Advances in the chemical vapor deposition (CVD) of Tantalum

Mugabi, James Atwoki; Bjerrum, Niels; Petrushina, Irina; Eriksen, Søren; Christensen, Erik

Publication date: 2014

Citation (APA):
Chemical Vapour Deposition (CVD) of Tantalum

- In Long narrow channels

James Atwoki Mugabi
PhD Student, DTU

Supervisors:
Niels J. Bjerrum
Irina Petrushina
Søren Eriksen
Erik Christensen

DTU Energy Conversion
Department of Energy Conversion and Storage
Why Tantalum?

Percentage Weight loss in 10 wt % HCl, room temperature, α-alumina abrasives and 1000 rpm for 168 hours.

Tantalum Coated Plate Heat Exchanger
**SYSTEM DESCRIPTION**

\[ Ta_{(s)} + 2.5 Cl_2 ((g)) \rightarrow TaCl_5 \]

\[ TaCl_5 + \frac{5}{2} H_2 \rightarrow Ta + 5 HCl \]
Modeling

Long narrow Channel: Tubes

Fluid Flow: Navier Stokes

Diffusion: Fick’s Law

Chemical Reaction: Arrhenius

Adsorption: Langmuir
Results:

Experiment 800°C, 25 mbar

![Graph showing Tantalum Thickness vs Position in tube for Try 1 and Try 2.](image)
Experiment 850°C, 25 mbar

Tantalum Deposition Rate [µm/h]

Position in tube [m]

- Try 1
- Try 2
- Try 3
Experiment 900°C, 25 mbar

Tantalum Deposition Rate [$\mu$m/h] vs. Position in tube [m]

- Try 1
- Try 3
- Try 4
Experiment 950\degree C, 25 mbar

Tantalum Deposition rate [\mu m/h]

Position in tube [m]

• Try 1

× Try 2
All Temperatures, 25 mbar

Tantalum Deposition rate [µm/h]

Position in tube [m]

- 800 C
- 850 C
- 950 C
- 900 C X 4
All Pressures, 800 °C

Tantalum Layer Deposition Rate [µm/h]

Position in the Tube [m]

- 25 mbar -- 50g Cl2/ h
- 100 mbar -- 50g Cl2/ h
- 300 mbar -- 30g Cl2/ h
- 1 atm -- 30g Cl2/ h
Model Fitting
Model

Fluid Flow: Navier Stokes

Diffusion: Fick’s Law

Adsorption: Langmuir

Chemical Reaction: Arrhenius

Geometry: 2D Axial Symmetry and 3D

Software: COMSOL MultiPhysics®
Mechanism

\[ \text{TaCl}_5(g) + \frac{1}{2}H_2 \rightarrow \text{TaCl}_4(g) \]

\[ \text{TaCl}_4(g) + \frac{1}{2}H_2 \rightarrow \text{TaCl}_3(g) \]

\[ \text{Ta}_5 + 4\text{HCl}(g) \rightarrow \text{Ta} + 4\text{HCl}(g) \]

\[ \text{Ta}_5 + 3\text{HCl}(g) \rightarrow \text{Ta} + 3\text{HCl}(g) \]

Gas Phase Reaction

Surface Reaction
Model Fitting – 800 °C

Tantalum Deposition Rate um/h vs. Position in tube [m]

Position in tube [m]

Tantalum Deposition Rate um/h
Model Fitting – 850 °C

Tantalum Deposition Rate µm/h

Position in tube [m]
Model Fitting – 900 °C

Tantalum Deposition Rate um/h vs Position in tube [m]
Model Fitting – 950 °C

Tantalum Deposition Rate um/h vs. Position in tube [m]
Application
CB30 – Channel
CB30 – Channel (X-Y Plane)
CB30 – Streamline: Velocity field Visualization
CB30 – Streamline: Velocity field Visualization
CB30 – 1st Run: Tantalum Layer Thickness
(i.e. Only treated from the right end)
CB30 – 1st Run: Tantalum Layer Thickness (i.e. Only treated from the left end)
CB30 – 2nd Run: Tantalum Layer Thickness (i.e. Treated from the both ends)
CB30 – 2\textsuperscript{nd} Run: Tantalum Layer Thickness (i.e. Treated from the both ends)
Thank you for your attention.