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


1. Leaky shells result from loose or open GB

2. Key requirement for Be shells: must be gas-tight & low-argon!

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

Hollow Be shell 150um thick
Hydrogen ice Layer (D, T)

Target shell, external view

200nm
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

We benchmarked the simulation against published measurements:

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Experiment (Field at al.)

Simulation (0.1X scale)

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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

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)
- **Simulation (MD)**

**Results on He → Cu: simul vs expt.**
- **1.5keV He+ → Cu(110), <211>**
- **Experiment**
- **Simulation**
  - surface
  - sub-surface

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.

**Surface: mean angle vs incoming E, θ**

- **Sputtered Be Mean Angle Contours**
  - Ion Incld. Angle (deg from normal) vs Ion Energy (eV)
  - Example of difference between Ar and Be: mean and σ of angle (for 300eV Ar+ at ⊥ incidence)

  - **50° ± 15° (1σ)**

- **Reflected Ar Mean Angle Contours**
  - Ion Incld. Angle (deg from normal) vs Ion Energy (eV)
  - 15° ± 9° (1σ)
3rd step - transport to substrate – VALIDATION: Simulation reproduces thickness profiles to within ~10%

Studying film thickness profiles vs distance:

![Graph showing normalized thickness or normalized Be flux vs distance (r cm)].

File is "uniformity vs distance.ep"

Map of percent Cu in gas
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 @ $P = 2\text{kW}$
• sputtering Cu in Ar
• $P = 4\text{Pa}$
Steps 1-3 RESULTS: At substrate, target-reflected Ar has more energy than the sputtered Be atoms

Energy distribution $N(E)$

- **Sputtered Be**
  - Mean $E = 4.3\text{eV}$
  - Total Flux = $2.72\times10^{19}\text{ m}^{-2}\text{s}^{-1}$

- **Reflected Ar**
  - Mean $E = 11.0\text{eV}$
  - Total Flux = $7.42\times10^{20}\text{ m}^{-2}\text{s}^{-1}$

Angle distribution $N(\theta)$ (from normal)

- **Sputtered Be**
  - Mean $\theta = 29.2\text{deg}$

- **Reflected Ar**
  - Mean $\theta = 26.4\text{deg}$
Steps 1-3 RESULTS
If substrate is biased negative, Ar⁺ ions hit the substrate at high energy

Energy Distribution of Ar hitting substrate

INTEGRATED FLUXES:
No bias: 7.25e20 m-2s-1
Bias: 9.32e20 m-2s-1
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.

**Stretch goal:** reproduce increase of roughness with pressure. (Not shooting for stress yet!)

For now: Simple approximation

1. Plasma dynamics (PIC)
2. Target impact (MD)
3. Neutrals Transport (DSMC)
4. Film Growth (MD&KMC)
Application to SiC: we obtain angle and energy distributions of all species leaving the target.

**Carbon**
- Angle distribution: Occurrences of $\theta$ vs $\theta$ (degrees)
- Energy distribution: Occurrences of Energy (eV) vs Energy (eV)
- Mean E = 11.2 eV

**Silicon**
- Angle distribution: Occurrences of $\theta$ vs $\theta$ (degrees)
- Energy distribution: Occurrences of Energy (eV) vs Energy (eV)
- Mean E = 0.135 eV

**Argon**
- Angle distribution: Occurrences of $\theta$ vs $\theta$ (degrees)
- Energy distribution: Occurrences of Energy (eV) vs Energy (eV)
- Mean E = 0.135 eV
- 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

Energy (eV)

Occurrences of E

Mean E = 11.1eV

Mean E = 8.7eV

Energy distribution

Occurrences of E

Angle distribution

Occurrences of θ

Energy (eV)

Occurrences of θ

Occurrences of θ (degrees)
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:

Orange: Si
Silver: C

Images and PSDs produced by TOPO code (D. L. Windt)
Roughness of simulated film shows very preliminary resemblance to experimental results

PSDs of experimental and simulated films:

$P = 1\text{mTorr}$

$P = 10\text{mTorr}$

Experimental results by Regina Soufli (LLNL)
Application to Be films: Increased Ar bombardment (for example from bias) causes decreased roughness

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

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

- $E_{Ar^+} = 2.5\text{eV}$
- $E_{Ar^+} = 10\text{eV}$
- $E_{Ar^+} = 20\text{eV}$
- $E_{Ar^+} = 30\text{eV}$
- $E_{Ar^+} = 40\text{eV}$
- $E_{Ar^+} = 50\text{eV}$
- $E_{Ar^+} = 60\text{eV}$

**RMS Roughness vs Thickness**

- **No bias**
- **Bias**
Application to Be films: Simulations show bias favoring (101) film texture, consistent with experiment.

**No Bias**

Our first Be growth simulations with two textures competing:

- Red: basal plane (0001)
- Blue: pyramidal (1011)

**Bias**

- 5mTorr, -40V bias
- 5mTorr, no bias
- 2 mTorr, no bias

**Without bias:** Basal plane texture beginning to dominate early.

**With bias:** Closer texture competition.

▸ Bias pushes texture competition toward (1011), 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 ⇒ 0.5 at% Ar in the film
(from MD implantation studies)

0.5 at% Ar ⇒ 200MPa stress change
(from MD stress tests)

Experiment:

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

Toggling -40V bias changes stress about 150MPa
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 = \( \Delta H_{\text{condens-Be}} + KE_{\text{Be}} + KE_{\text{reflected-Ar}} \approx 50 + 70 + 350 \approx 470 \text{W/m}^2 \)
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

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

Maps of particles collected on witness wafers at 3 locations in chamber:

**Simulation:**
- **Target** (867 defects)
- **Mask** (349 defects)
- **Hide** (94 defects)

**Experiment:**
- **Target**
- **Mask**
- **Hide**

Scenario modeled:
- Particles originate at target
- \( V_0 = 300 \text{ m/s} \)
- Cosine direction distribution

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

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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 \(E_{\text{Ar}^+}\) with PIC.

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: $N(r, E)$

Modeling a circular magnetron:
Temperature map of 2D axial model, single shell in center of pan:

Steady state:
\[ T = 415K \quad T = 410K \]

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 ~\( 135^\circ C \)
- Similar work with Troy’s 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. Interested in any experimental temperatures LLNL or GA has.
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)

Defect Maps Resulting:

Target

- 40 cm²

Mask

- 6.8 cm²

Hide

- 2.5 cm²

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:

**Prediction:** Increasing porosity (total GB area) with thickness implies stress will get more tensile with thickness.

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

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We are working on making this relationship quantitative!
Agreement with of predicted microstructure with experiment is also promising, but not yet satisfactory

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

<table>
<thead>
<tr>
<th>2nm</th>
<th>60 nm</th>
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<tbody>
<tr>
<td>Full cosine, ⊥</td>
<td>Narrower, tilted</td>
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