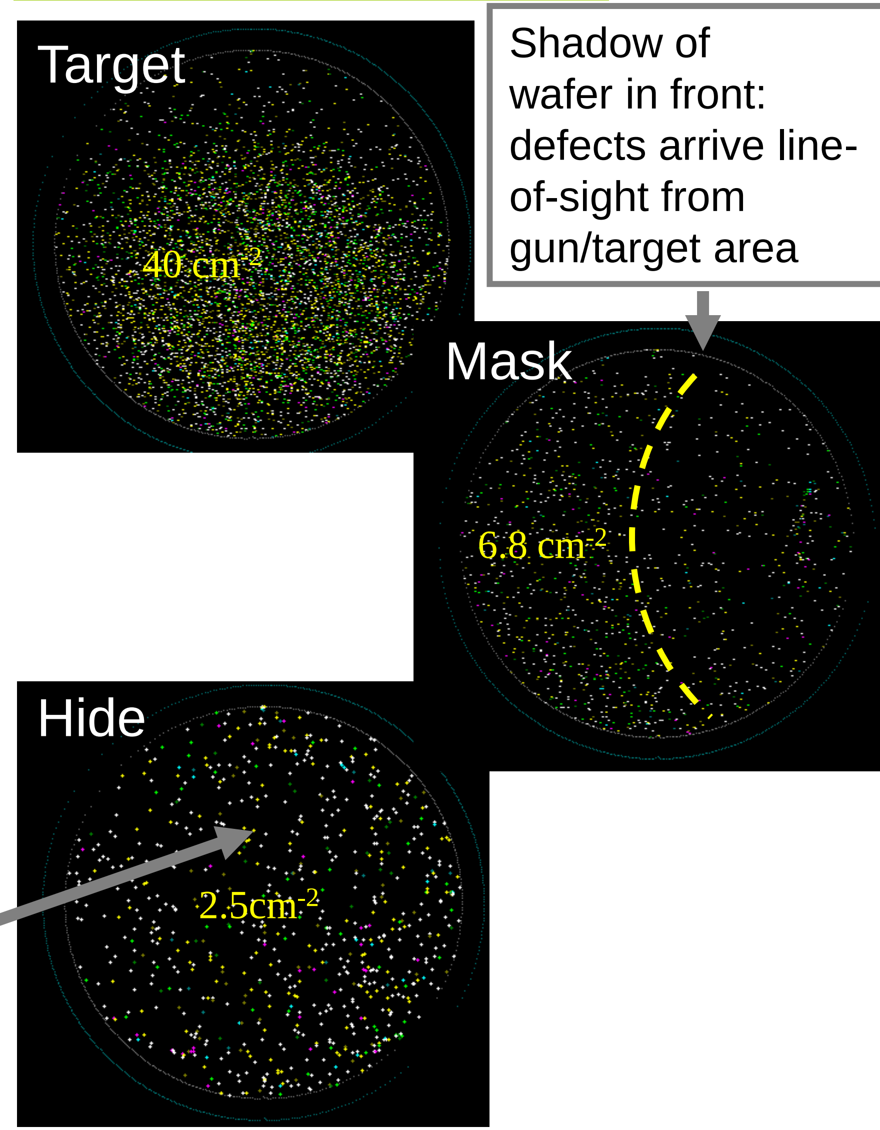
Comparison with experiment #2: spatial distribution of “native” particles over 3 witness wafers

Experiment in test chamber: (top view)



10cm

Defect Maps Resulting:



Shadow of wafer in front: defects arrive line-of-sight from gun/target area

Adders reach back surface: some bounce occurs also

We are working on using microstructure simulations to understand and control film stress

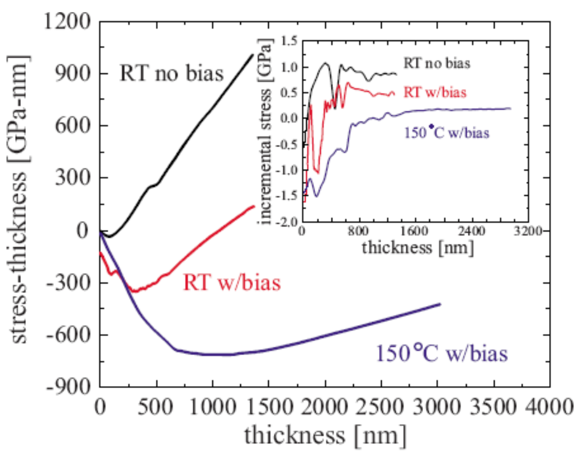
Film stress is generally believed[1] to be a competition between open grain boundaries producing *tension* and packed (or implanted) interstitials causing *compression*.

Approach: study grain boundary width and porosity vs thickness, using the KMC microstructure simulations discussed above. Simulated Be results:

SIMULATION[2]

Prediction: Increasing porosity (total GB area) with thickness implies stress will get **<u>more tensile</u>** with thickness

EXPERIMENT[2]



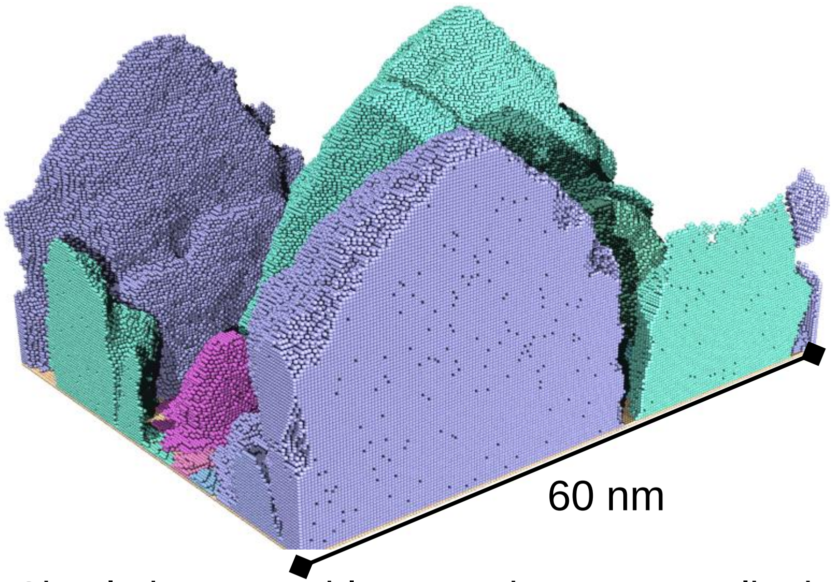
Experimental results: becomes more tensile with thickness under a variety of conditions.

We are working on making this relationship quantitative!

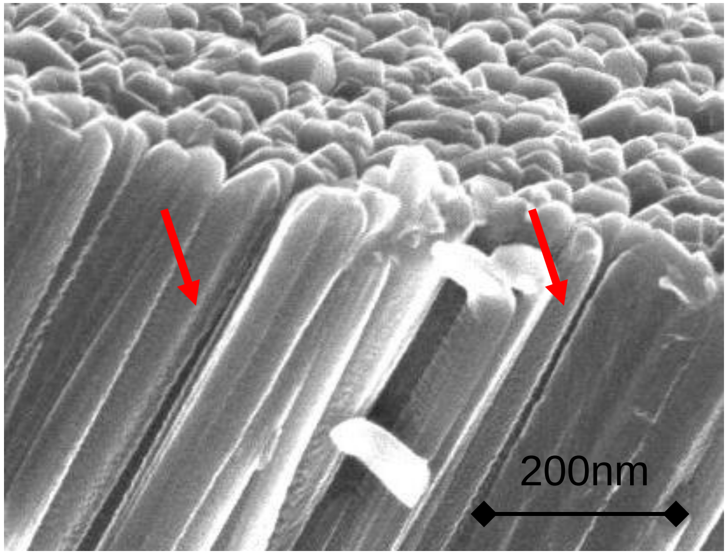
1. Chason, E., et al., *Origin of compressive residual stress in polycrystalline thin films.* Physical Review Letters, 2002. **88**(15): p. 156103/1-4.
2. Zepeda-Ruiz, L.A., et al., *Understanding the relation between stress and surface morphology in sputtered films: Atomistic simulations and experiments - art. no. 151910.* Applied Physics Letters, 2009. **95**(15): p. 51910-51910.

Agreement with of predicted microstructure with experiment is also promising, but not yet satisfactory

<u>Simulation:</u>



<u>Experiment:</u>



SEM photo courtesy
Andy Detor, LLNL

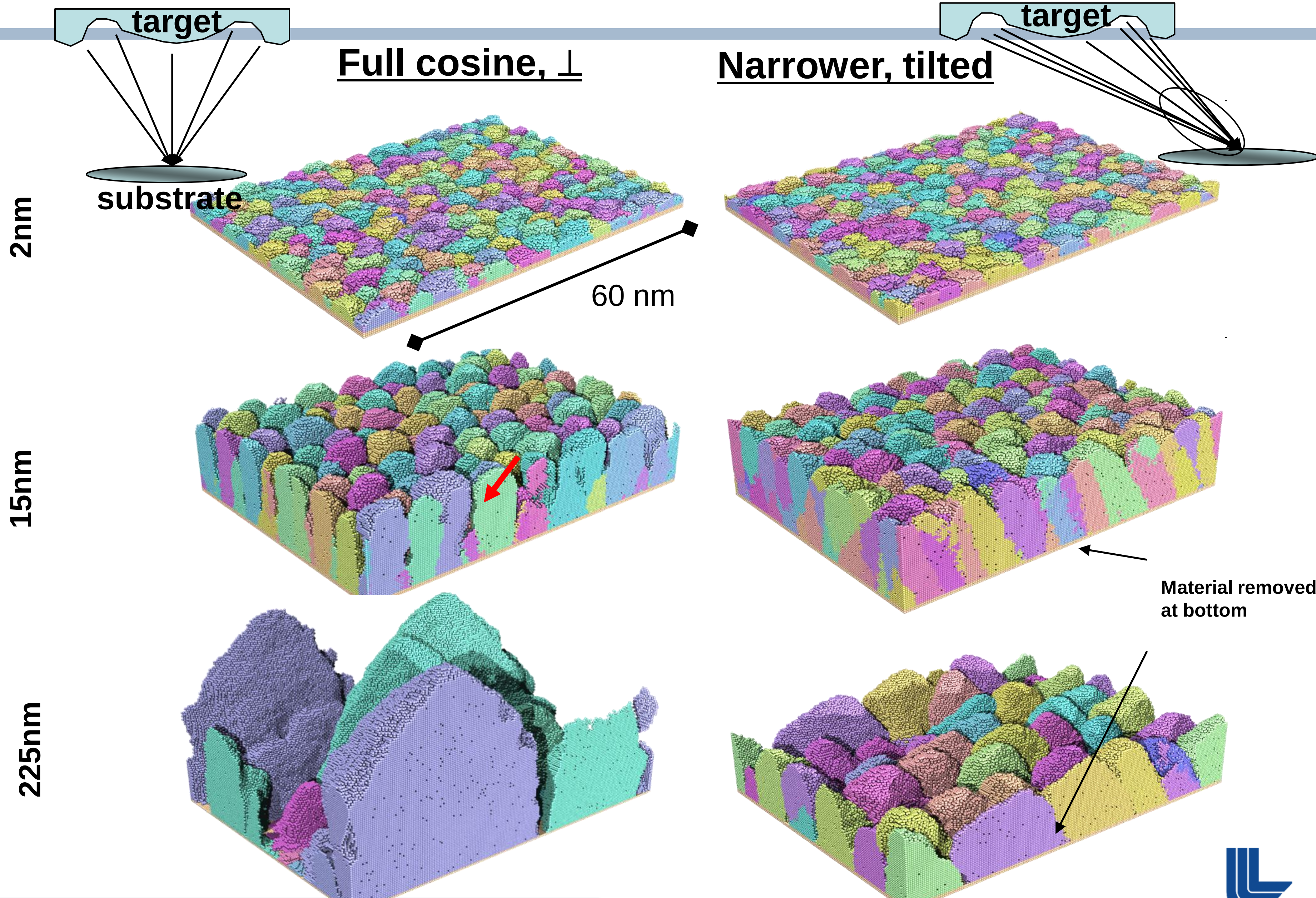
Simulation resembles experiment on qualitative points:

1) Columnar grain film structure, with grain coarsening
2) Tilting of grains with tilting of substrate
3) Separation of grain boundaries after first ~10nm
4) Dome-shaped grain tops

Disagreement with experiment remains on:

1) Asymptotic grain width
2) Onset thickness for grain separation. <u>Separation critical to film stress</u>.

We can simulate polycrystalline films and larger size scales with Kinetic Monte Carlo. Results show grain growth, grooving, and doming.



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