Modification of the Ion Angular Distribution in Plasma Sheath Modeling Approach under COMSOL Multiphysic

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Outline:

- Technological opportunity – IADF control
- Finding the approach
- What we need for feasibility study
- What we want to get from feasibility study
- Concept of prototype
- Model components
- Implementation within computational domain
- Results
- Next strategy
How is IADF generated?

- In existing technology the profile of the IADF is given by pressure, wafer bias and single or dual frequency choice.

- Isotropic IADF in plasma
  - Bulk plasma: \( W_{ion}^{random} \approx 0.05-0.1 \text{ eV} \)
  - Presheath: \( W_{ion}^{presheath} \approx \frac{T_e}{2} \approx \text{several eV} \)

- Sheath
  - Typical ion angular distribution observed in experiments

- \( E_{sheath} \)

- Anisotropic IADF
  - \( W_{ion}^{sheath} \approx 10\text{s}-100\text{s eV} \)

Technological opportunity – IADF control
semiconductor technology

➔ etch profile modification (in-situ)
➔ CD control & variation
➔ deposition conformality (sidewall coverage)
➔ plasma immersion ion implantation

➔ it is applicable for core plasma technology
Technological opportunity – IADF control
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- etch profile modification (in-situ)
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- it is applicable for core plasma technology
- Surface structuring w/o need of the pattern transfer (nanotechnology, ..., self-assembling, ..., MEMS, ...) – avoiding additional technological steps such as litho, resist, ...
- Creating conditions and impact on the film growth and its structure
- Surface roughness tailoring
- Tailoring film properties in PVD, ...

- it is applicable for new technology
Technological opportunity – IADF control

- Nanotubes (NT) growth in low temperature plasma
- NT alignment is perfectly the same as that of electric field in sheath\(^1\)
- The ion fluxes that are most responsive to the E-fields. Applying an external DC electric field parallel to the substrate surface – carbon NT can be bent in sharp predetermined angles = L-shaped NTs\(^2\)

\[^{1}\text{k. Ostrikov and S. Xu, Plasma-Aided Nanofabrication, Wiley-VCH Verlag GmbH & Co., KGaA, Weinheim (2007)}\]

Growing nanowires horizontally yields nano-LEDs

Source: image by NIST, OptoIQ, Sep 29, 2010

Technological opportunity – IADF control

- Nanotubes (NT) growth in low temperature plasma
  - NT alignment is perfectly the same as that of electric field in sheath\(^1\)
- Surface bombardment – impact on fragmentation & nanostructurization of catalyst layers that are widely used to synthesize carbon NT
  - The ion fluxes that are most responsive to the E-fields. Applying an external DC electric field parallel to the substrate surface – carbon NT can be bent in sharp predetermined angles = L-shaped NTs\(^2\)

Field emission scanning electron microscopy of carbon structures grown at different DC biases

DC variation has impact (A) on local T, and (B) even a modest change in the substrate bias (~50-100 V) results in in structural transformation (at unheated surfaces)\(^3\)

\[ V_b = \{0V, -60V, -100V, -200V, -300V, -400V\} \]

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Diversification of conditions on the single wafer and instant processing

• DC variation visualization of the parametrized growth on the single wafer

This is as an idea example only from previous slide…[4]
Technological opportunity – IADF control

- Polystyrene spheres used as a sort of scaffolding to create 3D nanostructures of semiconducting zinc oxide on various substrates\[^5\]

- The principle: spheres a few micrometers in diameter are placed on an electrically conducting surface where they orient themselves in regular patterns

- Exploitation: electronic and optoelectronic devices, solar cells, short wave lasers, LEDs and FEDs

- Excellent light scattering properties

- Use of ion-milling to control clustering of nanostructured, columnar thin films

- Nanostructured AlN\[^6\] is attractive for the future nanodevice applications – it is possible to direct the growth process by DC toward quasi-3D columnar structures. Similar case – vertically aligned gallium-zinc oxide nanorods\[^7\]

- From continuous to nanostructured columnar plasma polymer\[^8\] Deposition by sequential sputtering of Ti and polypropylene in Ar/hexane mixture at a glancing angles

\[^5\] Ref. in Advanced Materials by Jamil Elias and Laetitia Philippe of Empa’s Mechanics of Materials and Nanostructures Laboratory in Thun, Switzerland, Aug. 2, 2010
Technological opportunity – IADF control
numerical simulations suggested

- Selective manipulation of ions fluxes can be instrumental in maintaining a steady growth with a predetermined shape\(^9\), reshaping of caved cylindrical nanorods into conical spike-like microemitter structures\(^{10}\), etc.

**Properties to be influenced:**
- Alignment
- Spacing
- Ordering
- Composition

- Stoichiometry
- Crystallinity
- Size
- Shape

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• Ion fluxes have potential to have impact on the various shapes and structures\(^{11}\)

Properties to be influenced:
- Alignment
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- Ordering
- Composition
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- Crystallinity
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- from “0 dimensionality” (ultrasmall quantum dots, …)
- “1D” (high-aspect-ratio nanowires or nanotube-like structures, …)
- “2D” (nano-wall-like structures, nanowells, …)
- up to “3D” (nanoparticles, nanopyramides, nanocones, nanorods, …)

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Application opportunity for post-processing, coating with nanofilms, functionalization, or doping, …

Finding the approach

- **EEDF**
  - EEDF controls the spatial plasma distribution (uniformity), aimed RF power dissipation into plasma and chemistry

- **IEDF**
  - IEDF controls the quantitative and qualitative process performance (processing rates, etch or deposition profile, selectivity, damage, etc.)

- **IADF**
  - IADF is apparently uncontrollable factor (consequence of used pressure and bias, e.g. IEDF)

• How can one control the EEDF, IEDF and IADF in the plasma?

  - Reactor design, plasma source design, …
  - Bias power design, frequency, …
  - Any independent control knob?, …

• Can one design these distribution functions? “design at the kinetic level”
Concept: Modification of the IADF

Collimated beam and inclination of the rotating wafer will produce specific IADF.

Generate this specific IADF w/o motion and provide its control and variation.
Concept

Conductive grid structure embedded into a substrate holder

Generation of the E-field parallel to the wafer surface

• Application of ac voltage to grid conductors (cross-section shown is in the y-direction, analogically done in x-direction)
Concept application for plasma based technology\textsuperscript{[12]}

- Resulting effect will depend on the plasma and wafer bias
- Point where E-field is focused is moving on wafer surface in particular pattern

Conductors are superimposed one over another – creating rectangular grid

Example of electrical scheme to bias grid structure

\[ V^{2k-1} = V_0 \sin(\omega t) \]

\[ V^{2k} = V_0 \sin(\omega t + \pi) \]
Multiple options to control ion trajectories

Controlling parameters

- Grid electric field:
- Phase $\Delta \varphi_{xy}$ of wires
- Amplitudes
  - $V_x$ and $V_y$ in x and y directions, respectively and/or their ratio
- Frequency
  - $f_x$ and $f_y$ and/or their ratio
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We used Lieberman's formulation for collisionless DC sheath [14].

- Maxwellian electrons at temperature
- Cold ions in bulk domain
- Quasi-neutrality in bulk plasma
- Quasi-neutrality in presheath
- Boltzmann relation for electrons in sheath
- Ion energy conservation

Sheath model (1D)

\[
\begin{align*}
n_e &= n_i \\
\Phi_p &= 0 \quad x = 0
\end{align*}
\]

\[\Phi(0) = 0\]
• We used Lieberman’s formulation for collisionless DC sheath\cite{14}
  
  - Maxwellian electrons at temperature $T_e$
  - cold ions in bulk domain $T_i = 0$
  - quasi-neutrality in bulk plasma $n_e = n_i = n$
  - quasi-neutrality in presheath $n_{es} = n_{is} = n_s$
  - Boltzmann relation for electrons in sheath
    
    $$n_e(x) = n_{es} \exp\left(\frac{\Phi(x)}{T_e}\right)$$

  - ion energy conservation
    
    $$n_i(x) = n_{is}\left(1 - \frac{2e\Phi(x)}{m_iu_s^2}\right)^{-1/2}$$

**Extension sheath model into 2D (3D) and BC**

### Poisson equation

\[-\nabla \cdot \varepsilon_r \varepsilon_0 \nabla \Phi = \rho = -e(n_i - n_e)\]

### Plasma-sheath interface conditions

\[
n_i = \begin{cases} 
  n_s & \text{when } 2\eta > 1 \\
  n_s (1 - 2\eta)^{-1/2} & \text{when } 2\eta < 1 
\end{cases}
\]

\[
n_e = \begin{cases} 
  n_s & \text{when } V > 0 \\
  n_s \exp(V/T_e) & \text{when } V < 0 
\end{cases}
\]

\[
\eta = eV/(m_i u_s^2)
\]

- Under GUI in AC/DC module in Comsol we set following conditions:
  - surface boundary conditions (BC) are set to symmetrical at the vertical sidewalls of each sub-domain
  - top surface boundary is set to relative plasma potential \( V_{plasma} = 0 \) V
  - surface boundary at electrode are VDC
  - Surface boundary conditions at grid’s conductors in dependence on tested potential, Vx, Vy
  - Grid potentials were extended into transient
  - Interior boundaries are represented by continuity BC
2D results from sheath simulation\textsuperscript{[a]}
plasma potential @ 20 V, wafer at -100 V

Plasma (+20 V)
sheath
wafer (Si)
insulating (Al\textsubscript{2}O\textsubscript{3}) coating with grid
electrode (-100 V)

+50 V
grid conductors
electric field lines (red contours)

electric potential (blue contours, 25 levels)
(surface color plot)

\textsuperscript{[a]} Simulation by Multiphysics COMSOL
Sequential biasing the groups of the specific conductor lines

Phase I

+50 V 0 -50 V 0 +50 V 0 -50 V 0 +50 V 0

Phase II

-50 V 0 +50 V 0 -50 V 0 +50 V 0 -50 V 0

• In average overall surface of the wafer will be exposed by ions with specific IADF
Grid potential

Ion density in plasma

Ion path in sheath

Potential contours

+200 V to -200 V

-200 V to +200 V

Grid

wafer

Animation object - ionpath200red1.avi
3D grid structures

Slice: Electric potential [V]  Isosurface: ni
Particle Tracing: Electromagnetic force (emes)

+2.5V

-23.5V

Max: 5.708e15  Min: 2.575e15

IADF-01-transient-symmetric-in_phase(red1).avi
Full scale reactor

- Feasibility stage – virtual prototype for specific plasma reactor
- Plasma reactor choice of model
  - In-house sw for specialty modeling,
  - Plasma module of Comsol

- Profile evolution:
  - String model, Cell mode, level set model
IADF determination

- **Analytical model**\(^{[b]}\)
- **Collisionless rf sheath – cold-ion plasma model**
- **Extended collisional rf sheath model**\(^{[a]}\)
- **Monte-Carlo sheath model or hybrid codes**
- **Spatiotemporal sheath electric field**

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Opportunity for collaboration

- Focus: Application driven R&D
- Inside company development (engineering) & partnership with university (computational aspects and experimental evaluation)

Virtual prototype by simulation for design to developed library

Manufacture optimal design

Experimental test & validation

University #1: plasma technology

University #2: nanotubes

University #3: bio-applications

Testing in parallel
Conclusions

• We introduced idea and described concept on control of the IADF

• Sheath model was developed to investigate properties and performance of such device

• More robust scheme of model is proposed to include input data and output performance, more complex geometry and biasing schemes under same modelling platform

• Several emerging applications were indicated where it can be used and given call for collaboration on this subject