Experiments and Modeling of Mass Transfer for Cross-Contamination in Plasma Processes

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Thrust B: Subtask B5-3

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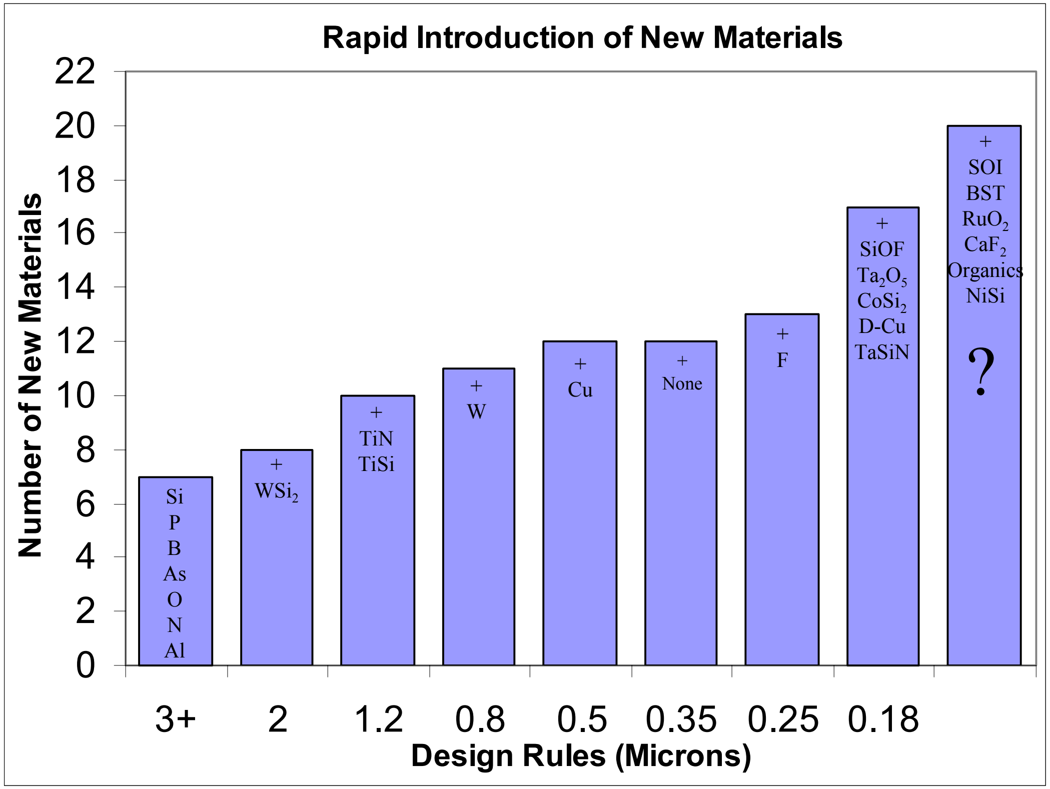
Outline

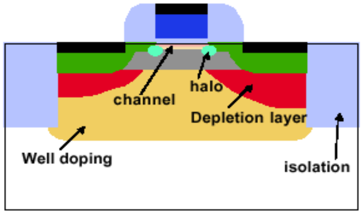
- Background on issues
- Motivation
- Cross-contamination experiments
    - Procedure and results
- Mass transfer model
    - Comparison to experimental results
    - Transfer coefficients, k
- Other contaminants
- Conclusions and future applications

Background

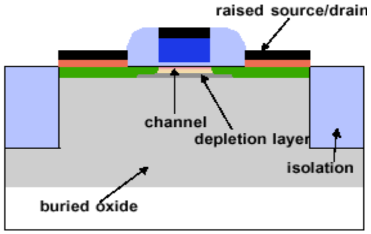
- Material diversity increases as process complexity increases



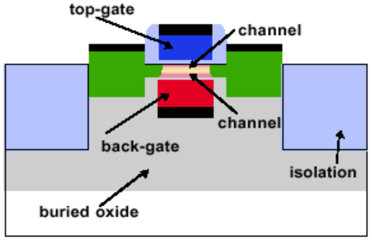
After Peercy, P.S, IEEE1998



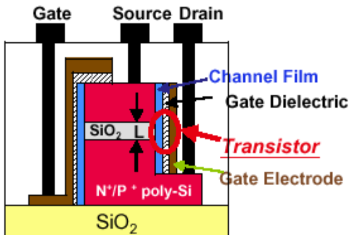
Bulk CMOS



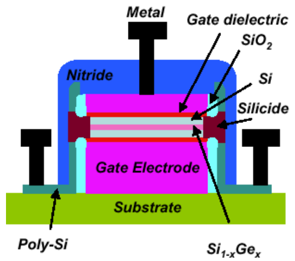
FD SOI CMOS



Double-Gate CMOS



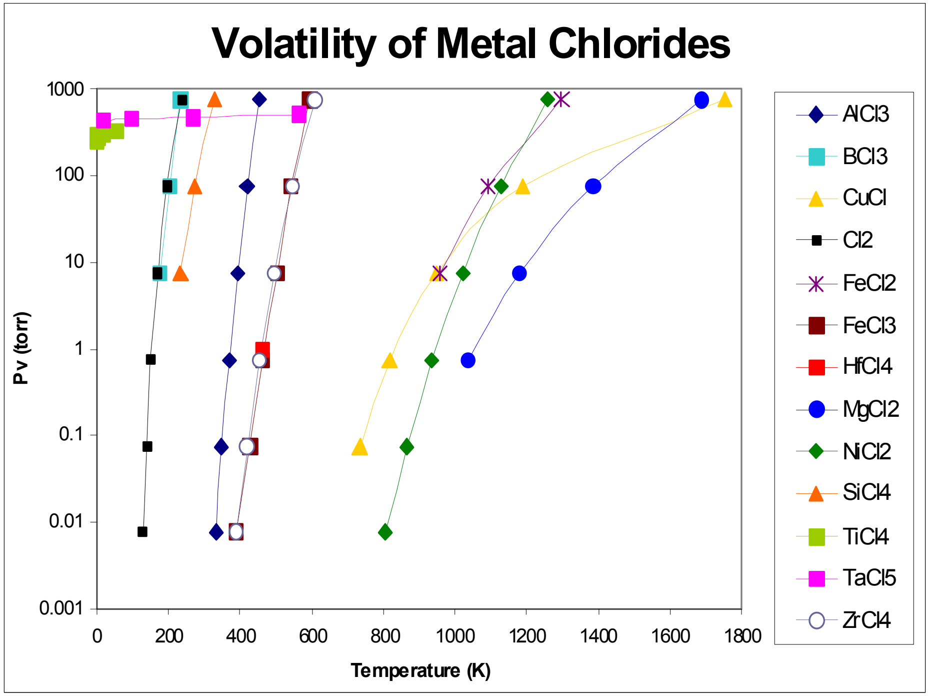
Vertical MOS



Planar Double-Gate

Background (2)

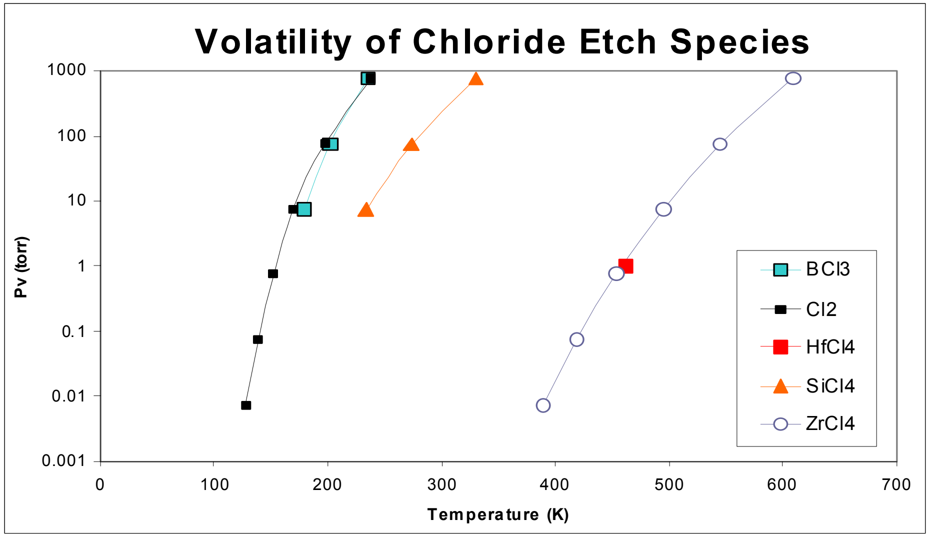
- Issues of cross-contamination
  - Low volatility material is hard to remove from chamber
  - New materials may require their own dedicated chamber
  - Mass transfer mechanism between chamber wall and wafer needs to be understood



Volatility of Metal Chlorides

Motivation for Studying Zr Contamination Rate Transfer

- ZrO_2 is promising candidate for gate dielectric
- Calculations suggest that interstitial Zr and Hf have mid-gap trap levels
- Interstitial Zr and Hf expected to have high diffusion rates in Si
- ZrO_2 etch by-products are less volatile than SiO_2 etch by-products
- Good vehicle for studying contamination rate transfer



Motivation for Studying Zr Contamination Rate Transfer (2)

ESH:

- Understanding mass transfer can help optimize chamber cleaning, wafer cleaning

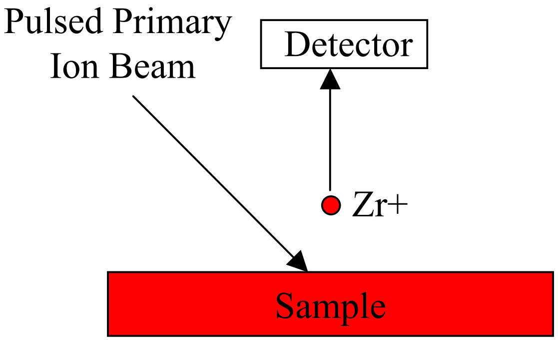
- Know how long chamber needs to be seasoned to reduce cross-contamination

- Help choose cleaning scheme to increase yields and reliability

Experimental Setup

- Applied Materials P5000 MERIE plasma etcher
- Measure contamination on wafers following ZrO_2 etching
- Use TOF-SIMS (collaborated with Physical Electronics, Inc.)
  - detection limit ~7e7 atoms/cm^2 for Zr

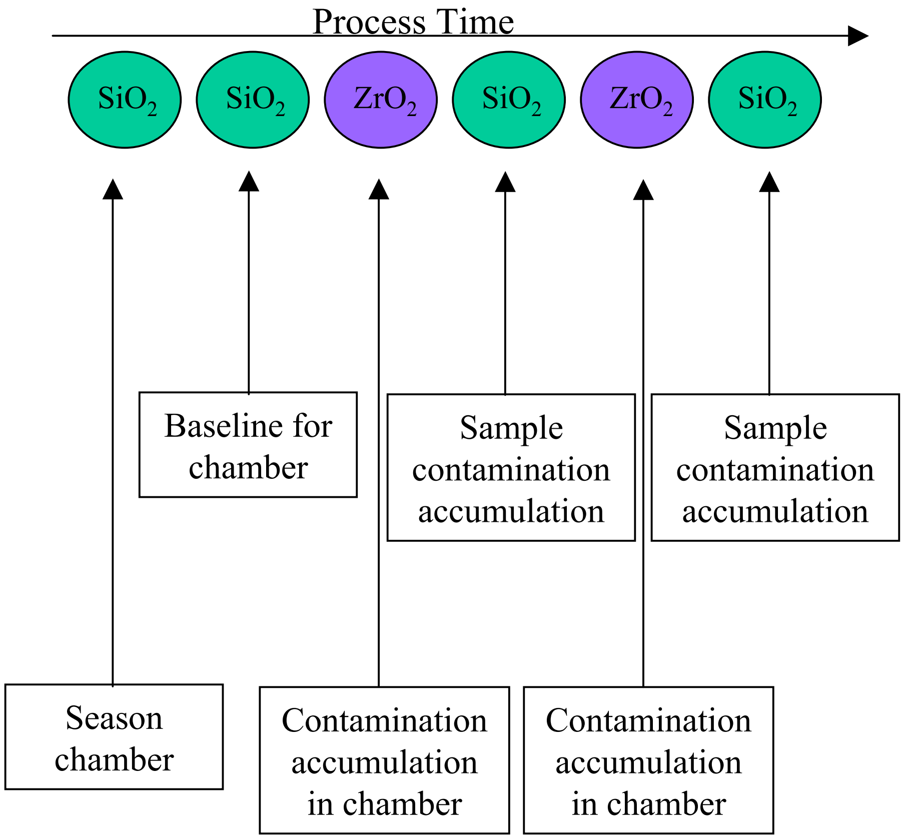
PHI THRIFT III



Time-of-Flight Secondary Ion Mass Spectrometry (TOF-SIMS)

Experimental Setup (2)

Accumulation



Process Time

SiO_2 SiO_2 ZrO_2 SiO_2 ZrO_2 SiO_2

Season chamber

Baseline for chamber

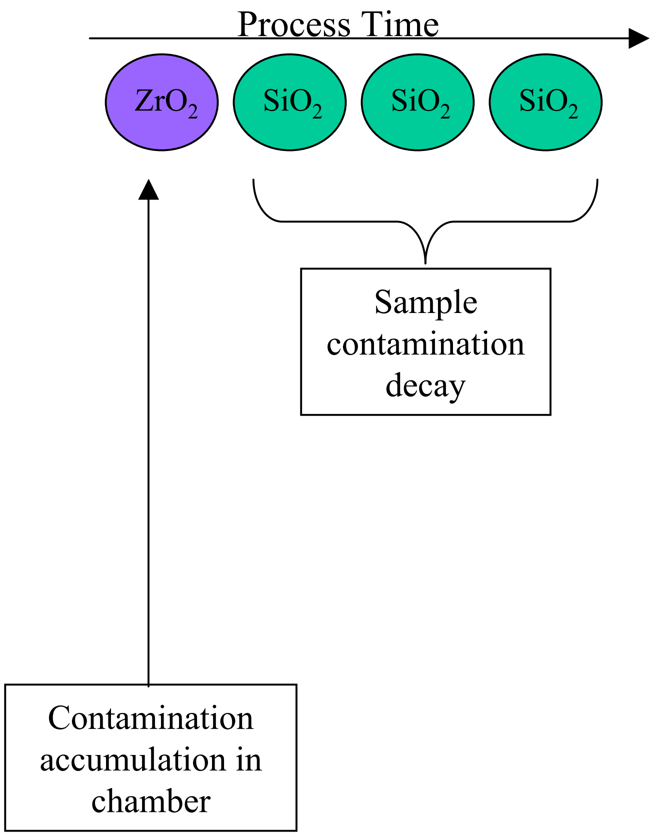
Contamination accumulation in chamber

Sample contamination accumulation

Contamination accumulation in chamber

Sample contamination accumulation

Decay



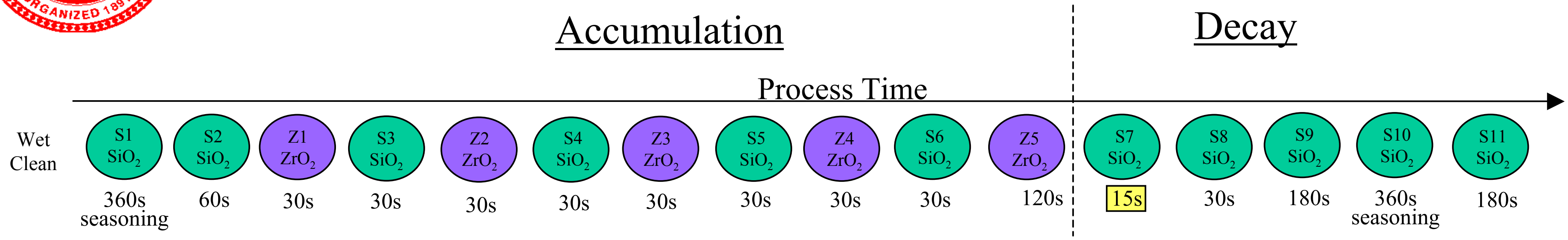
Process Time

ZrO_2 SiO_2 SiO_2 SiO_2

Contamination accumulation in chamber

Sample contamination decay

Experiment 1 Results

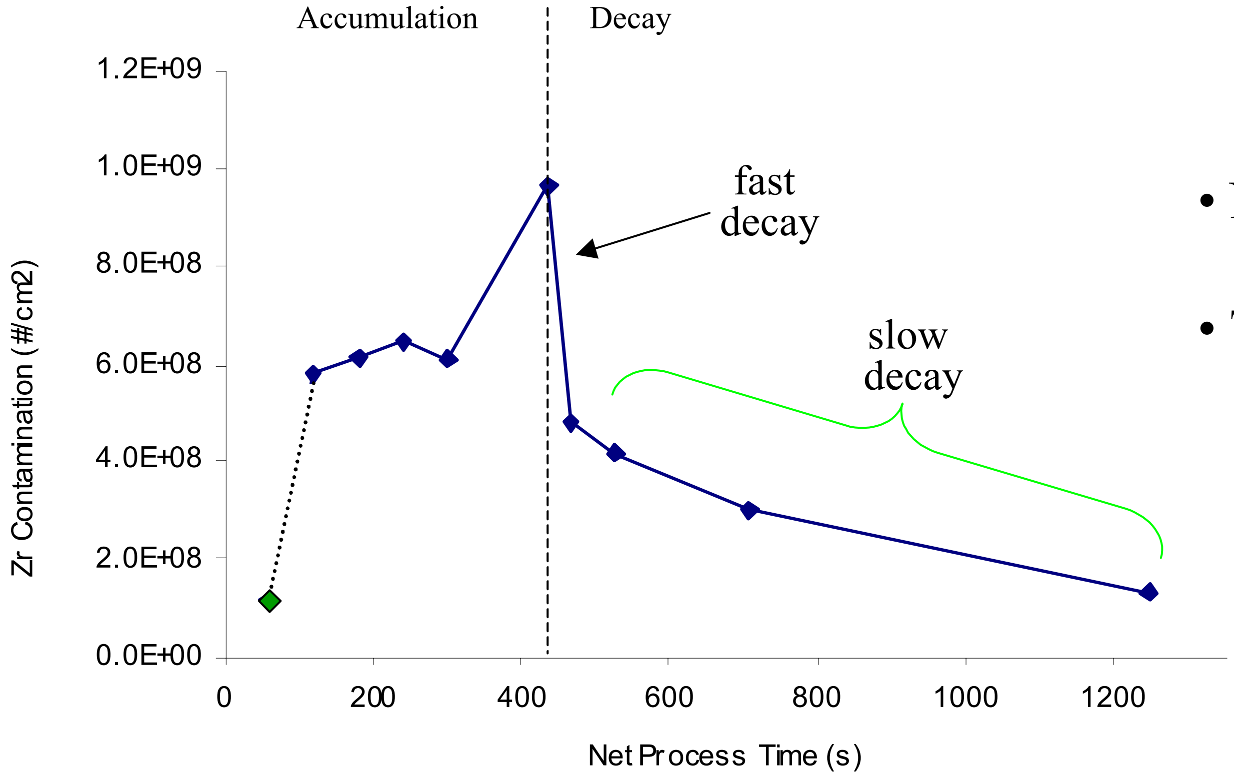


Accumulation

Decay

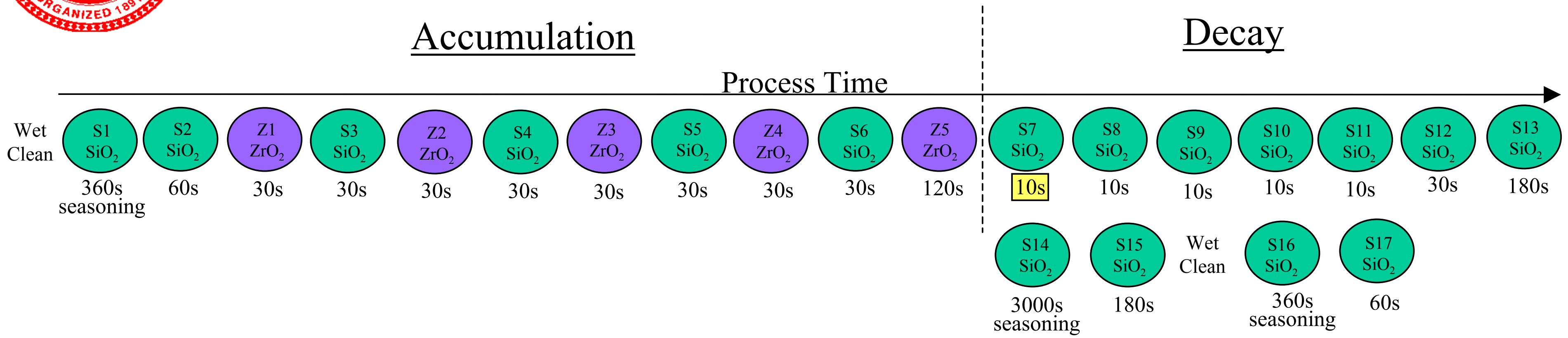
Process Time

Wet Clean	S1	S2	Z1	S3	Z2	S4	Z3	S5	Z4	S6	Z5	S7	S8	S9	S10	S11
	SiO_2	SiO_2	ZrO_2	SiO_2	ZrO_2	SiO_2	ZrO_2	SiO_2	ZrO_2	SiO_2	ZrO_2	SiO_2	SiO_2	SiO_2	SiO_2	SiO_2
	360s seasoning	60s	30s	30s	30s	30s	30s	30s	30s	30s	120s	15s	30s	180s	360s seasoning	180s



- Non-linear accumulation
- Two decay stages

Experiment 2 Results



Accumulation

Decay

Process Time

Wet Clean

S1 SiO_2 360s seasoning

S2 SiO_2 60s

Z1 ZrO_2 30s

S3 SiO_2 30s

Z2 ZrO_2 30s

S4 SiO_2 30s

Z3 ZrO_2 30s

S5 SiO_2 30s

Z4 ZrO_2 30s

S6 SiO_2 30s

Z5 ZrO_2 120s

S7 SiO_2 10s

S8 SiO_2 10s

S9 SiO_2 10s

S10 SiO_2 10s

S11 SiO_2 10s

S12 SiO_2 30s

S13 SiO_2 180s

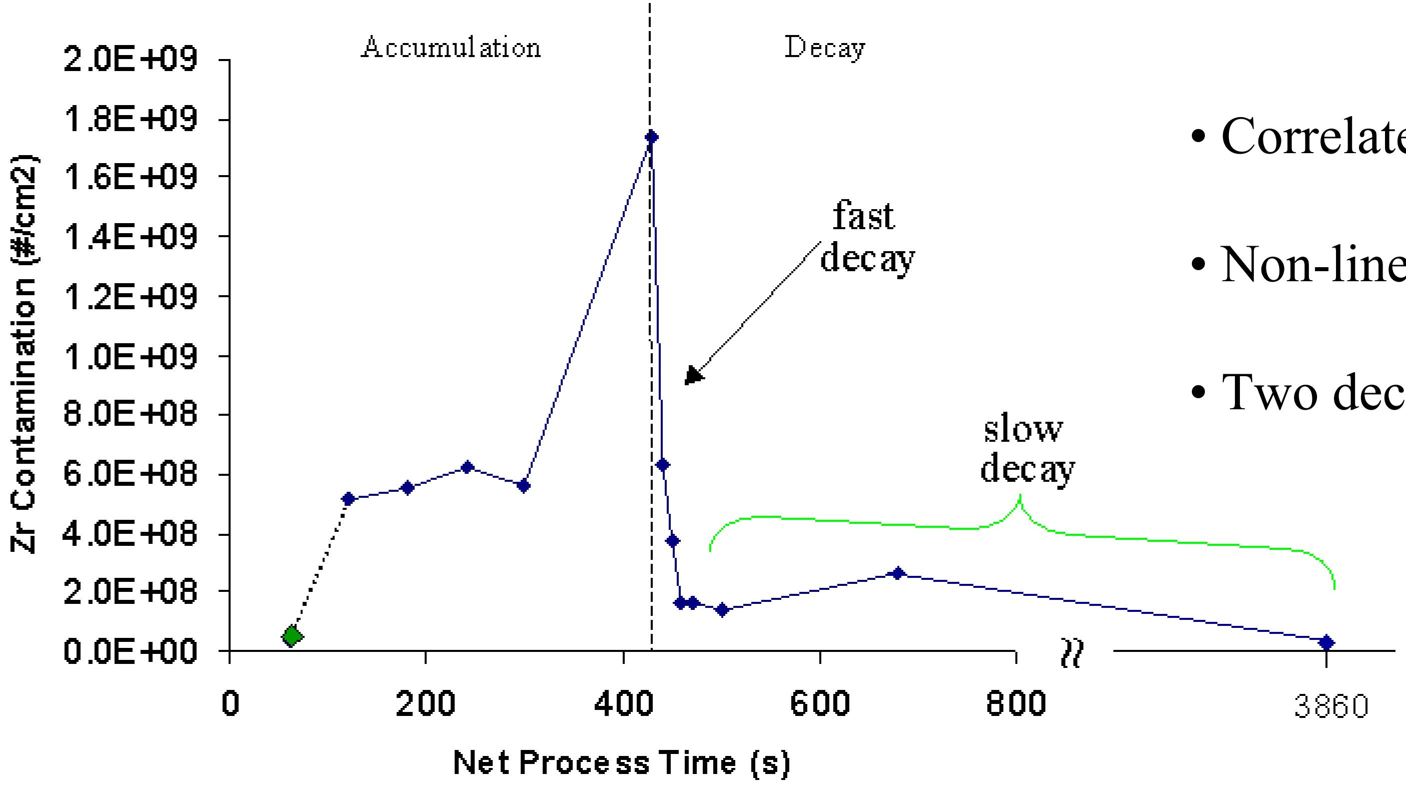
S14 SiO_2 3000s seasoning

S15 SiO_2 180s

Wet Clean

S16 SiO_2 360s seasoning

S17 SiO_2 60s



- Correlates well with expt.1
- Non-linear accumulation
- Two decay stages

Experiment 3 Results

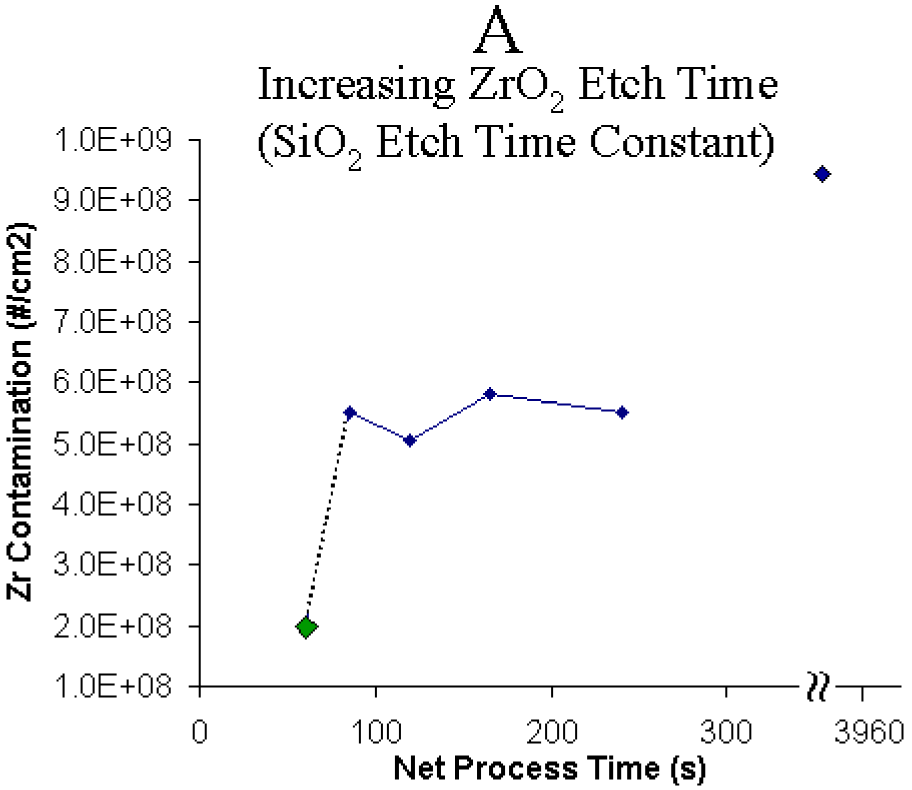
A — Process Time →

Wet Clean	S1	S2	Z1	S3	Z2	S4	Z3	S5	Z4	S6	Z5	S7
	SiO_2	SiO_2	ZrO_2	SiO_2	ZrO_2	SiO_2	ZrO_2	SiO_2	ZrO_2	SiO_2	ZrO_2	SiO_2
	1800s seasoning	60s	10s	15s	20s	15s	30s	15s	60s	15s	120s	3600s no plasma

B — Process Time →

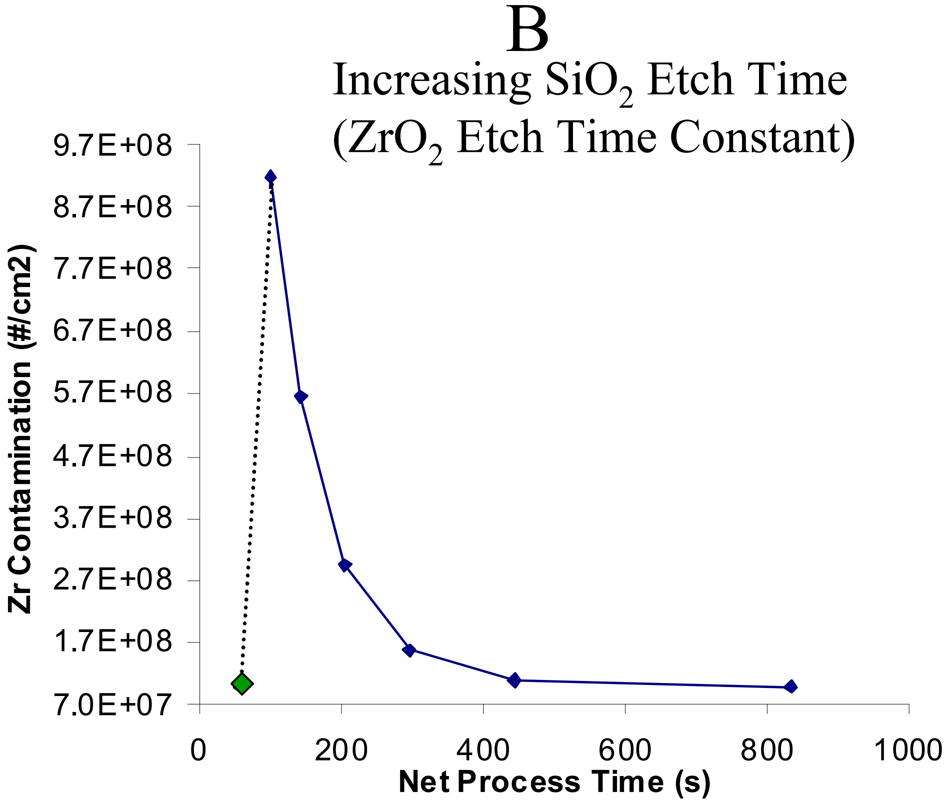
Wet Clean	S8	S9	Z6	S10	Z7	S11	Z8	S12	Z9	S13	Z10	S14
	SiO_2	SiO_2	ZrO_2	SiO_2	ZrO_2	SiO_2	ZrO_2	SiO_2	ZrO_2	SiO_2	ZrO_2	SiO_2
	1800s seasoning	60s	30s	10s	30s	30s	30s	60s	30s	120s	30s	360s

- Highest Zr concentration for wafer without plasma



A

Increasing ZrO_2 Etch Time (SiO_2 Etch Time Constant)



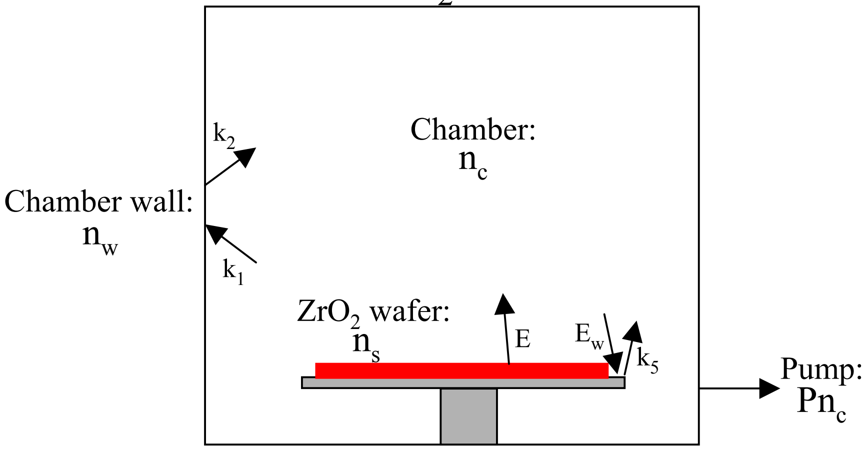
B

Increasing SiO_2 Etch Time (ZrO_2 Etch Time Constant)

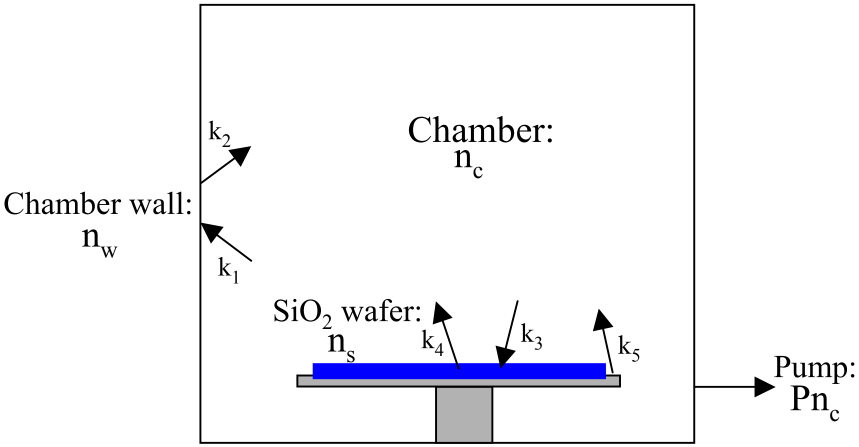
Model Basis

- Contamination transfer rate ∝ vapor pressure and sticking coefficient
- Use ideal gas approximation for impingement rate
- Transfer rate coefficients are constants
- Assumptions:
    - no spatial variations
    - constant pump rate
    - no wall sputtering

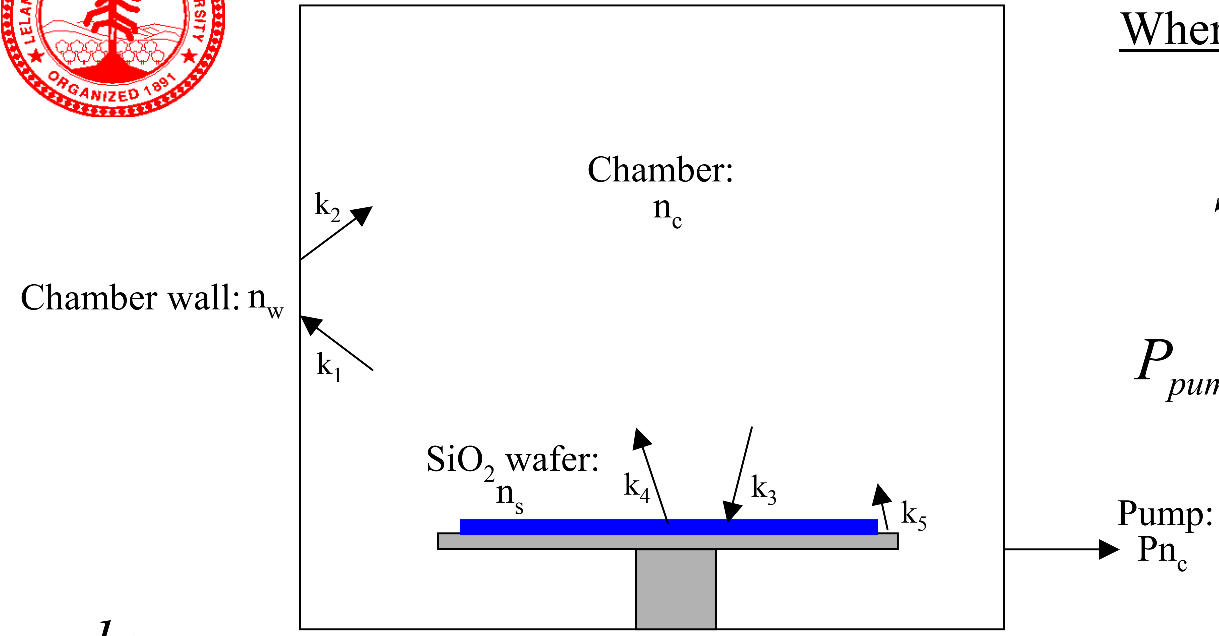
ZrO_2 Etch



SiO_2 Etch



Modeling Contamination Accumulation and Decay



Where:

$S \cdot n_w = x$ S is chamber area

$S_s \cdot n_s = y$ S_s is wafer area

$V \cdot n_c = z$ V is chamber volume

$P_{pump} / V = B$ P is pump speed

E is sputtering component

$$E = \frac{E_{Zr} \cdot S_s \cdot \rho_{Zr} \cdot N_A}{Weight_{Zr}}$$

$$\frac{dw}{dt} = E_w - k_5 \cdot w$$

$$\frac{dx}{dt} = k_1 \cdot z - k_2 \cdot x$$

$$\frac{dy}{dt} = k_3 \cdot z - k_4 \cdot y + b \cdot k_5 \cdot w$$

$$\frac{dz}{dt} = -k_1 \cdot z + k_2 \cdot x - k_3 \cdot z + k_4 \cdot y - B \cdot z + E$$

Boundary conditions:

At $t = 0 : n_w = n_o$

$n_s = 0$

$n_c = 0$

- During ZrO_2 etch, k3,k4=0,b=0
- During SiO_2, E=0, E_w=0

Obtaining k Constants

k_1 and k_3:

- Mass transfer from chamber to wall, chamber to SiO_2 wafer
- $\propto$ Zr impingement rate, R, times sticking coefficient
- R $\propto$ chamber partial pressure of Zr

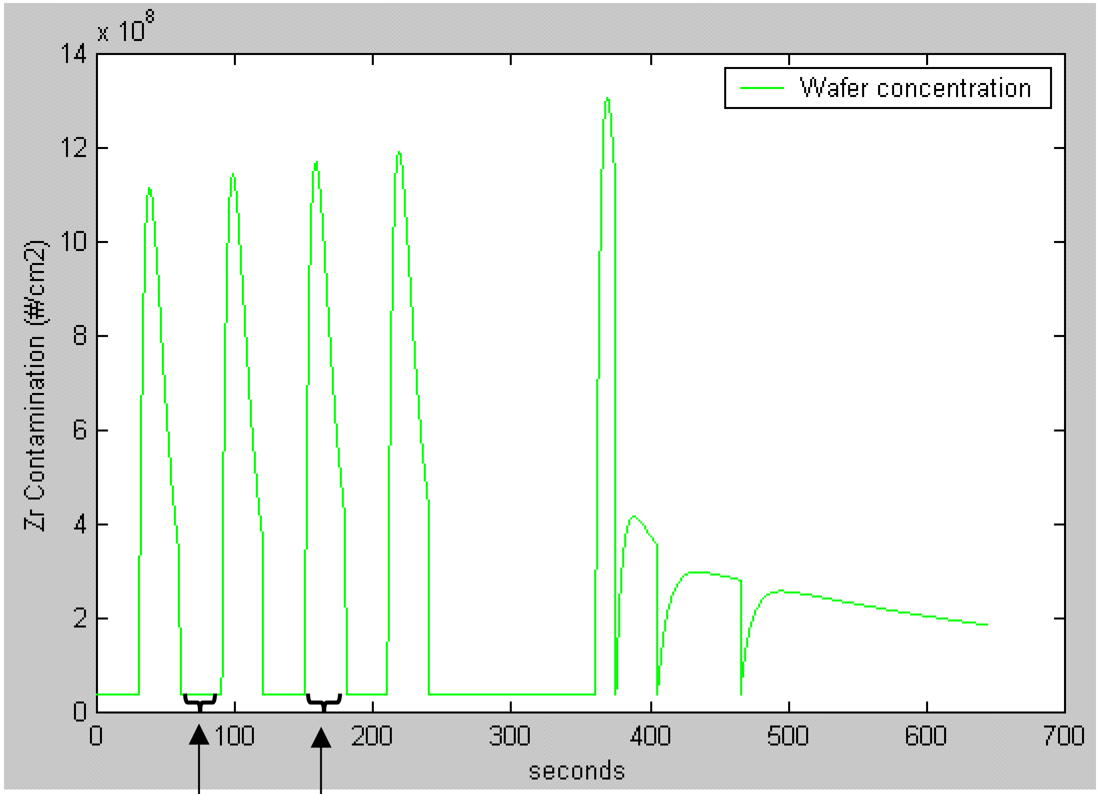
k_2 and k_4:

- Mass transfer from wall to chamber, chamber to SiO_2 wafer
- Escaping rate from surface is balanced with the impingement rate at the volatility vapor pressure
- Extra sputtering term is added to k_4 for etching of newly deposited Zr

k_5:

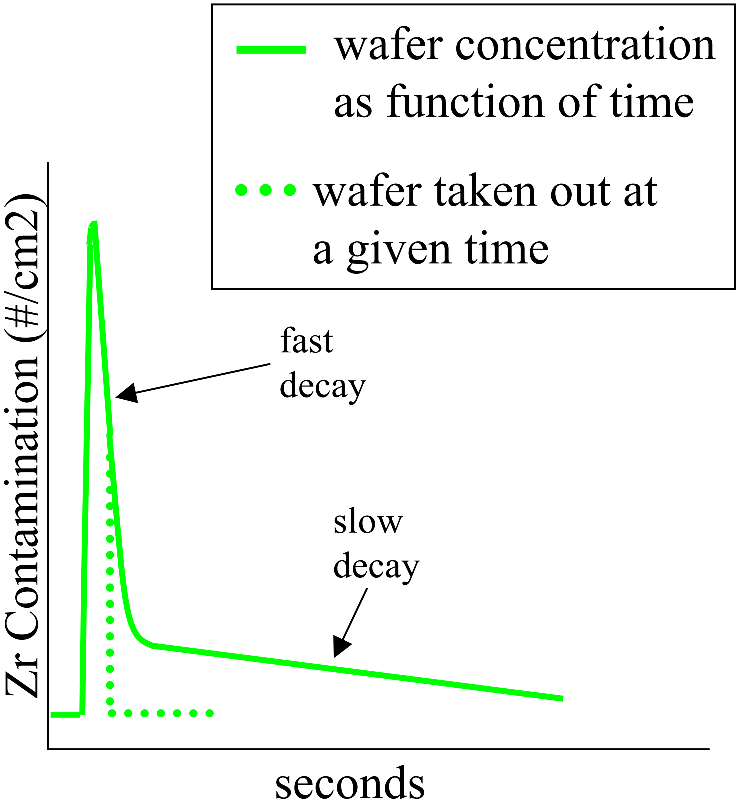
- Mass transfer from surrounding area (re-sputtering)

Model: Experiment 1

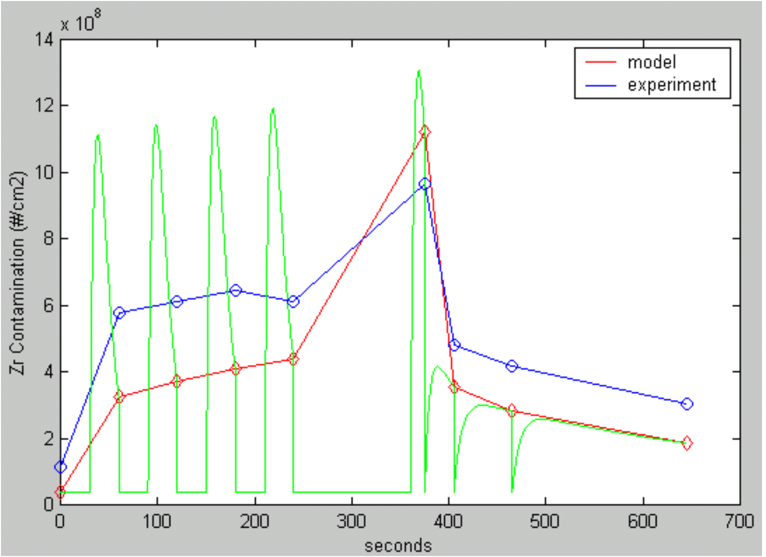


ZrO_2 wafer being etched

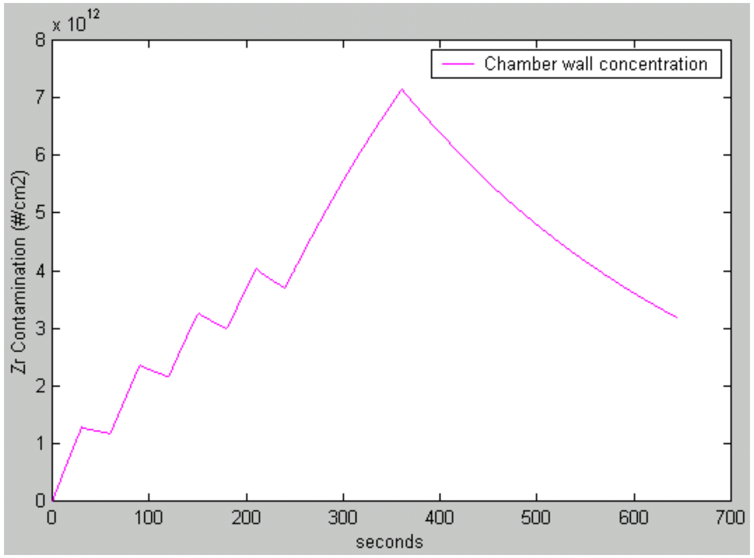
SiO_2 wafer being etched



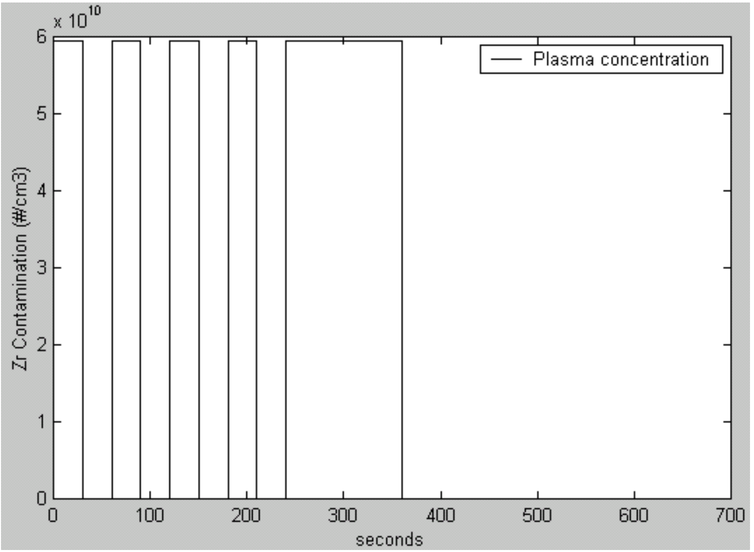
Model: Experiment 1 (continue)



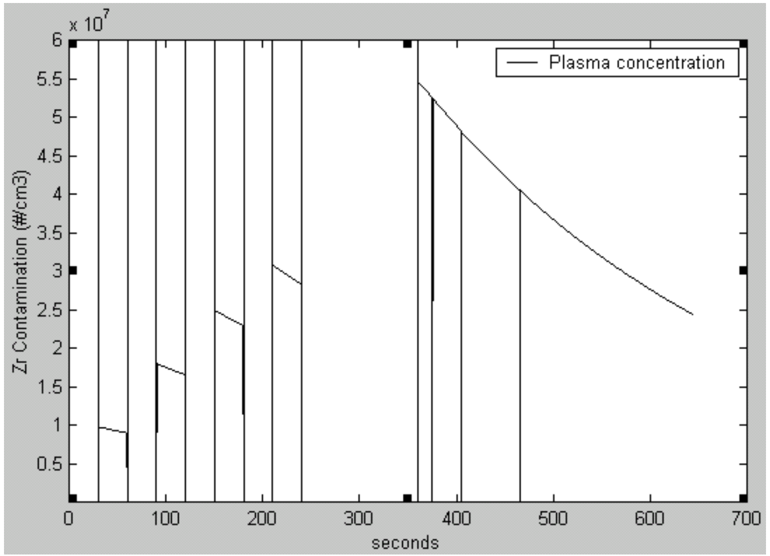
Fitting



Wall concentration



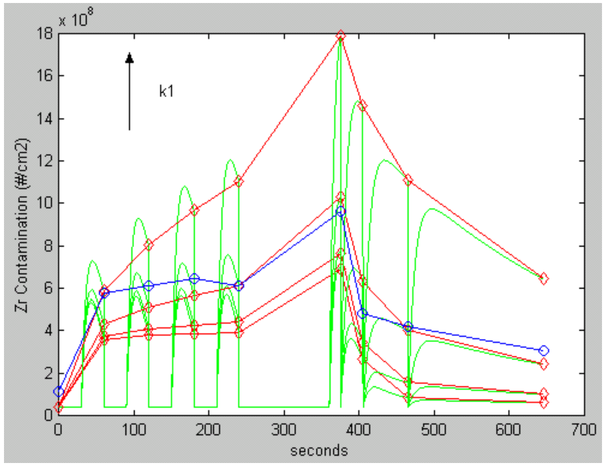
Chamber concentration



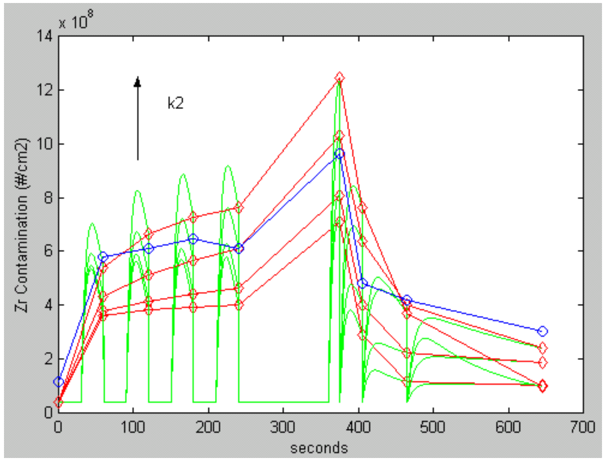
Zoomed-in on chamber concentration

- Model fit experiment reasonably well
- Plasma concentration saturates quickly
- Wall concentration increases ~ linearly

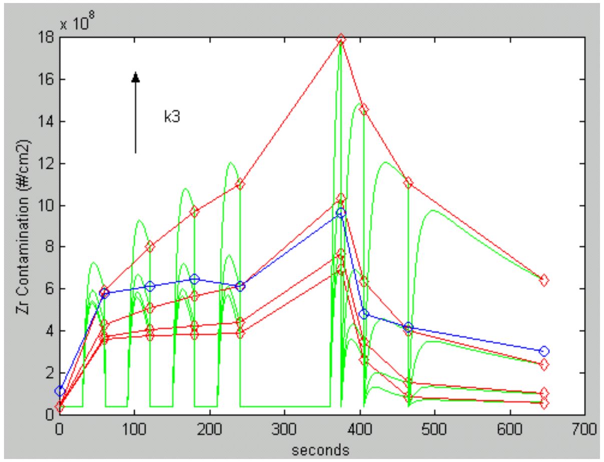
Model: Varying k's for Experiment 1



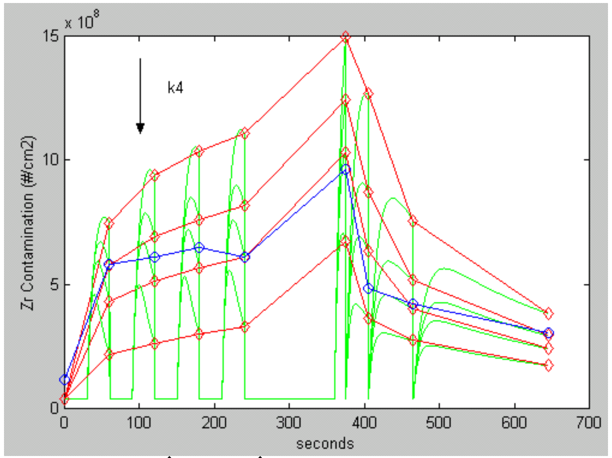
- ↑k_1 ,↑n_c →higher wafer concentration



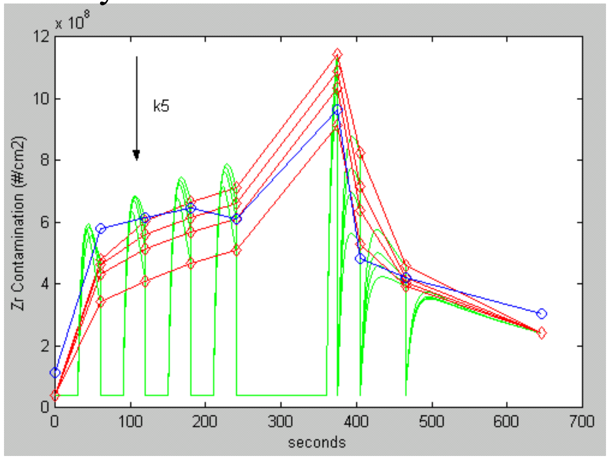
- ↑k_2 ,↑transfer from chamber wall, ↑wafer concentration
- Faster decay from wall, faster total decay with time



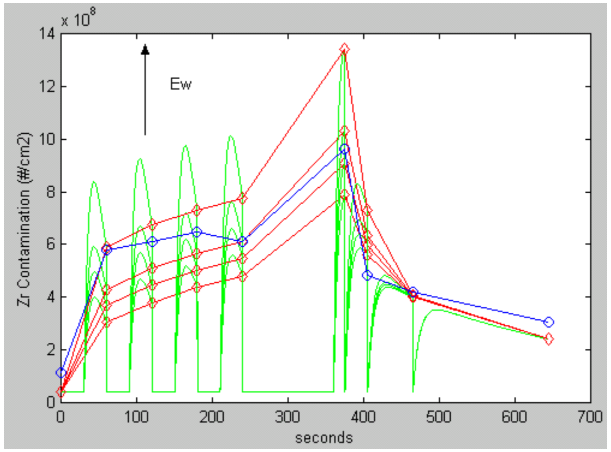
- ↑k_3 ,↑wafer impingement, ↑wafer concentration



- ↑ k_4 ,↑ wafer escape, lower wafer concentration

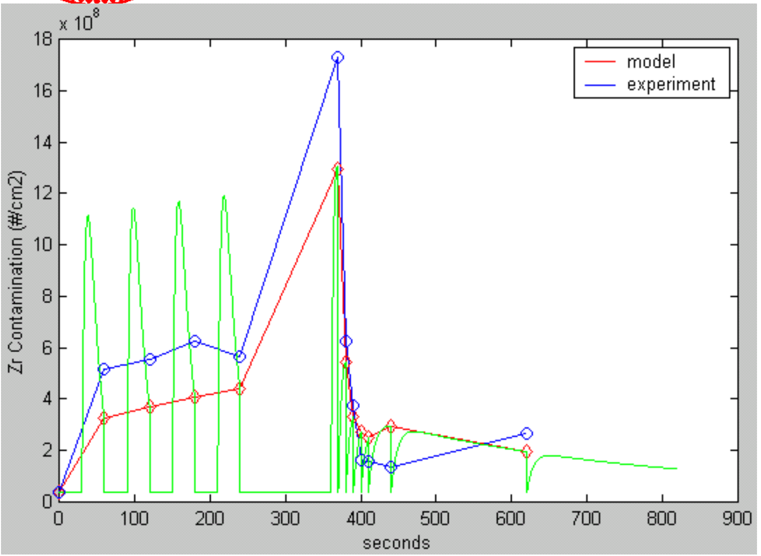


- ↑ k_5 ,↑ surrounding area escape, ↓ wafer

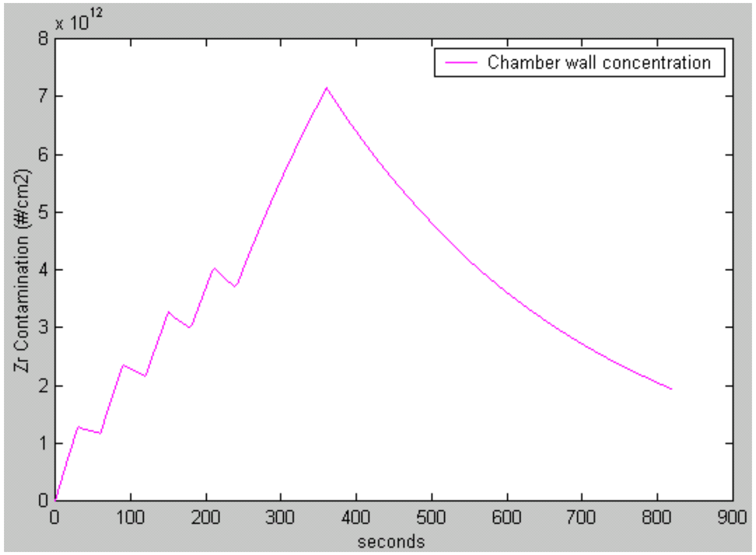


- ↑E_w , ↑surrounding area, ↓wafer due to re-sputtering

Model: Experiment 2

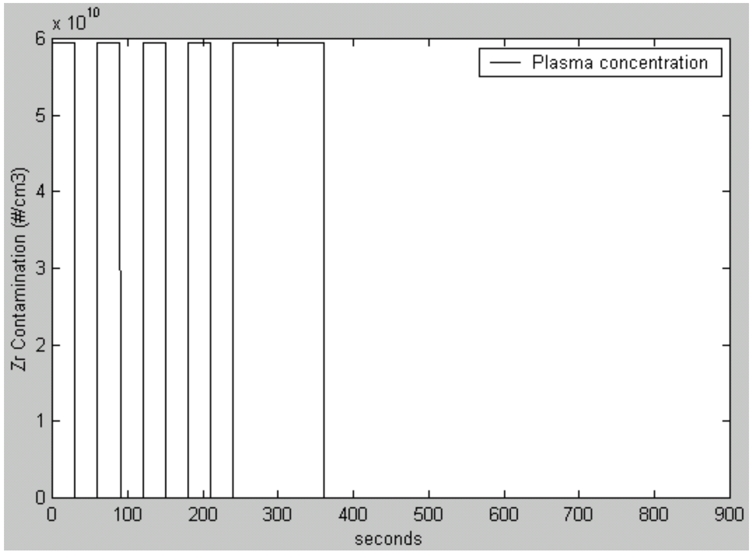


Fitting



Wall concentration

- Same fitting parameters as experiment 1



Chamber concentration

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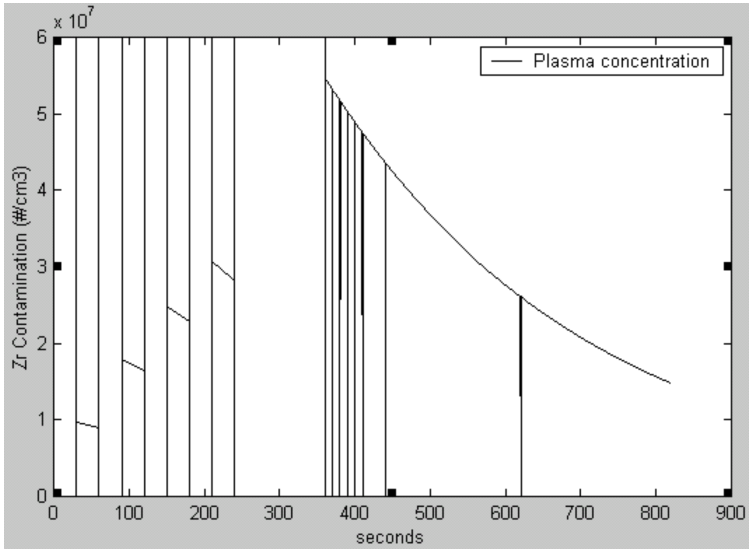
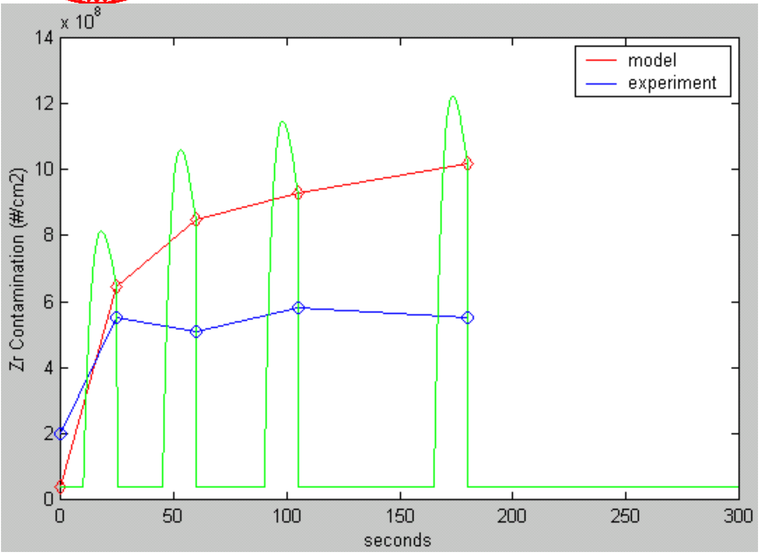


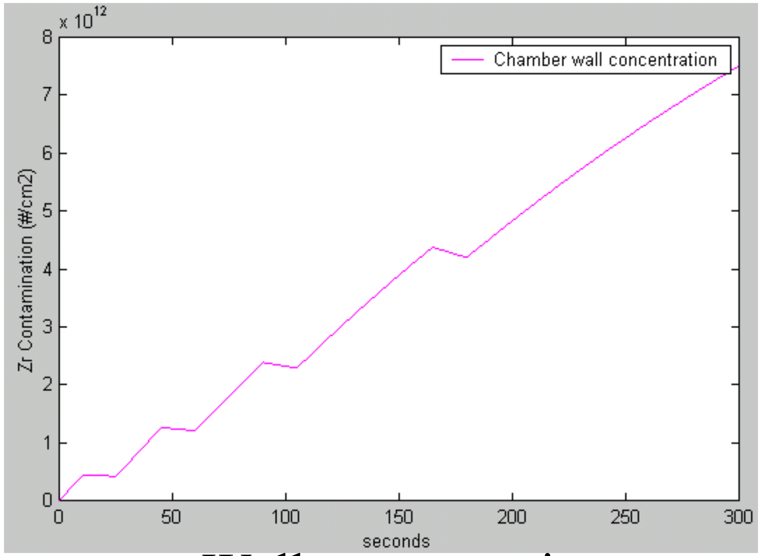
Zoomed-in on chamber concentration

Model: Experiment 3A (SiO_2 Etch Time Constant)

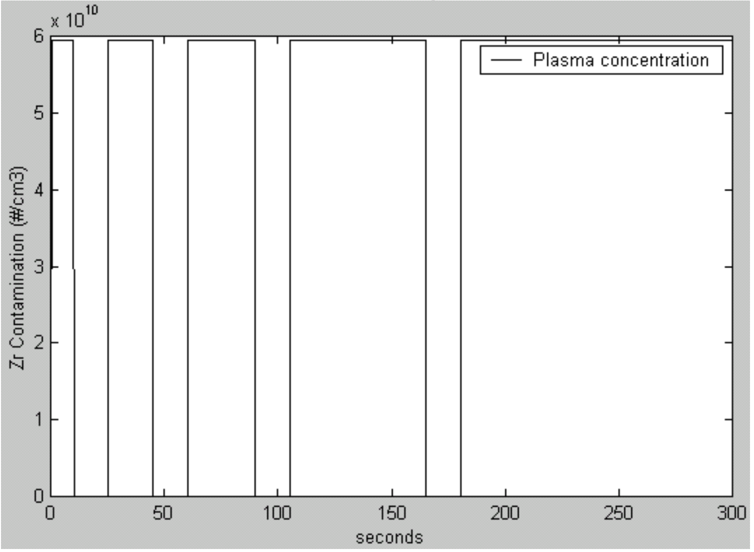
- Same fitting parameters as experiment 1,2



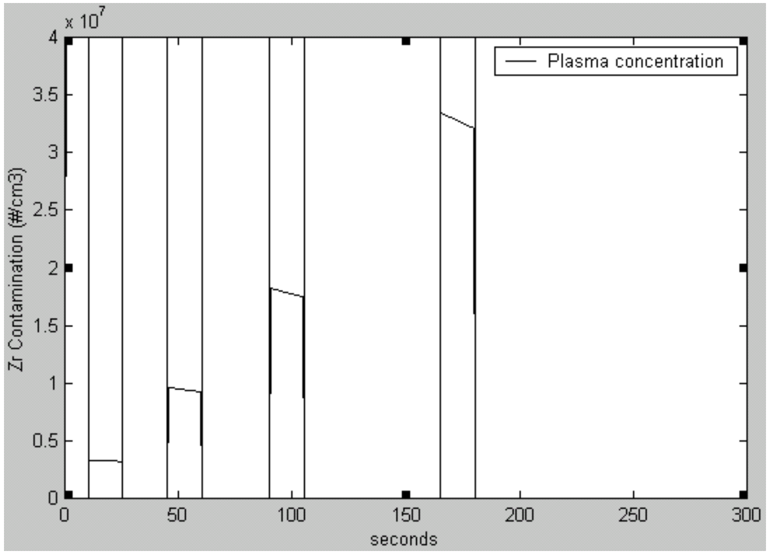
Fitting



Wall concentration

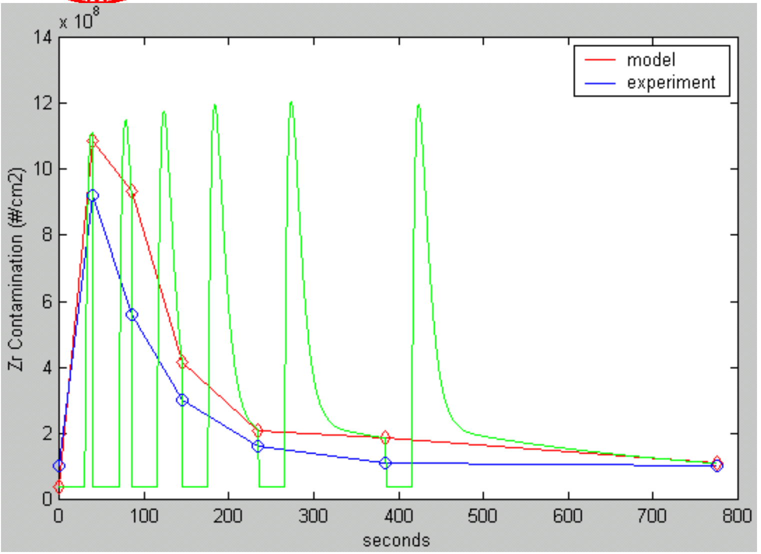


Chamber concentration

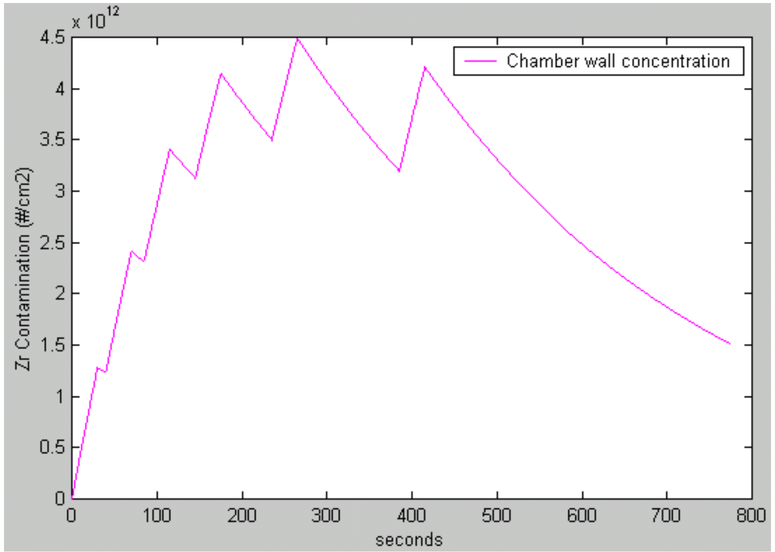


Zoomed-in on chamber concentration

Model: Experiment 3B (ZrO_2 Etch Time Constant)

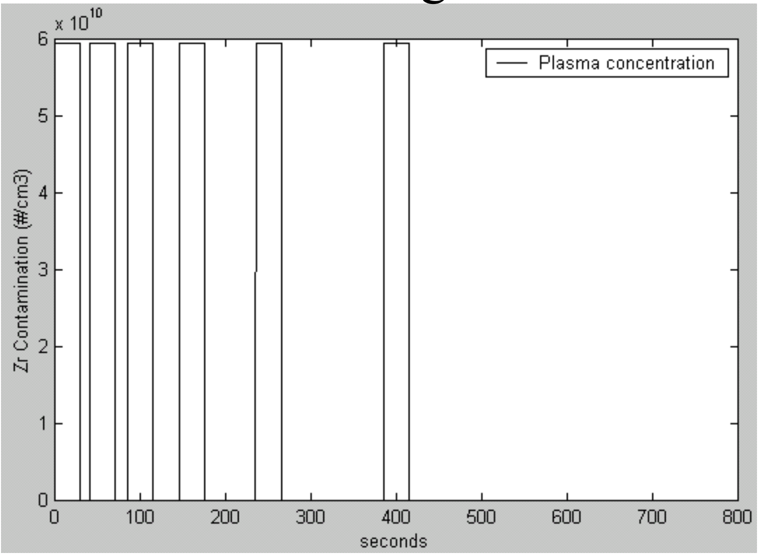


Fitting

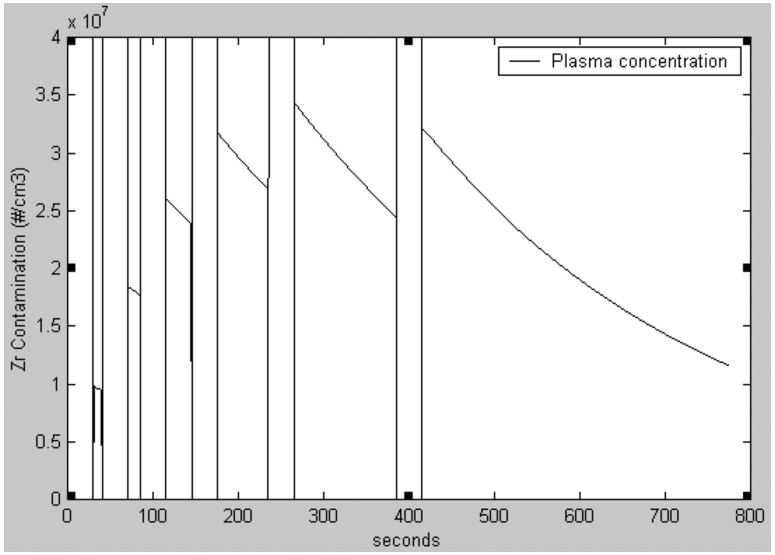


Wall concentration

- Same fitting parameters as experiment 3A



Chamber concentration



Zoomed-in on chamber concentration

Advantages of the Mass Transfer Model

- Straightforward kinetics model

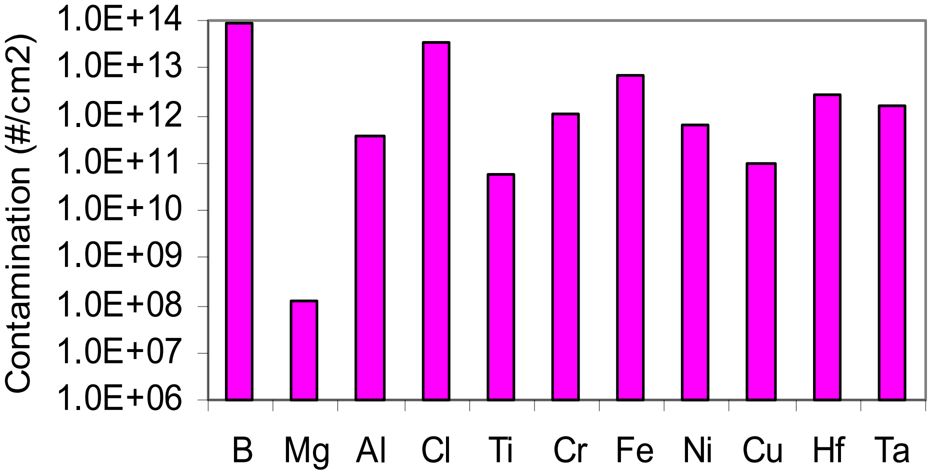
- Model gives insight into the different time scales and sources for the transfer mechanism

- Relationship between the chamber wall and wafer surfaces in mass transfer can be seen

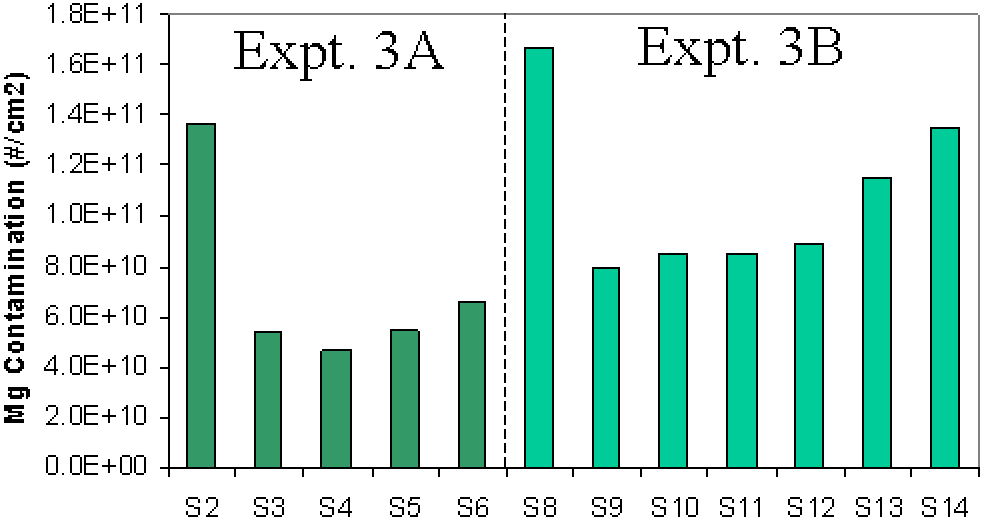
- Can see sensitivity of rate transfer factors (k's)

Other Contaminants

- Initial ZrO_2 wafers have other contaminants



- Interesting behavior for Mg
  - Contaminant from walls and wafer



Conclusions and Future Application

- Cross-contamination becoming more important
- Experimental results show complex accumulation and decay behaviors
- Developed mass transfer model based on volatility and sputtering
- Reasonable fit with experimental data
- Opportunity to investigate other materials