Getting more insight into reactive magnetron sputtering by modelling and experiments

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RSD2009

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www.DRAFT.ugent.be

Setting the problem …

Large area coaters use rotating cylindrical magnetron …

What about their behaviour during reactive magnetron sputtering?

Photo provided by W. De Bosschere, Bekaert N.V.

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Setting the problem …

Scaling down for a fundamental study

Downscaling
Rotation speed
Model
Parameters
A first result
Sputter cleaning
Including
deposition
Understanding
the effect
Conclusions
Acknowledgements

Influence of rotating speed

Hysteresis shifts to lower oxygen flow on increasing the rotation speed

Modelling of this effect...a first try

Principle: solving continuity equations of the form

$$\frac{\partial \rho}{\partial t} + \nabla \cdot F = S$$

The vacuum chamber

$$q_b = P \cdot S$$

$$\frac{dP}{dt} = \frac{k_B T}{V} \left[ q_b - (q_r + q_s + q_t) \right]$$

Modelling of this effect … a first try

**Deposition from the target**

\[ F_c = \frac{(1 - \varepsilon) I_{\text{tot}} (Y_c \theta_c + Y_m \theta_m)}{A_s} \]

\[ F_m = \frac{(1 - \varepsilon) I_{\text{tot}} Y_m \theta_m}{A_s} \]

\[ \Delta x = \frac{2F_s \alpha_s (1 - \theta_s)}{z} \]

**Flux to the underlying layer defined by the deposition rate**

\[ d \frac{d n_t}{dx} (1 - \theta_s) = \frac{(1 - \varepsilon) I_{\text{tot}} (Y_c \theta_c + Y_m \theta_m)}{A_s} \]

\[ d \frac{d n_t}{dx} = \frac{(1 - \varepsilon) I_{\text{tot}} (Y_c \theta_c + Y_m \theta_m)}{A_s} \theta_s \]

---

**Target surface**

\[ h_s \theta_m \frac{v_{1/2}^{n_m}}{n_m} \]

\[ h_s \theta_m \frac{v_{1/2}^{n_m}}{n_m} \]

\[ h_s \theta_m \frac{v_{1/2}^{n_m}}{n_m} \]

**Modelling of this effect … a first try**

**Target bulk**

\[ \theta_s \]

**Chemisorption**

\[ \theta_s \]

**Knock on implantation**

\[ \theta_s \]

**Direct ion implantation**

\[ \theta_s \]
Modelling of this effect … a first try

\[ v^{i}_{s}(n_{o} - n^{i}_{m}) \]

\[ v^{i}_{m}n^{i}_{m} \]

\[ v^{i}_{s}(n_{o} - n^{i}_{m}) \]

\[ v^{i}_{m}n^{i}_{m} \]

\[ v^{i}_{s}(n_{o} - n^{i}_{m}) \]

\[ v^{i}_{m}n^{i}_{m} \]

\[ \Delta x \]

Target bulk

Implanted reactive atoms form compound with the target material

\[ v^{i}_{s}n^{i}_{s} - v^{i}_{m}n^{i}_{m} \]

\[ \Delta x \]

The input parameters

Race track is calculated using an electron trajectory code
The input parameters

<table>
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<th>PARAMETER</th>
<th>VALUE</th>
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<tr>
<td>Volume chamber (experimental value)</td>
<td>0.1 m³</td>
</tr>
<tr>
<td>Pumping speed (experimental value)</td>
<td>111 L/s</td>
</tr>
<tr>
<td>Discharge current (experimental value)</td>
<td>0.4 A</td>
</tr>
<tr>
<td>Sputter yield metal (measured value)</td>
<td>0.65</td>
</tr>
<tr>
<td>Sputter yield oxide (measured value)</td>
<td>0.05</td>
</tr>
<tr>
<td>Knock-on yield (SRIM calculation)</td>
<td>0.22</td>
</tr>
<tr>
<td>Projected range of ions (SRIM calculation)</td>
<td>1.5 nm</td>
</tr>
<tr>
<td>Ion straggle (SRIM calculation)</td>
<td>0.7 nm</td>
</tr>
<tr>
<td>Incorporation coefficient (measured value)</td>
<td>0.13</td>
</tr>
<tr>
<td>Sticking coefficient on the target (fitting parameter)</td>
<td>0.01</td>
</tr>
<tr>
<td>Reaction rate constant (fitting parameter)</td>
<td>4x10⁻²³ cm³s⁻¹</td>
</tr>
<tr>
<td>Substrate area (fitting parameter)</td>
<td>1000 cm²</td>
</tr>
<tr>
<td>Oxygen gas flow (variable)</td>
<td>0-3 sccm</td>
</tr>
</tbody>
</table>


Simulation result

WRONG: gradual change but experimental abrupt effect
WRONG: minor effect of the rotation speed

poisoned mode
metallic mode
More experiments …

Sputtering a stationary target, and then sputter cleaning in pure argon while rotating

Metallic mode

Start sputtering cleaning

X.Y. Li, D. Depla, W.P. Leroy, J. Haemers, R. De Gryse
More experiments … interpretation

Stationary track

Position 1
Position 2

Position 3
Position 4

In poisoned mode: faster sputter cleaning than in metallic mode

Reason: the deposited layer is much thinner because the deposition rate is much lower
Deposition profile: result

(a) distance (cm)
(b) distance (cm)

Simulation result

RIGHT: abrupt effect is mimicked
poisoned mode

RIGHT: a more gradual decrease
metallic mode

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Cleaning experiments…

Including deposition enables to mimic the sputter cleaning experiments.

Important as this shows that the kinetics are well described.
Cleaning experiments …

Target condition after 30 s in stationary mode

Influence of deposition

Target condition during steady state
Understanding the effect

- $\Delta S$ enters plasma region fully oxidized
- Increase RPM $\rightarrow$ smaller $t_{\text{in}}$ = less time for oxide removal
- Critical gas flow decreases with increasing RPM

Without deposition, we would expect a similar behaviour, i.e. 1/RPM behaviour

- Lower rotation speed means a thicker layer, but there is more time to sputter the layer
- Higher rotation speed means a thinner layer, but there is less time to sputter the layer

But with deposition
Conclusions

Rotation speed influences the reactive sputtering behaviour of a rotation cylindrical magnetron

A model enables to understand its behaviour

Deposition explains its behaviour

Acknowledgements

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K. Van Aeken : Development of SIMTRA and electron trajectory code
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R. De Gryse : Scientific (and other) discussions

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