Multiscale Modeling of Kinetics and Dynamics of Heterogenous Catalysis and Material Degradation

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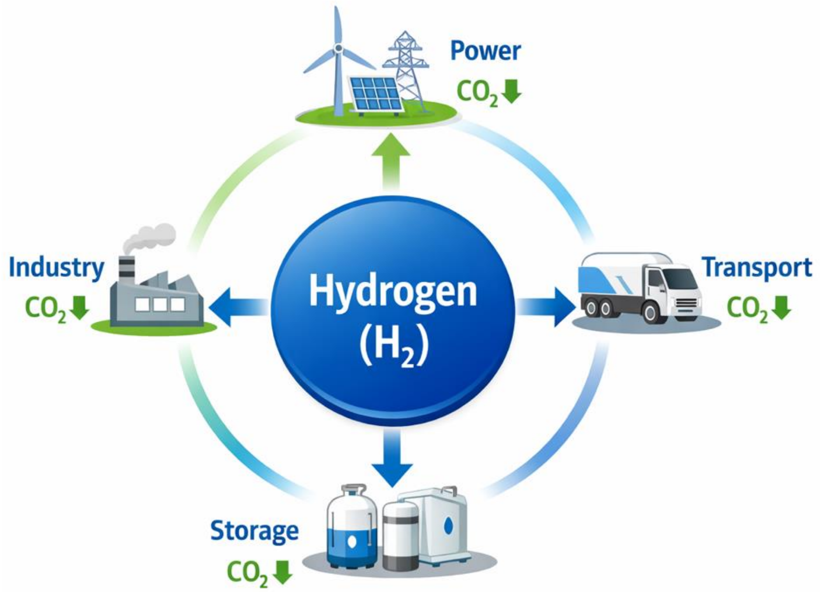
The Hydrogen Economy's $11 Trillion Promise – and Peril

- Hydrogen will supply **10-20% of global energy** demand by 2050
- Global hydrogen economy**: $2.5-11 trillion** by mid-century
- **700,000+ km** of existing natural gas pipelines could be repurposed for hydrogen
- But infrastructure must safely operate at **70-100 bar** for 30-50 years
- A single high-profile failure could delay adoption by decades



1998-2019: Four major incidents, 1,300+ fatalities

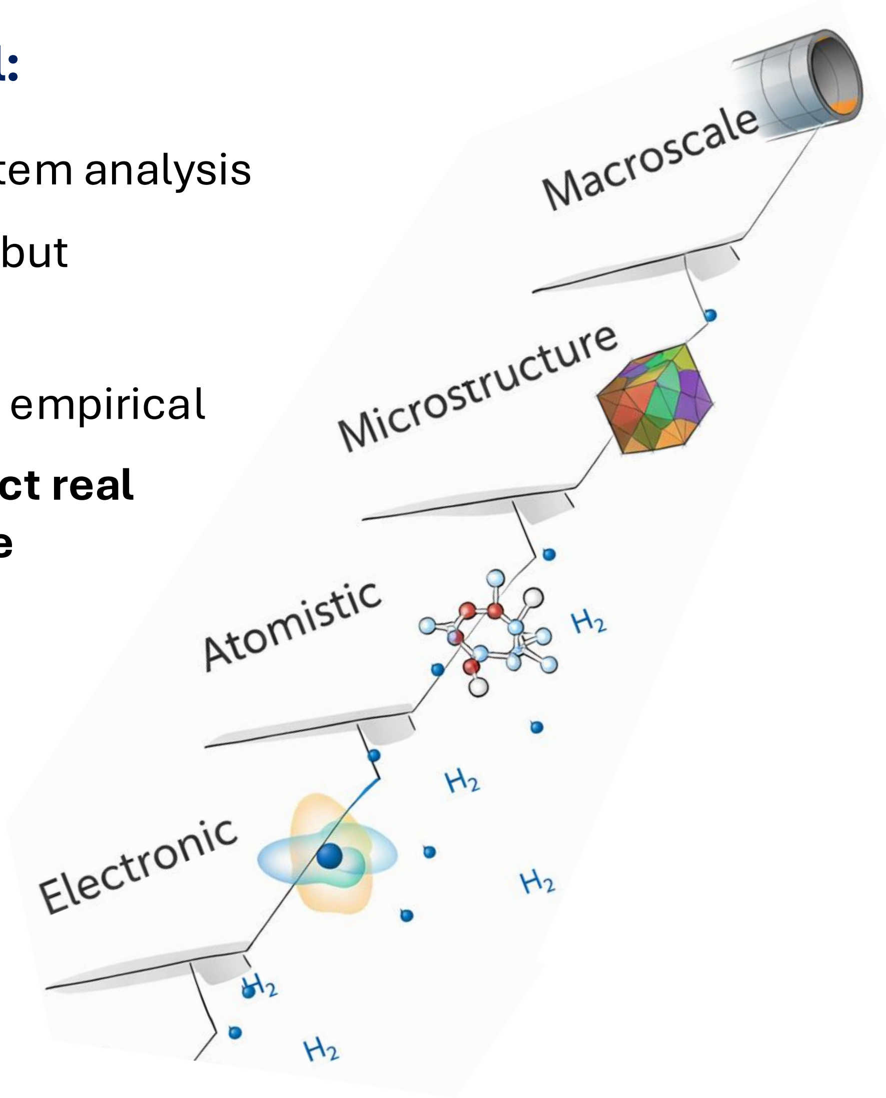
Why Hydrogen is Different: The Invisible Threat

The Permeation Problem

- **Hydrogen is the smallest atom** → diffuses directly through solid metals
- Traditional seals, welds, and gaskets **don't stop permeation**
- Accumulation causes **embrittlement and sudden fracture**
- **Damage is invisible** until catastrophic failure

Why existing approaches fail:

- Experiments: only post-mortem analysis
- Quantum models: accurate but microscopic
- Continuum models: fast but empirical
- **Result: Can't reliably predict real infrastructure performance**



The Scale Gap Crisis

> Despite 150 years of hydrogen research, we cannot reliably predict infrastructure performance

- The scale gap: Ångströms to meters, picoseconds to decades

Cracking the Hydrogen Bottleneck: Predictive, Multi-Scale Modeling

Hydrogen permeation is controlled by coupled processes across all scales

gas phase → oxide layer → metal–oxide interface → bulk metal

For the first time: Physically meaningful parameters across all scales, not empirical fitting

Our Strategy:

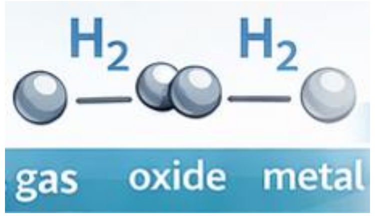
- **Aim 1**: Develop a multi-phase continuum model spanning gas to bulk metal
- **Aim 2:** Use sensitivity analysis to identify dominant transport mechanisms
- **Aim 3:** Compute critical parameters using quantum-accurate Machine-Learned-enabled Molecular Dynamics
- **Aim 4:** Incorporate surface reconstruction as dynamic boundary conditions

Continuum Model

Sensitivity Analysis

MLMD

Validation + Iteration



Accurate Permeation Prediction

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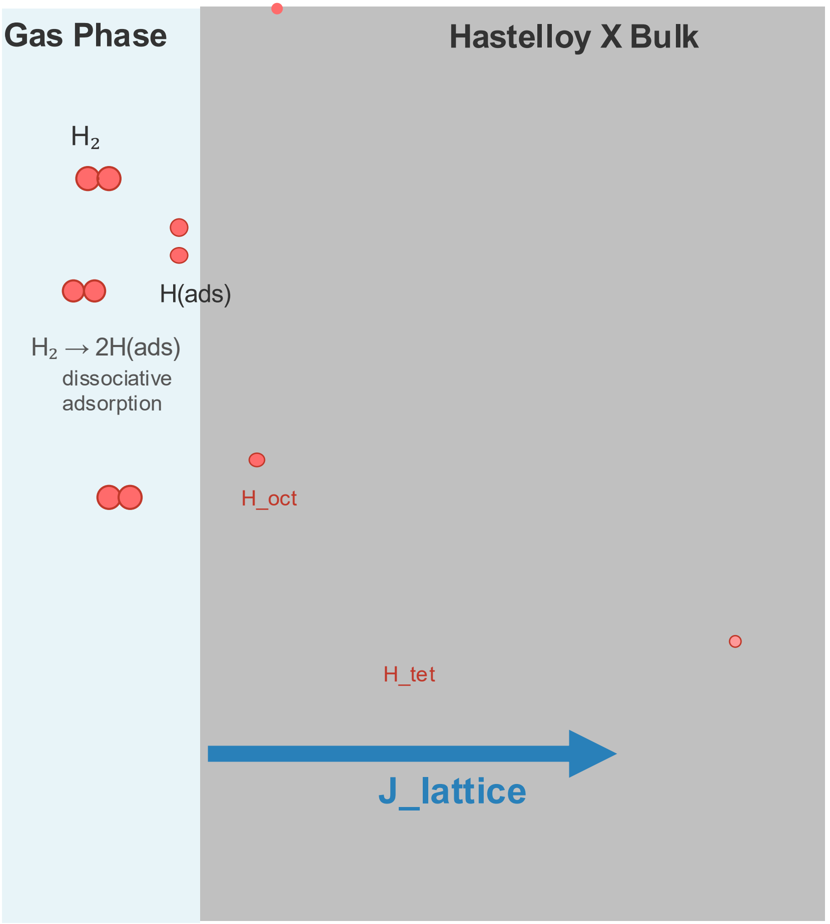
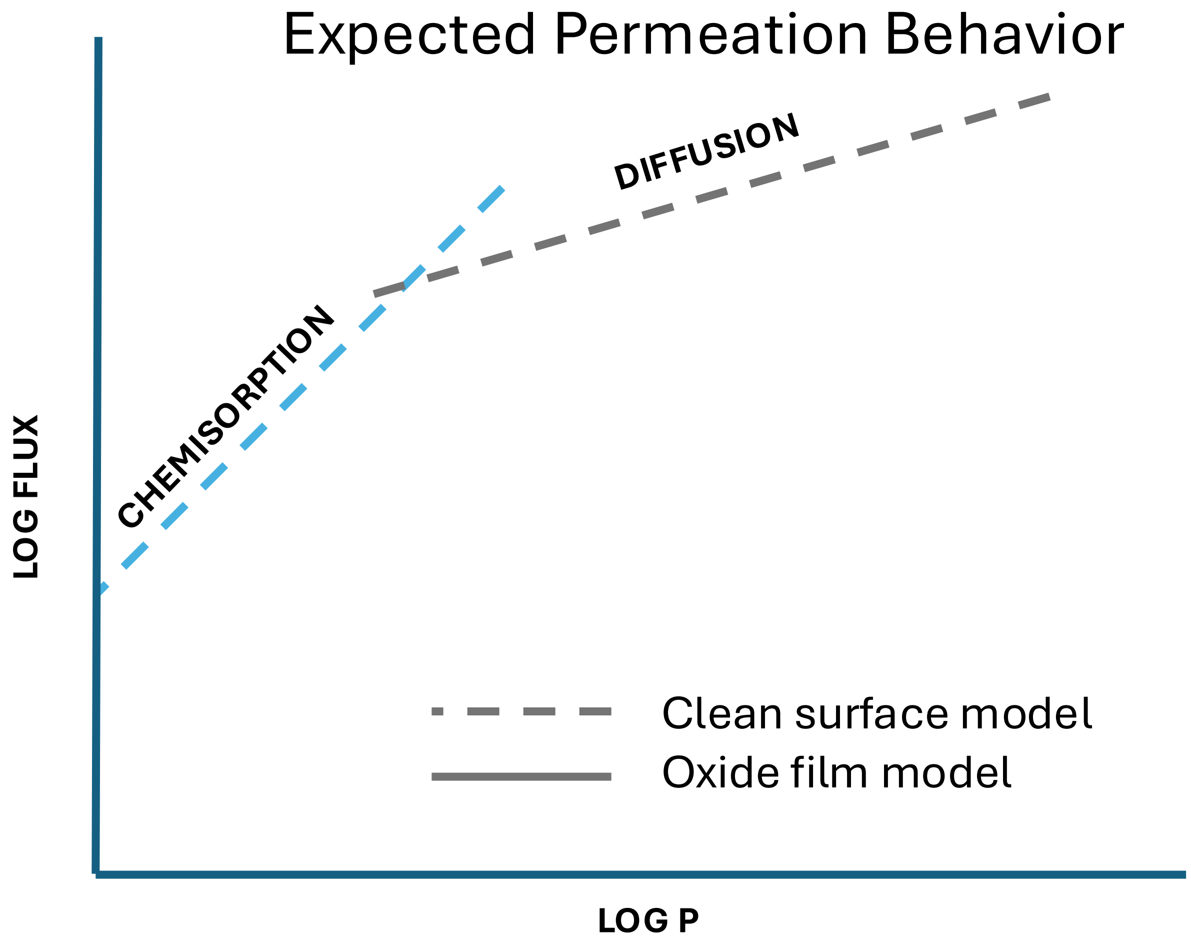
Development of Hydrogen Permeation Continuum Model



H atom in Perfect Metal



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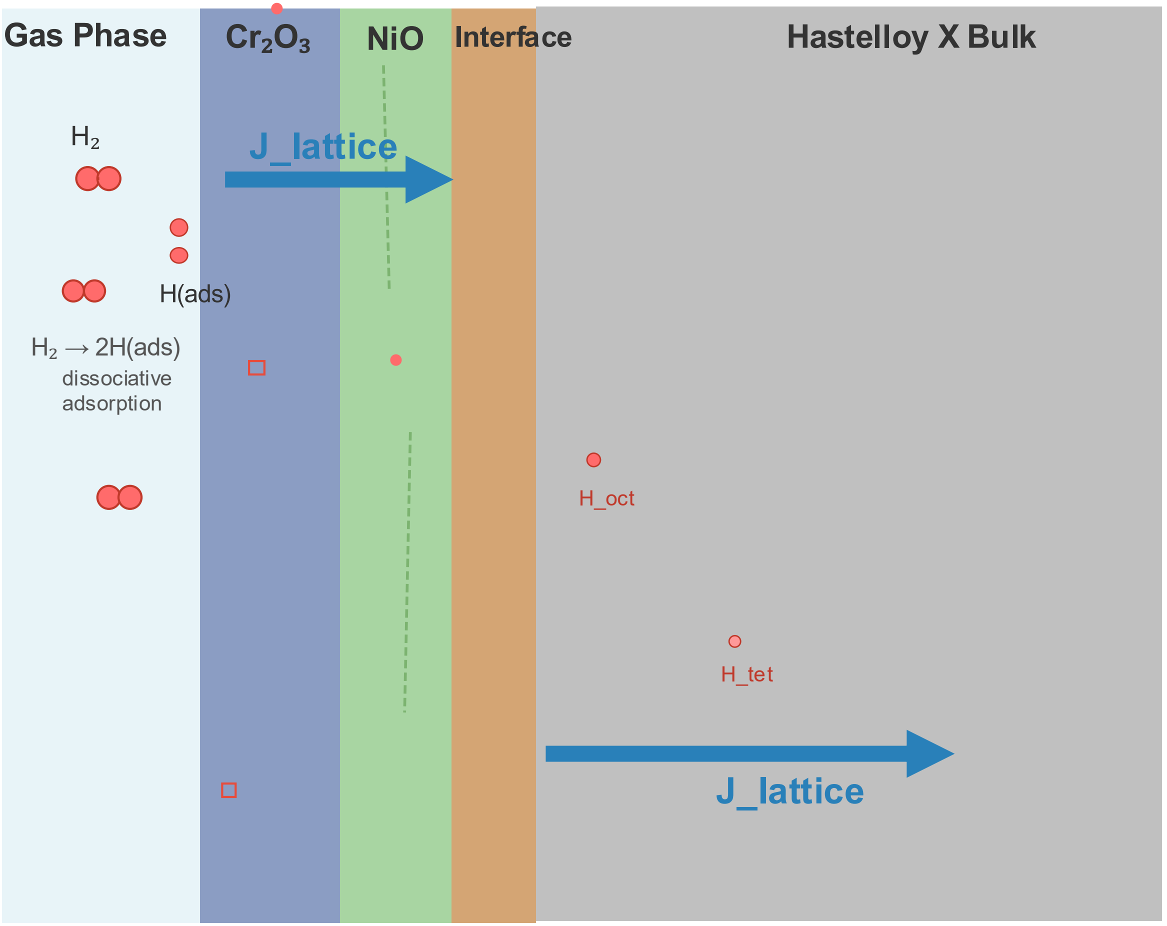
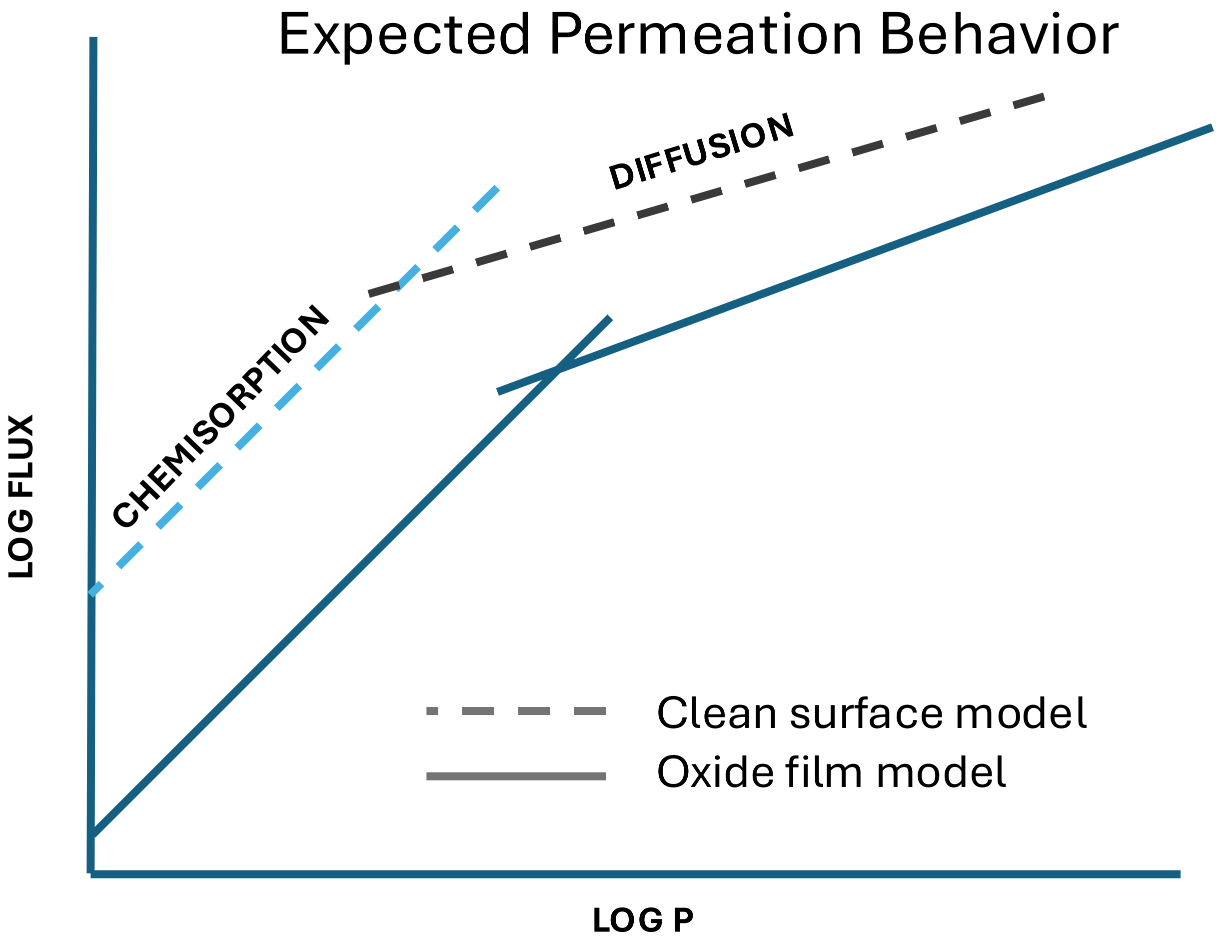


H2 through oxide layer into Perfect Metal



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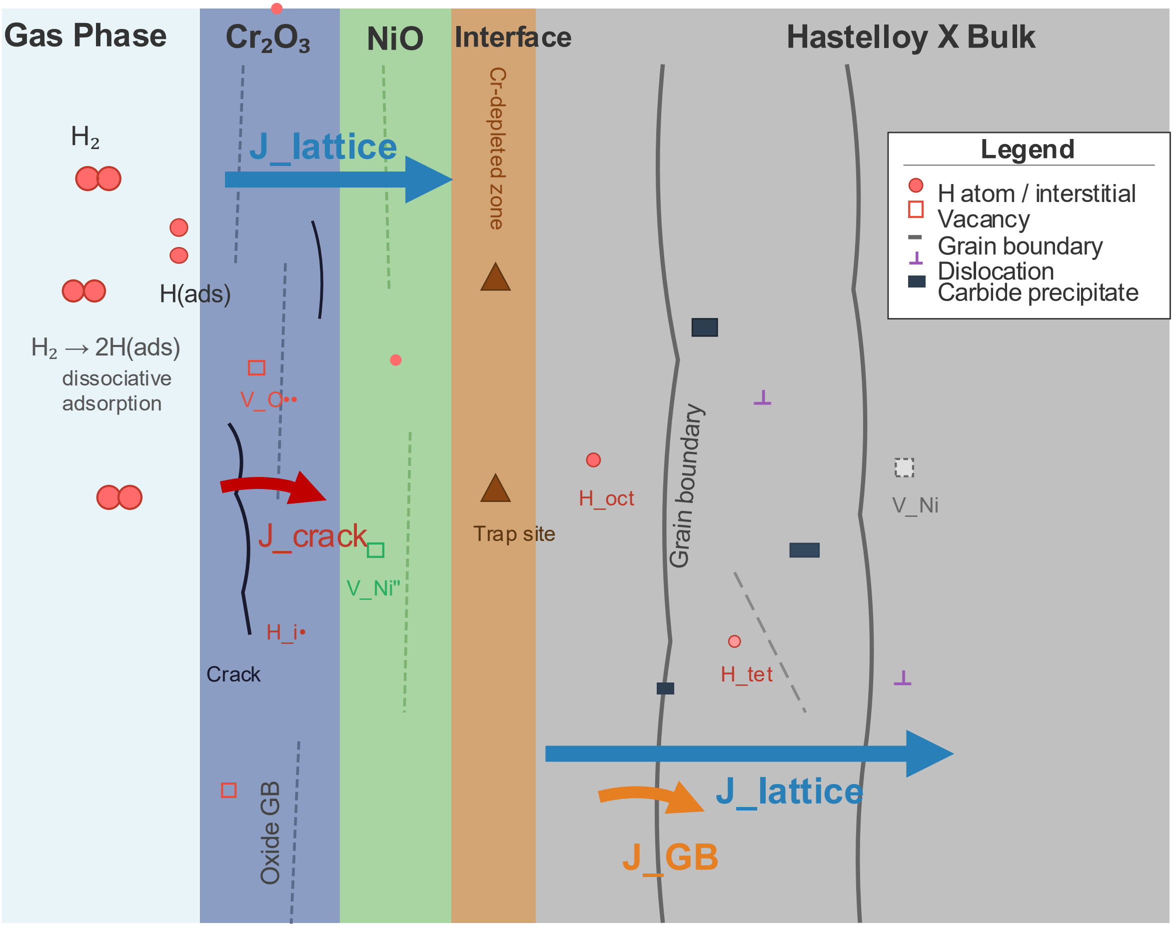
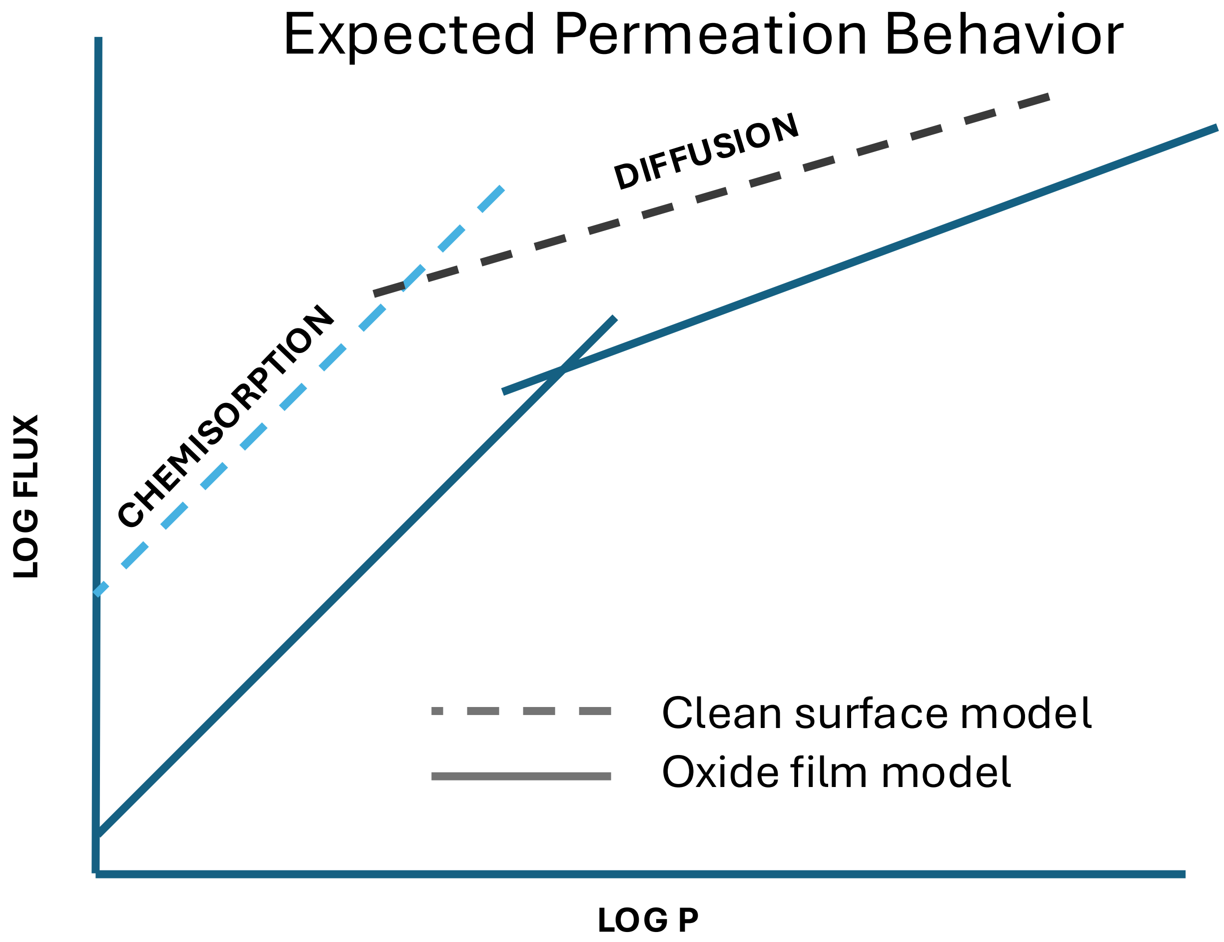


H2 through Defective Oxide layer and Metal



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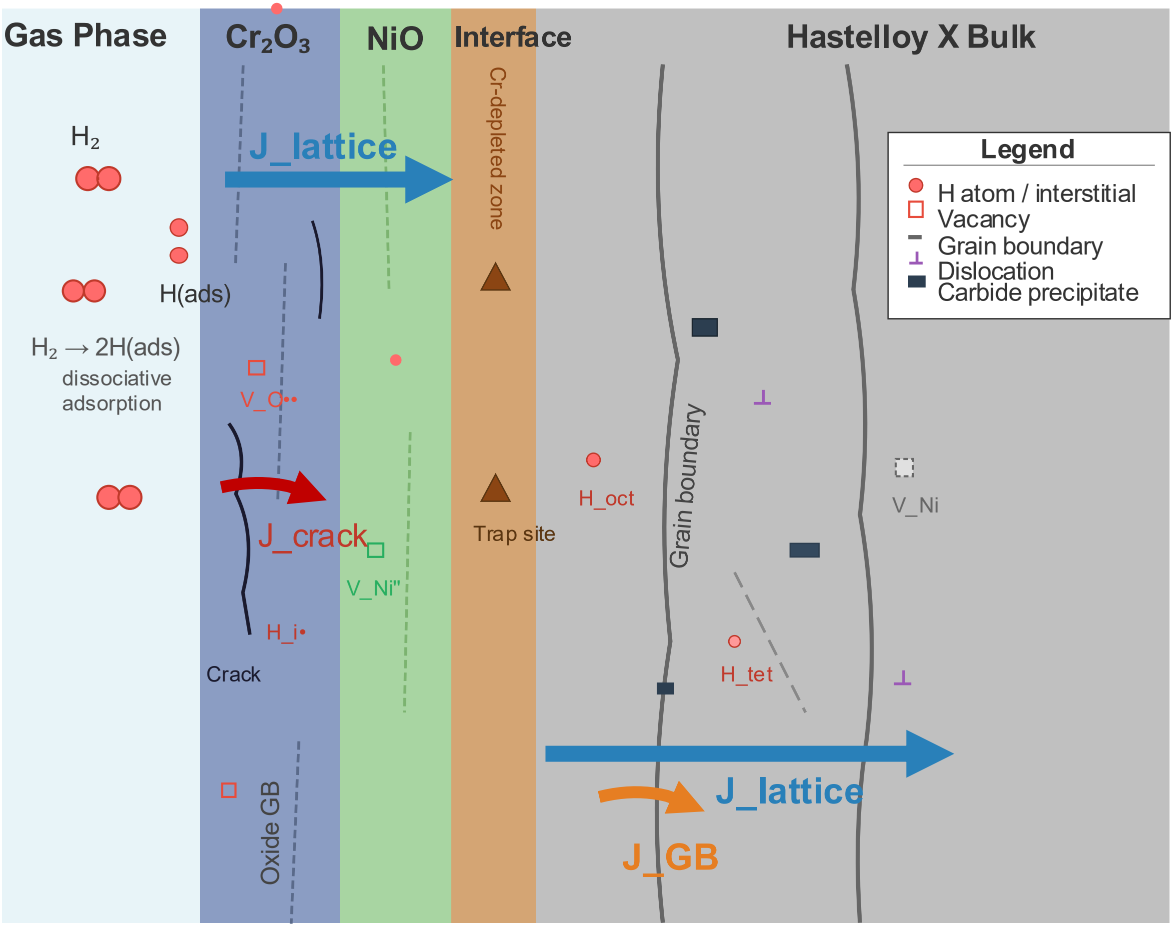

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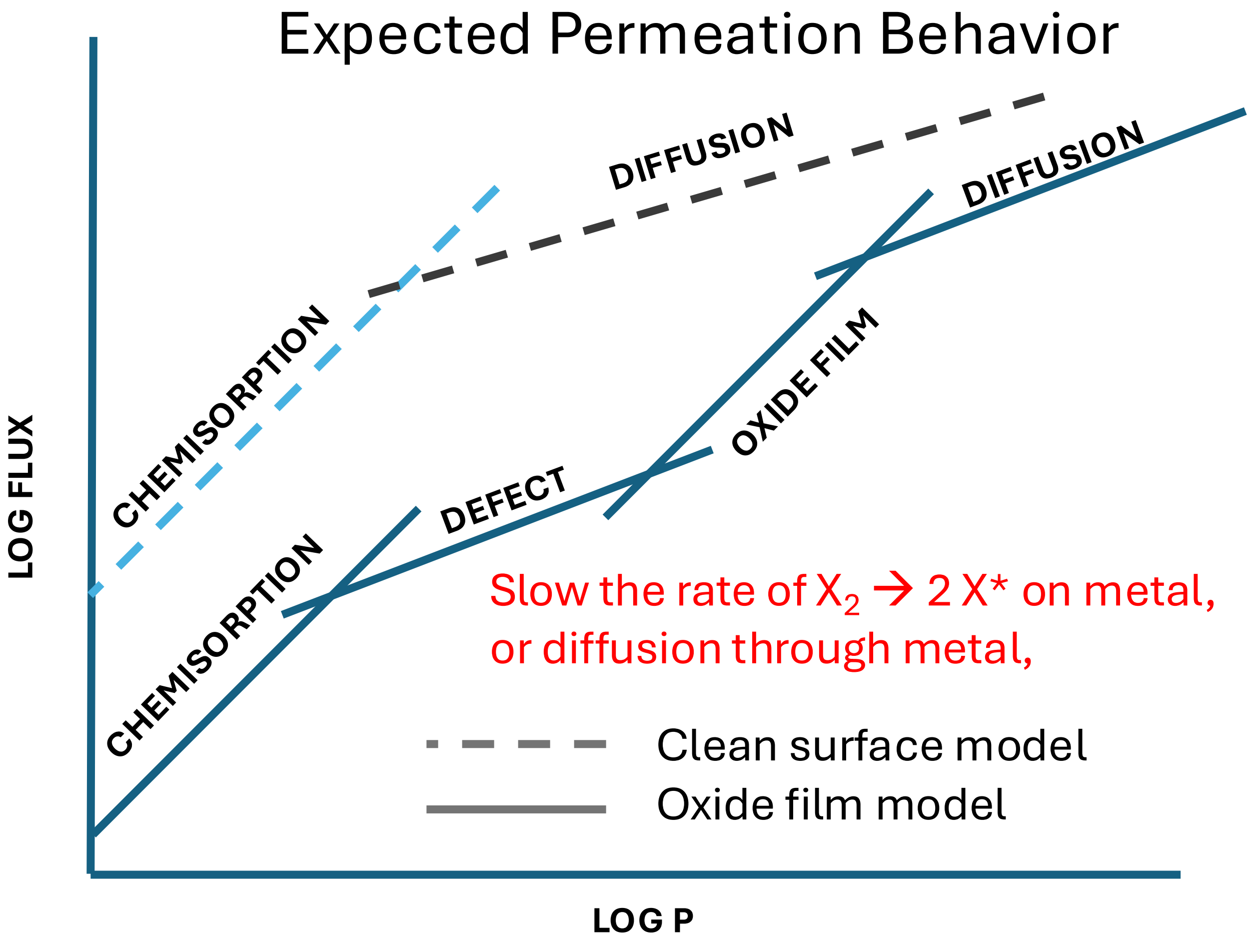

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Perfect Metal
Atomic Diffusion
(Level 1)

Perfect Oxide
Molecular Diffusion
(Level 2a)

Perfect Oxide
+Perfect Metal
Series Resistance
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Defective Oxide
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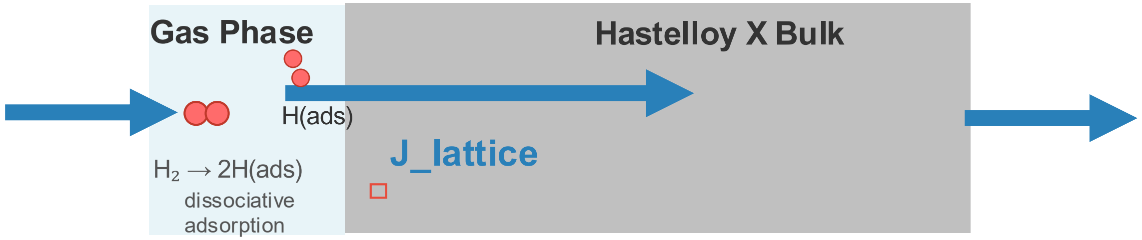
Perfect Metal Continuum Model (Baseline)



Physics: Sieverts' Law + Fick's Law

- Sievert's Law (surface equilibrium)

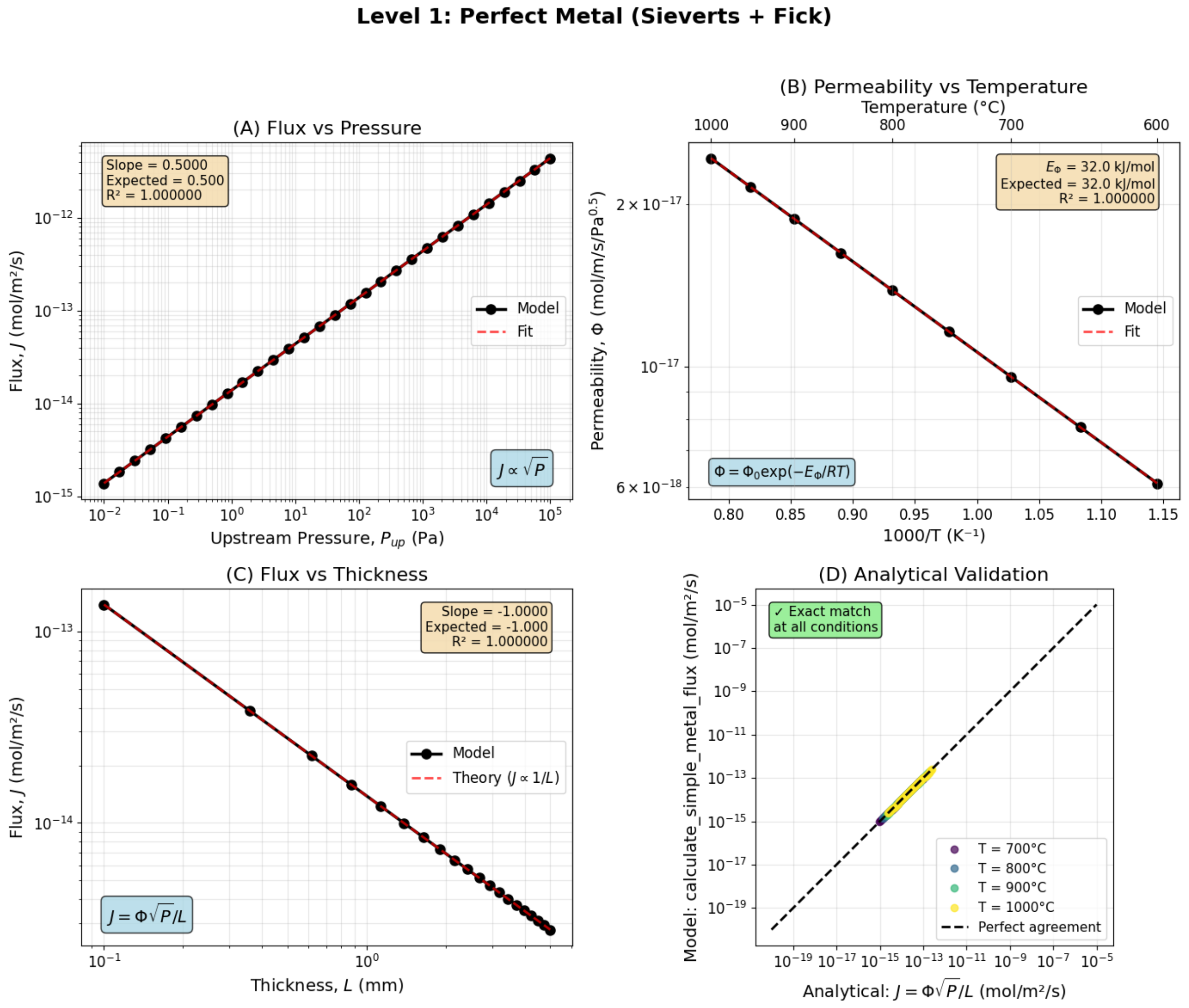
$$C = K_s \,.\, \sqrt{P}$$

- Fick's Law (Bulk diffusion)

$$Flux\ J = \frac{D\left(C_{up} - C_{\mathrm{down}}\right)}{L}$$

- Combined:

$$\boxed{J = \left(\frac{DK_s}{L}\right) . \left(\sqrt{P_{up}} - \sqrt{P_{down}}\right)}$$



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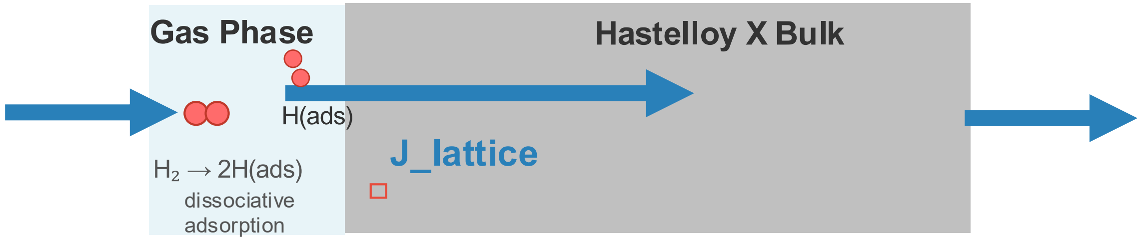

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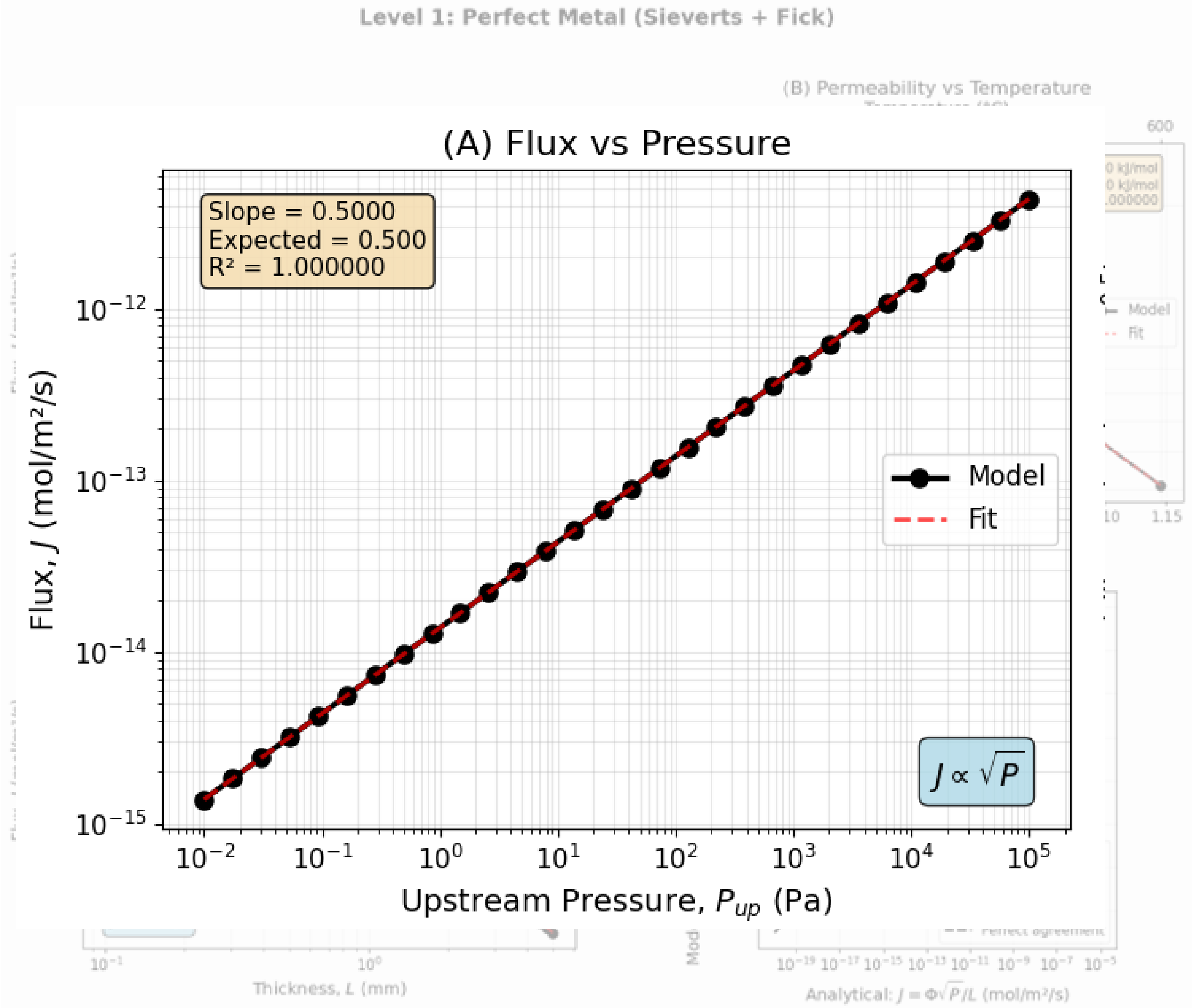

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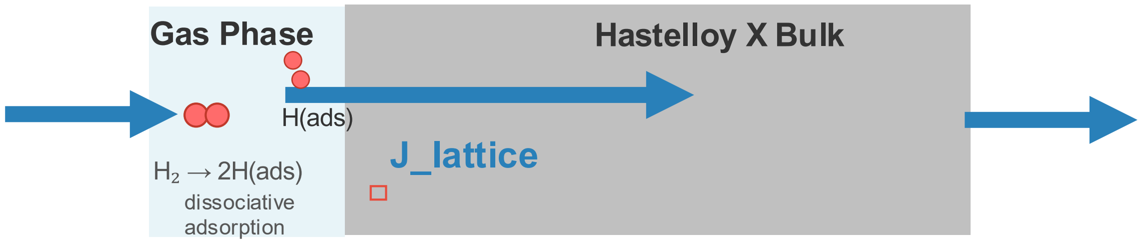

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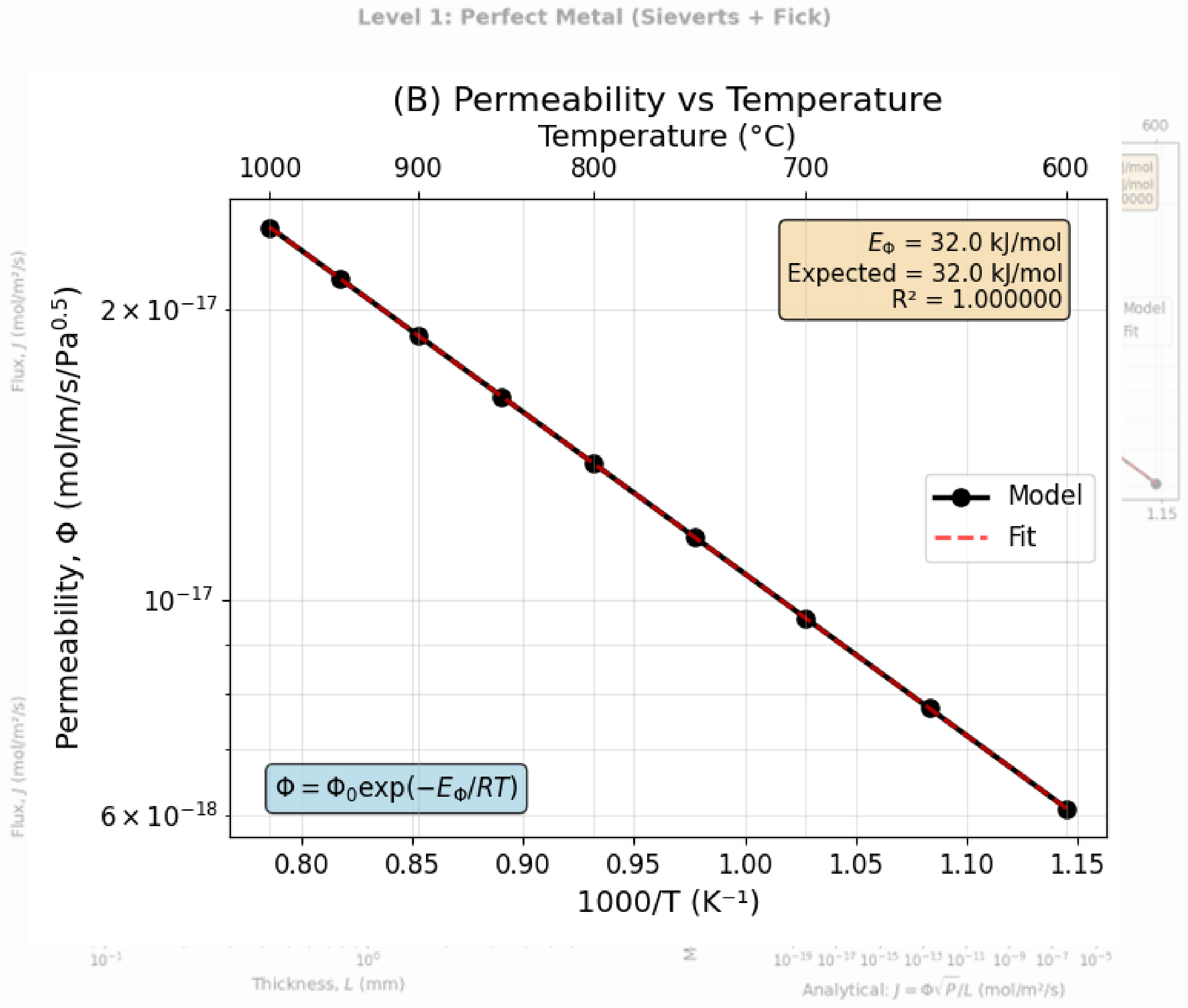

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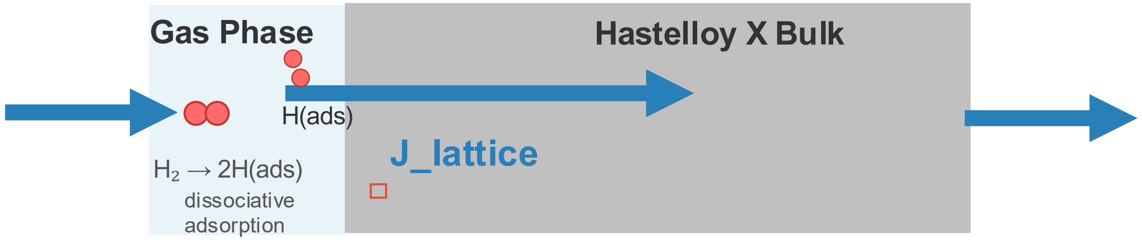

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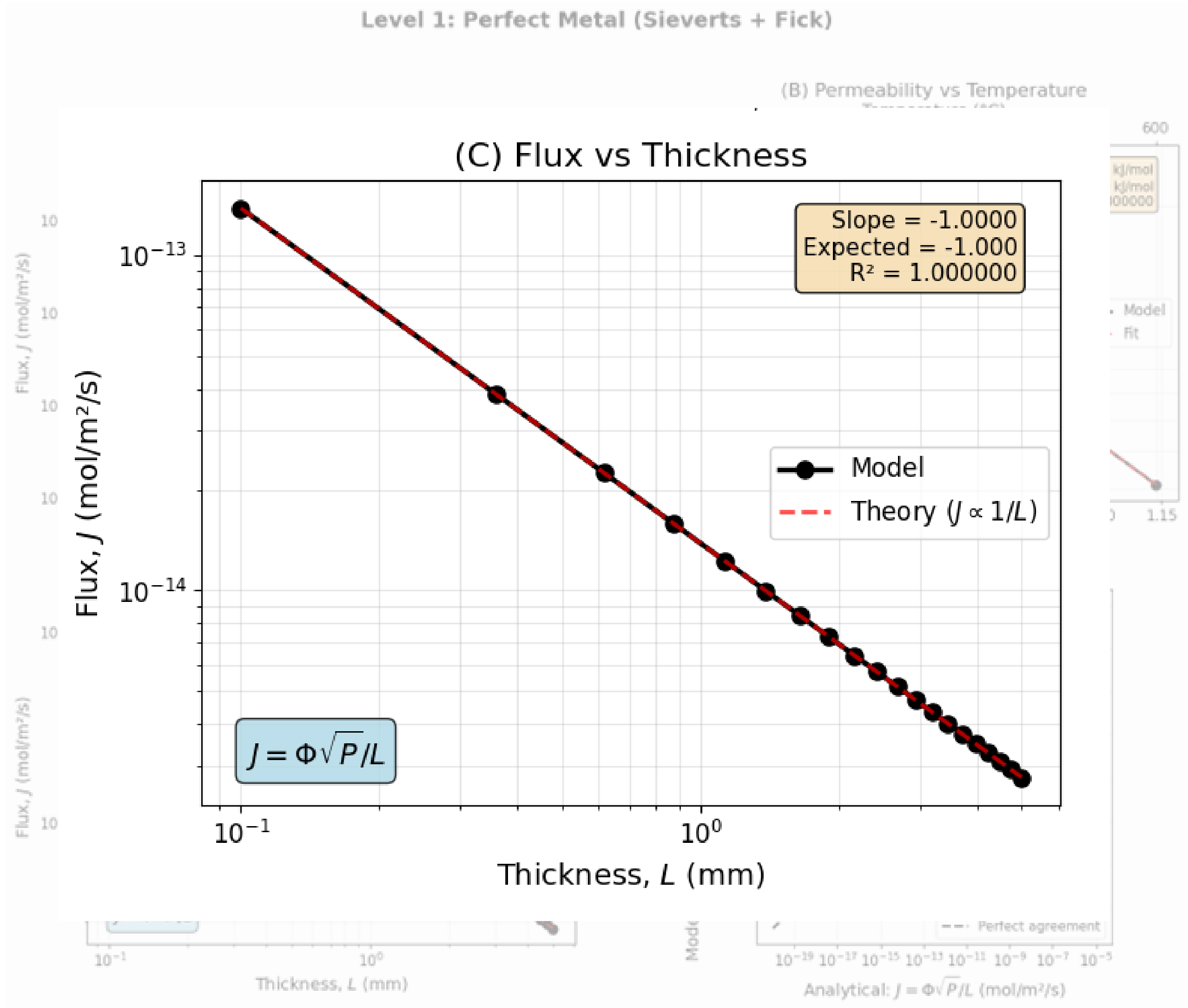

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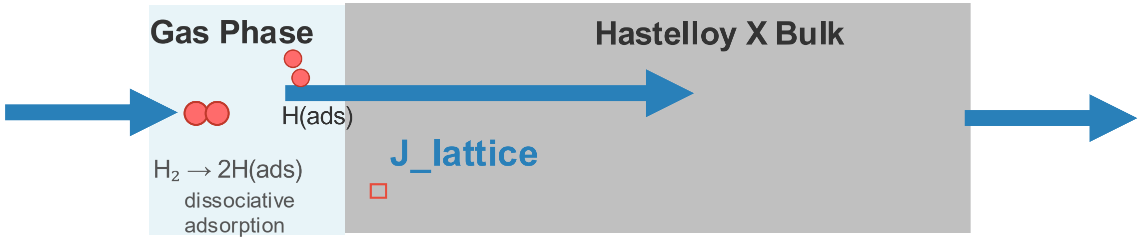

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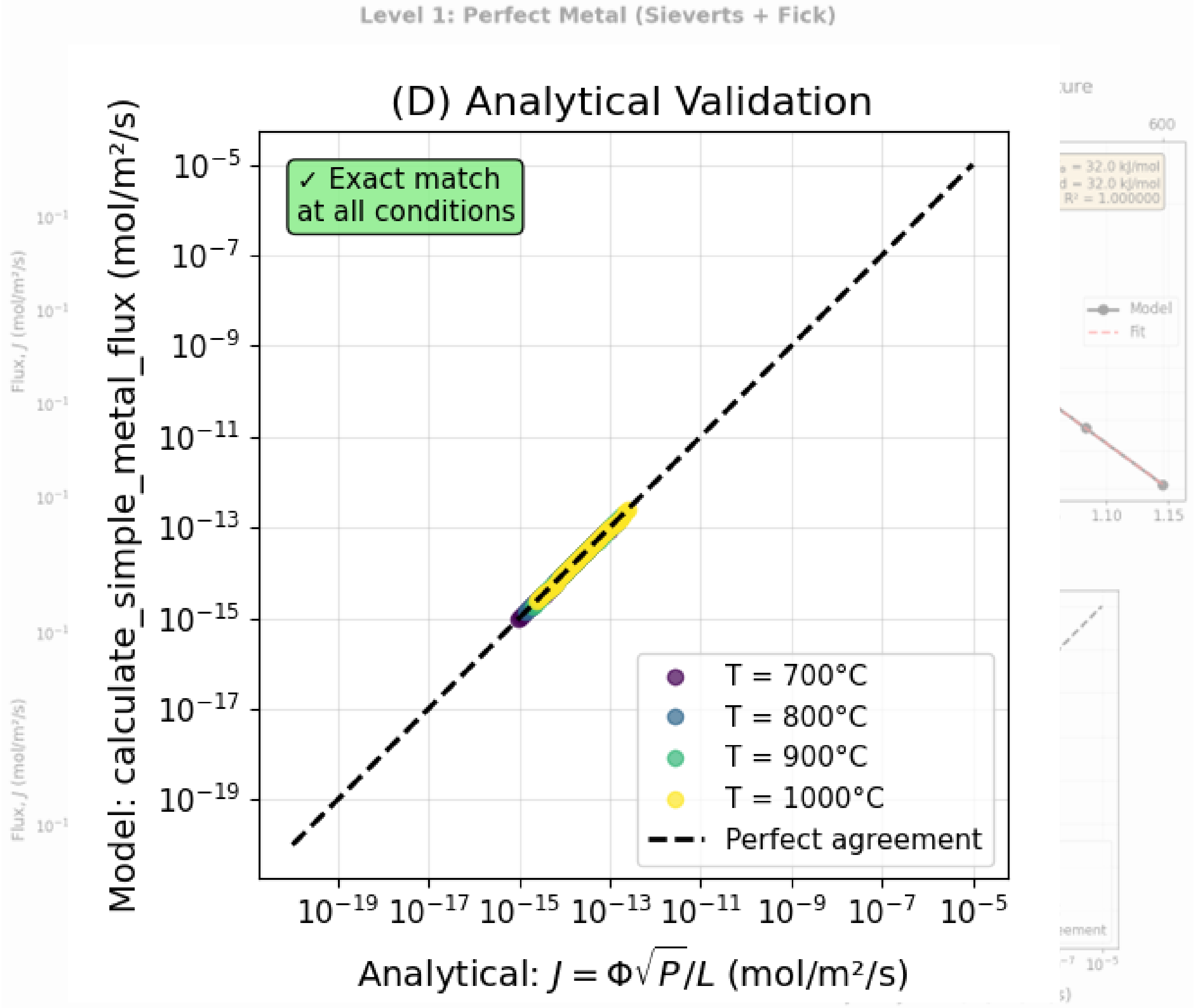

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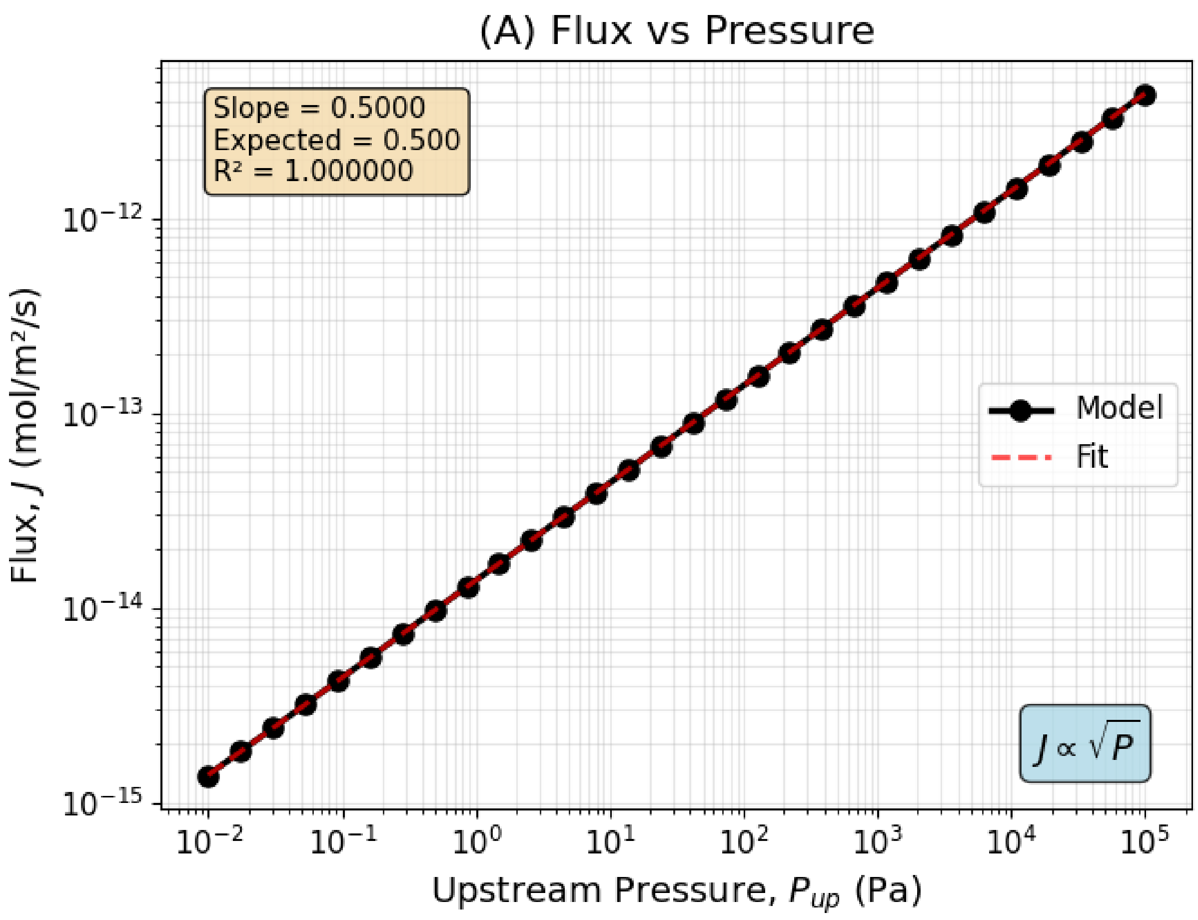

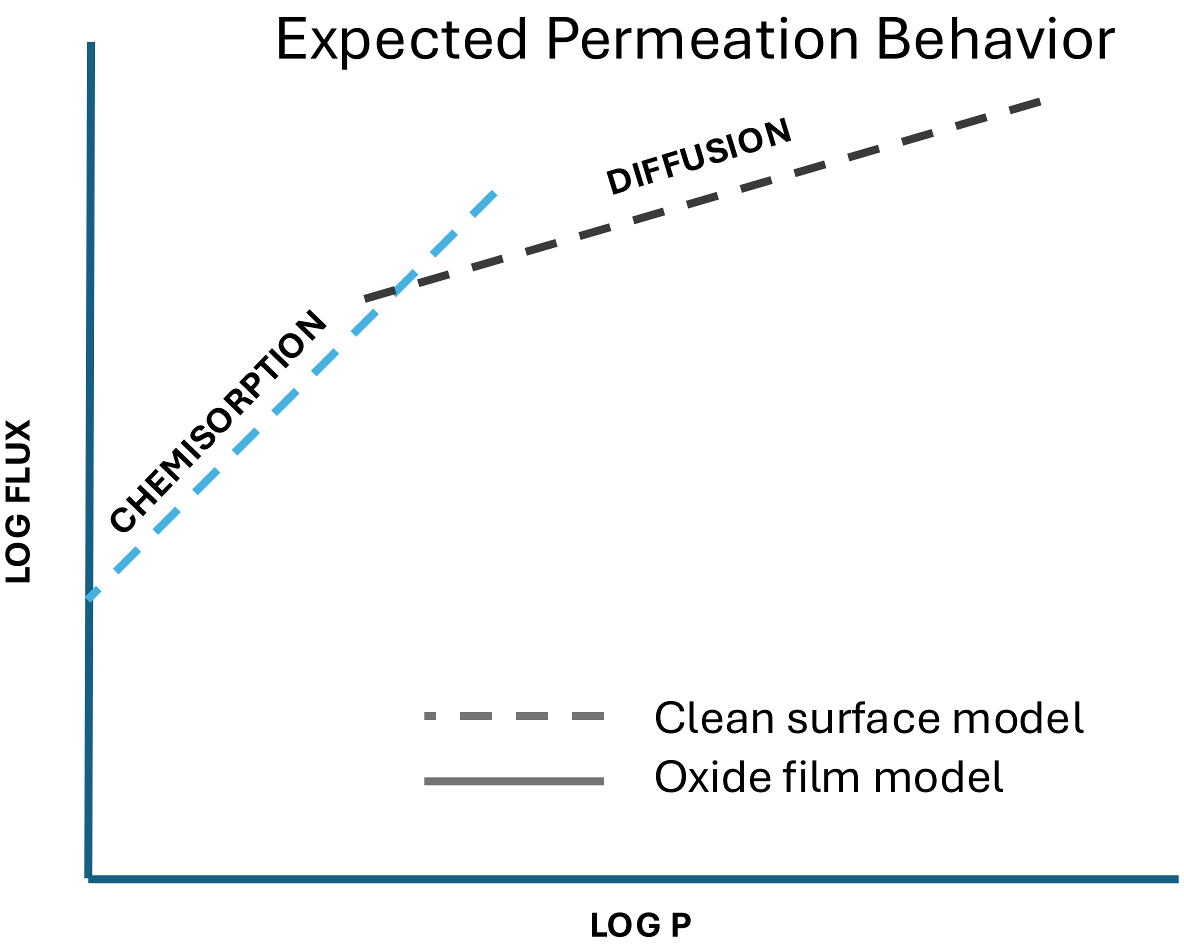

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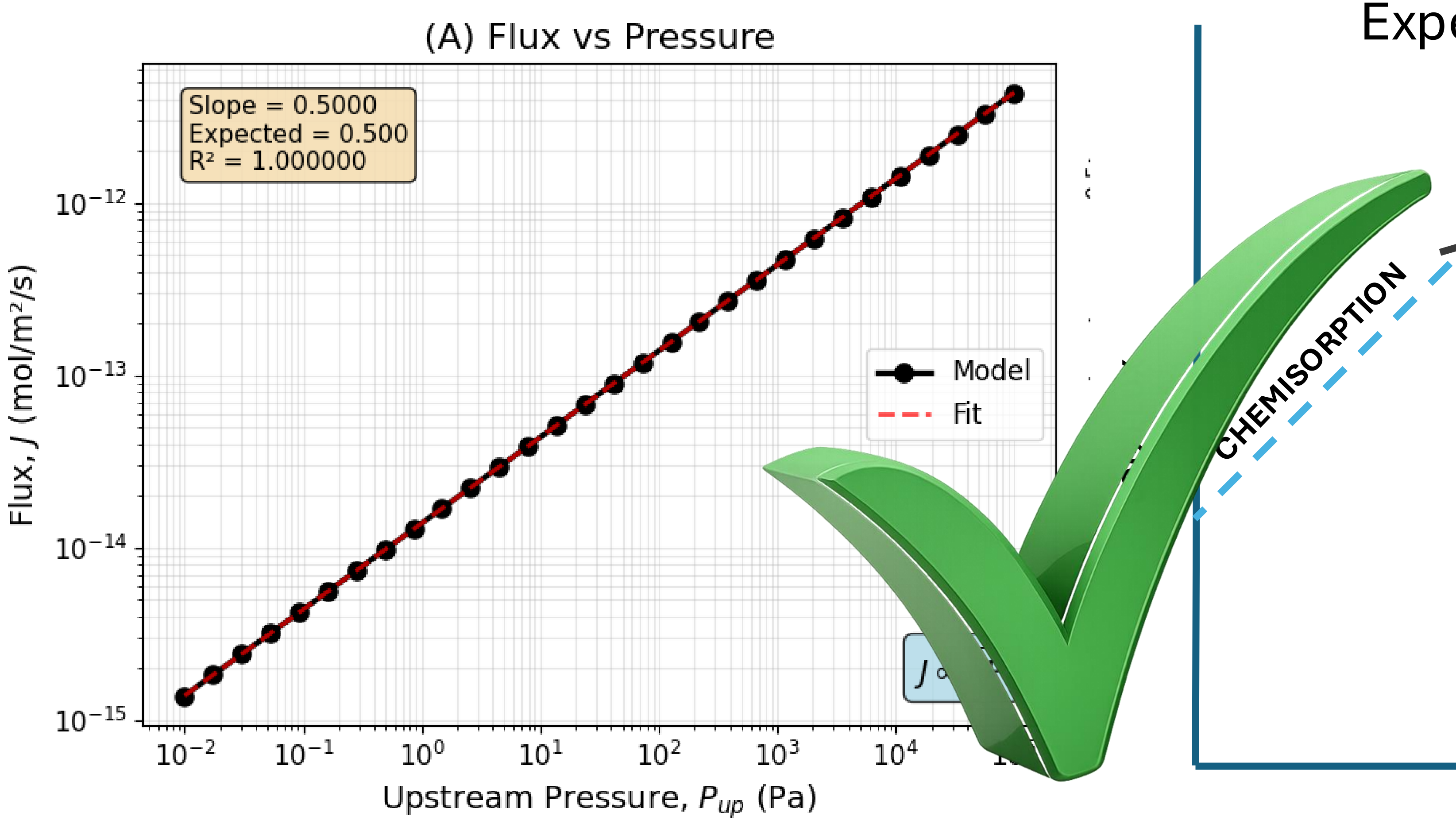
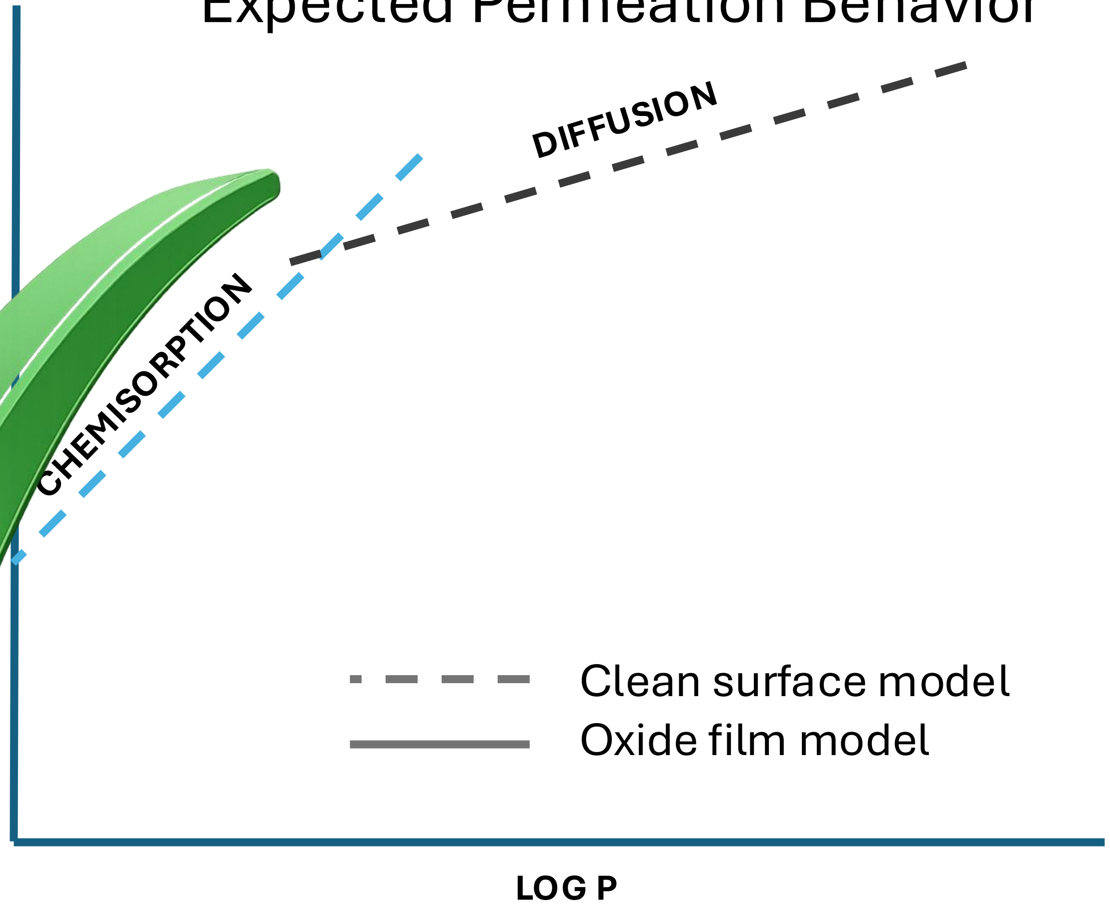


Expected Permeation Behavior



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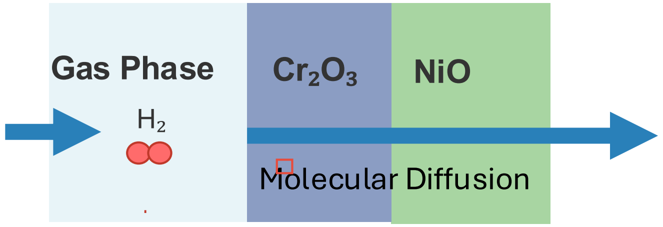
Perfect Oxide Only (Molecular Diffusion)



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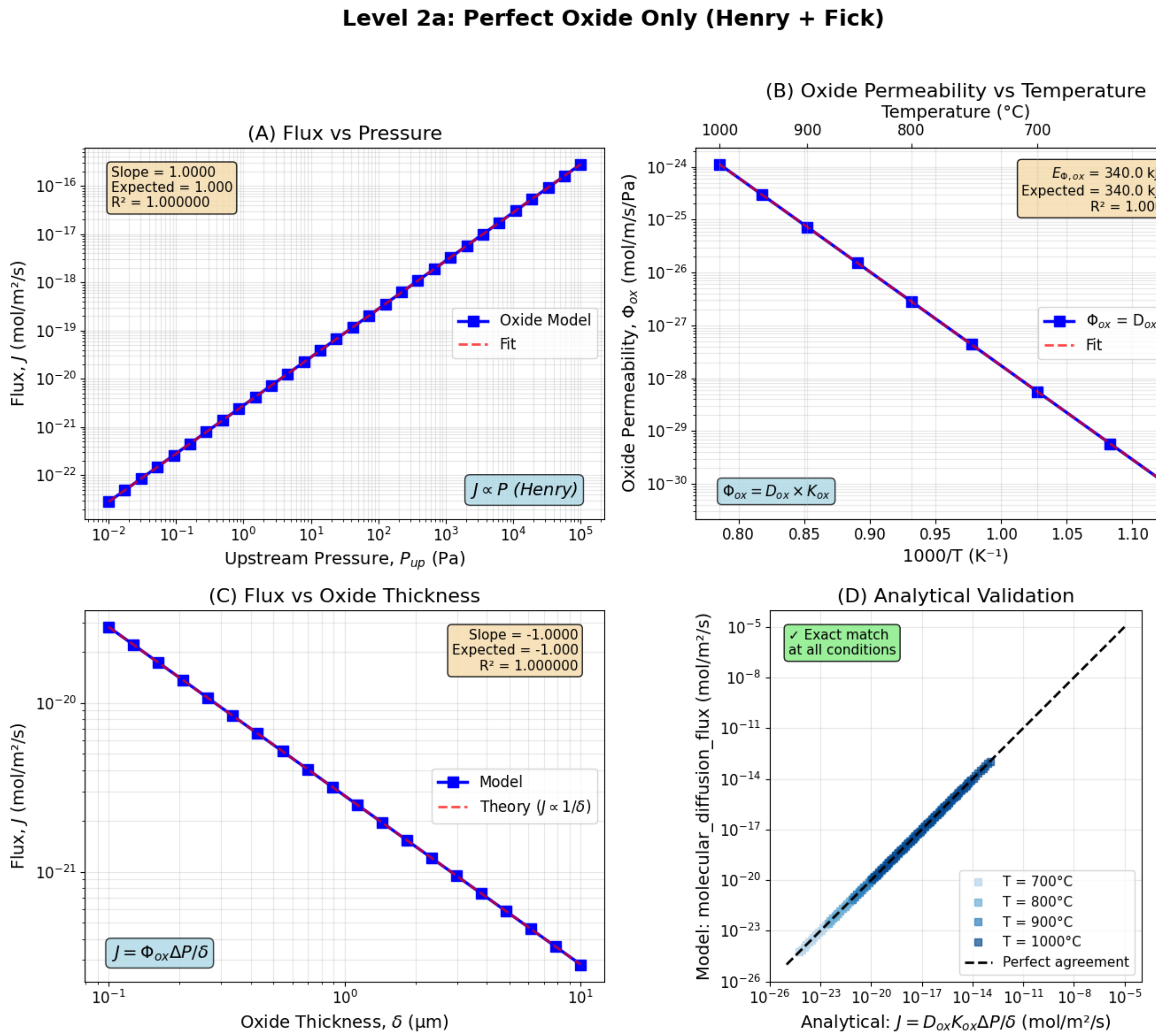

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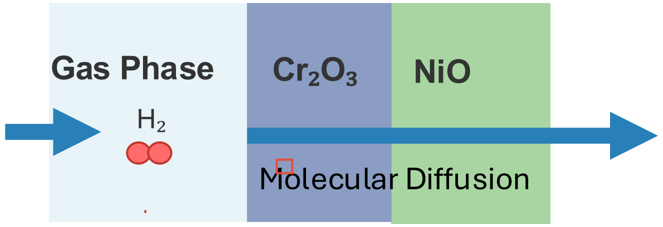

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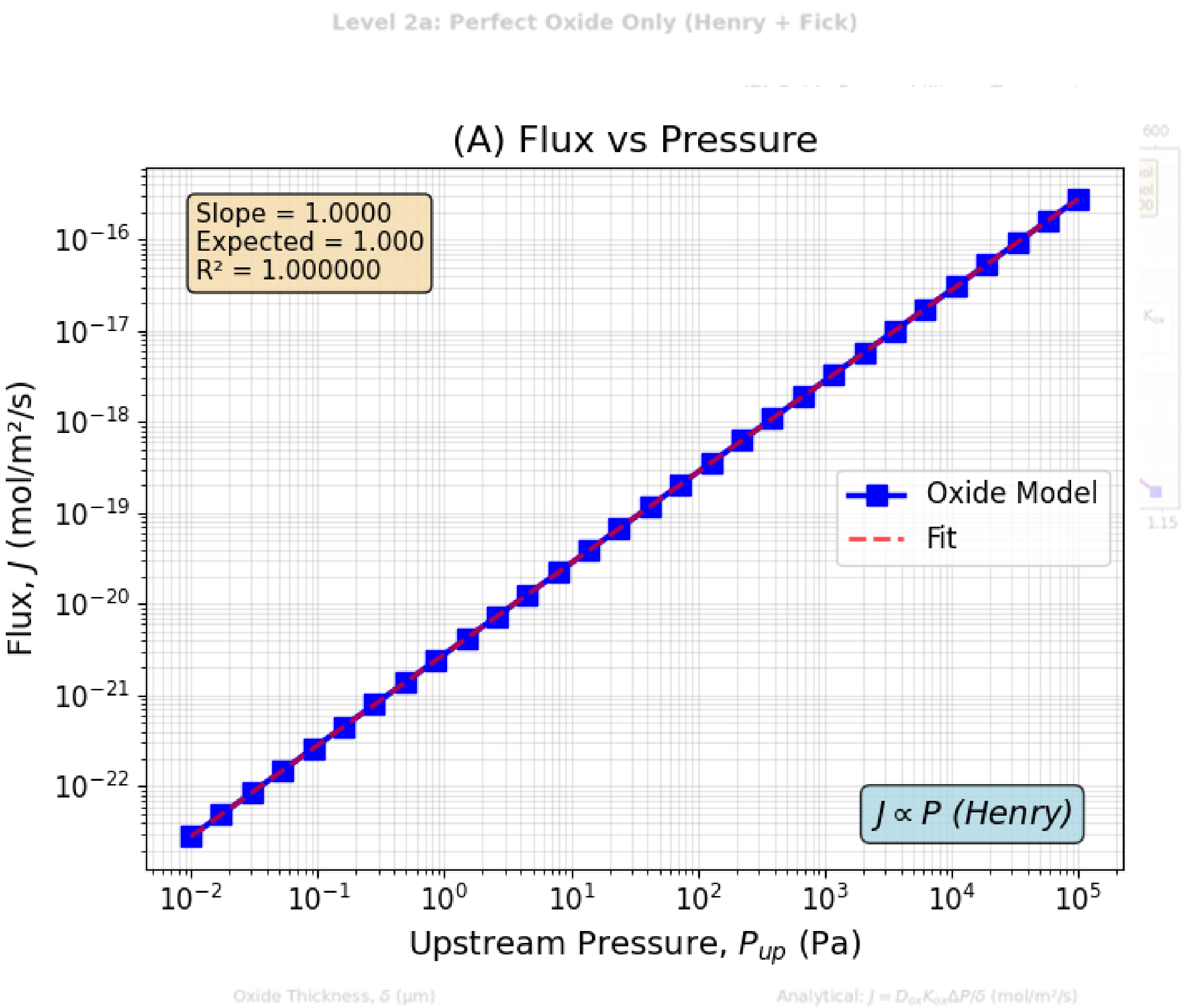

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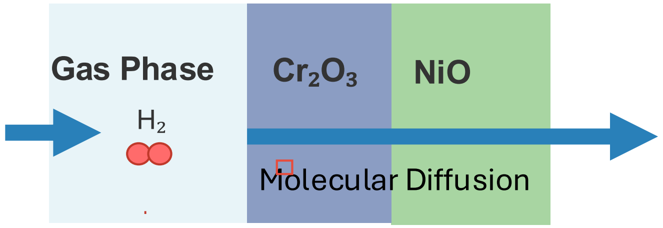

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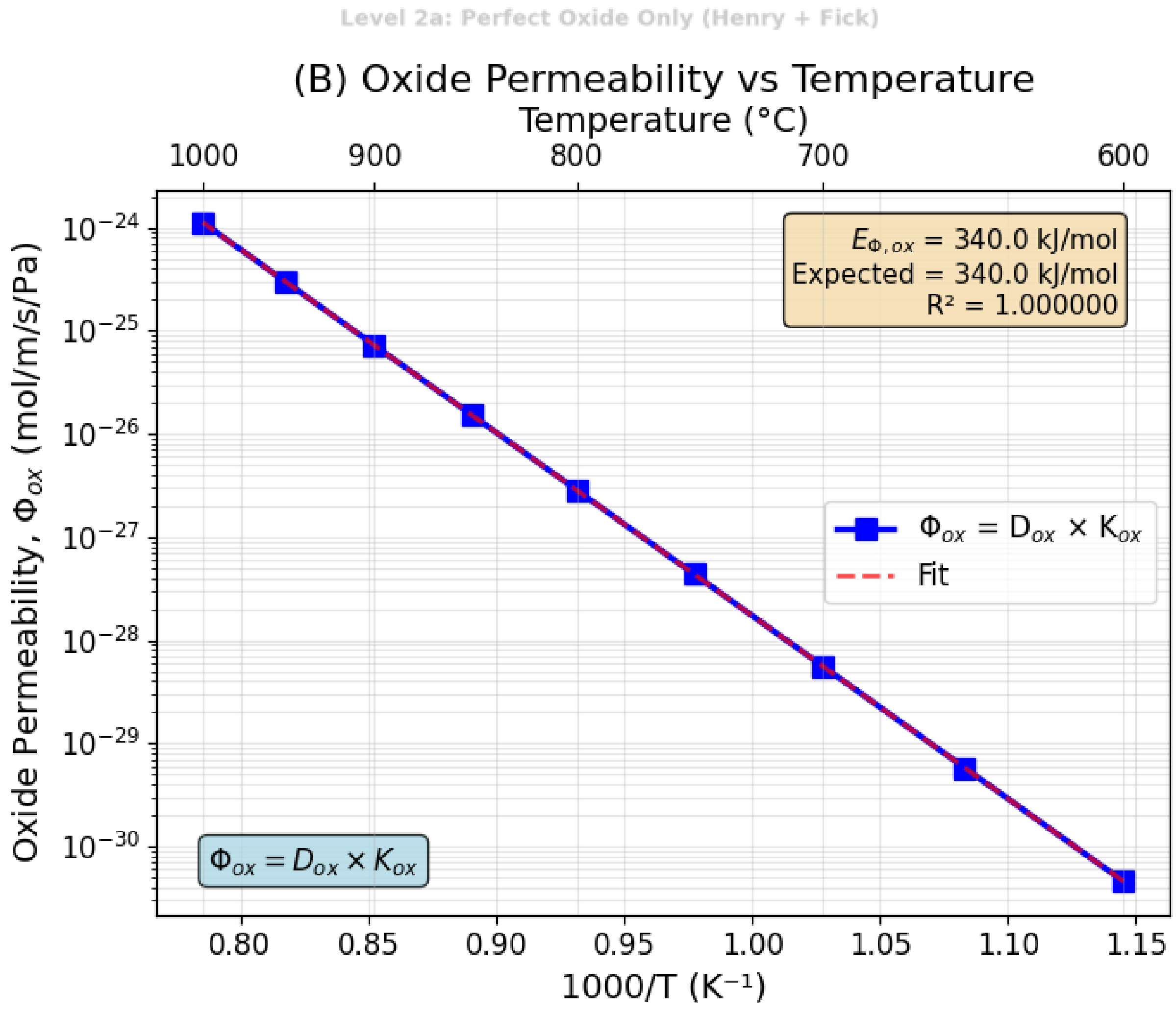

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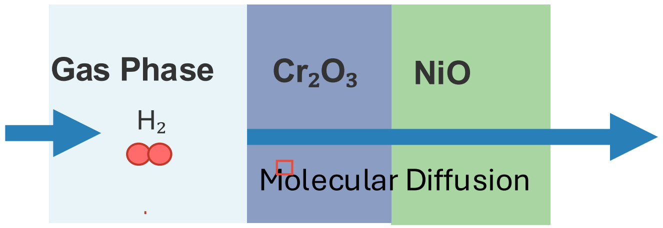

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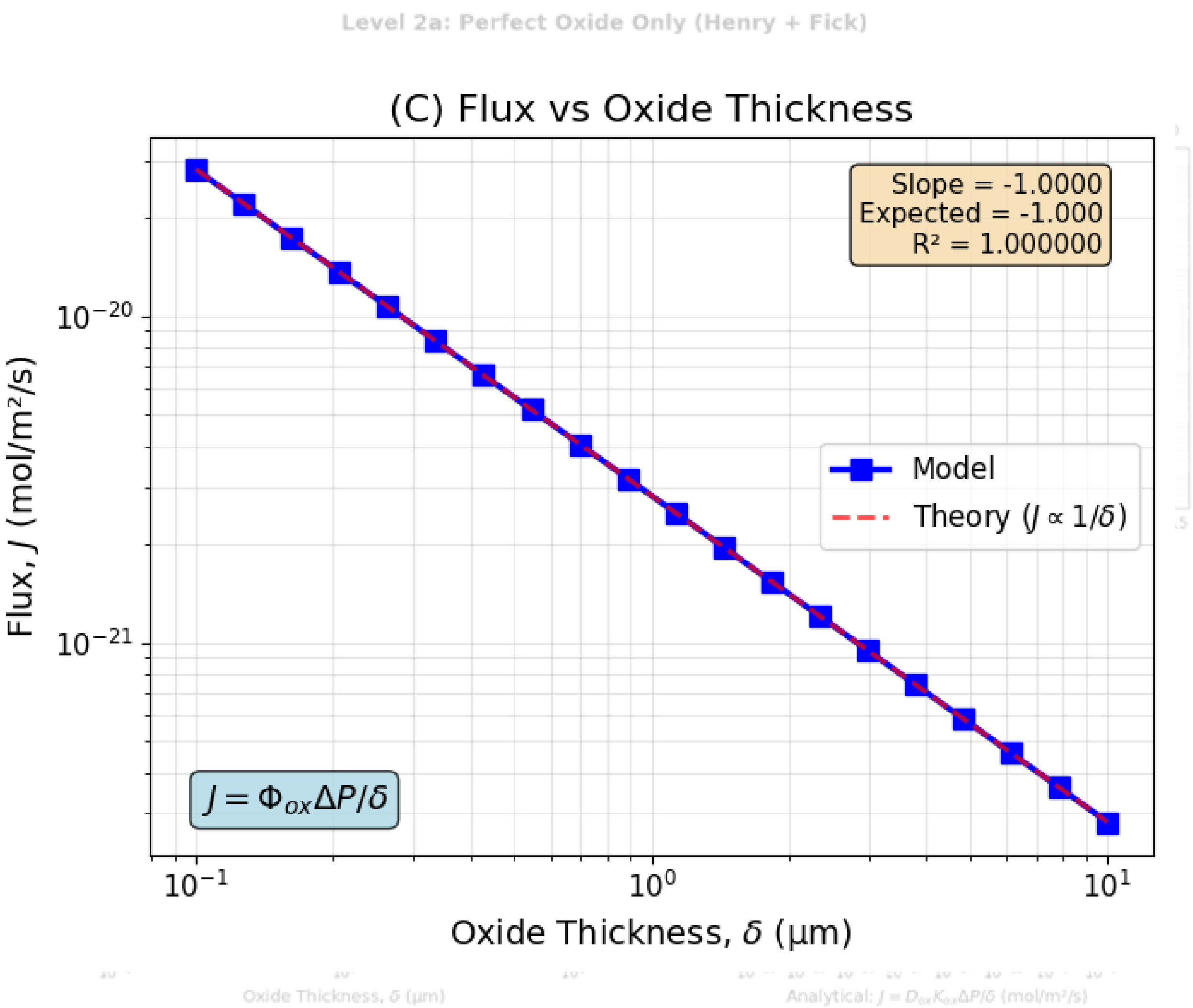

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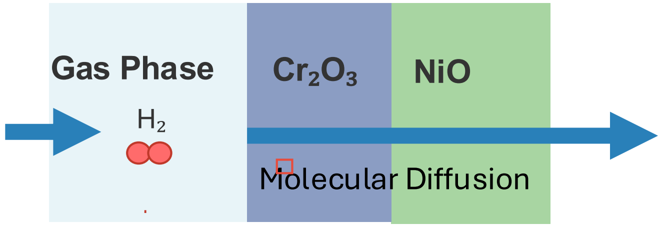

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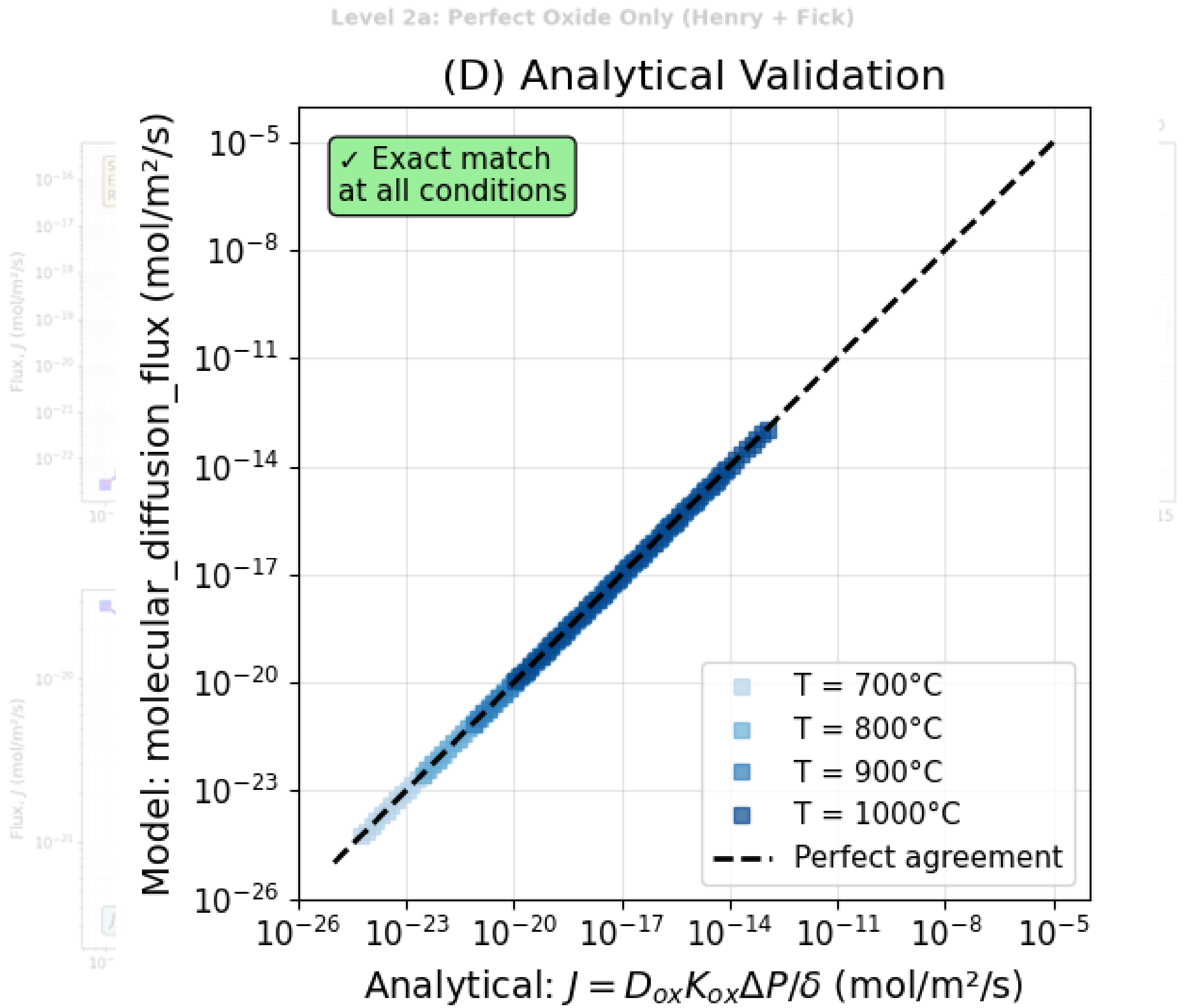

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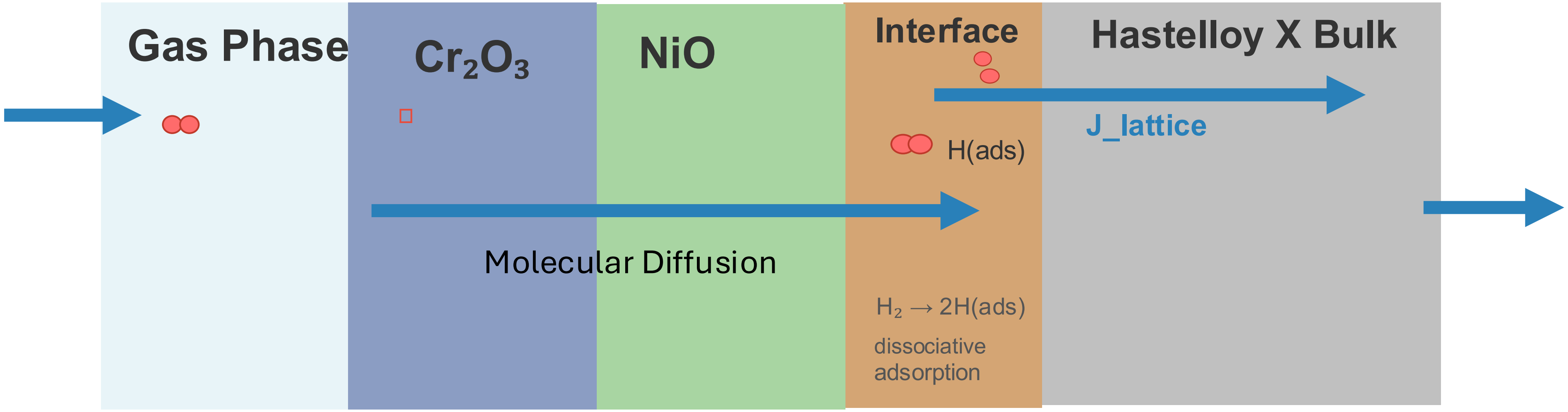
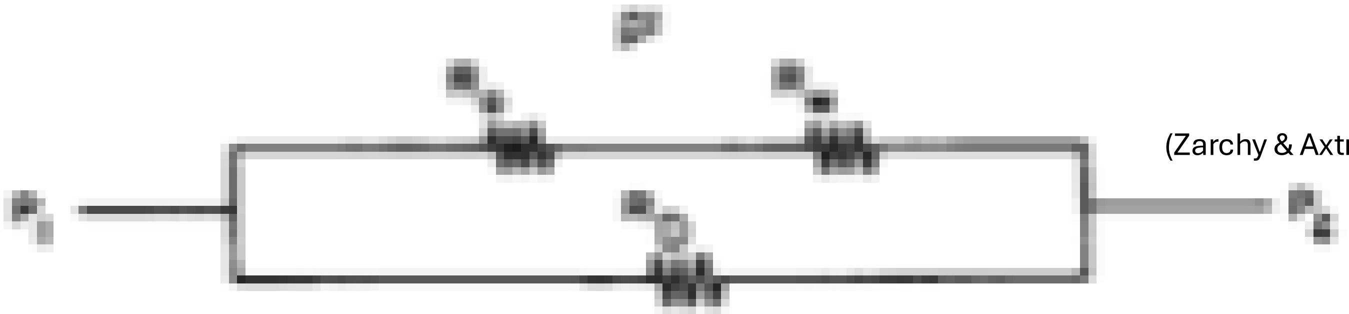
Perfect Oxide + Perfect Metal (Series Resistance)





(Zarchy & Axtmann, 1979)

Perfect Oxide + Perfect Metal (Series Resistance)

Flux Balance Equation

$$\text{Metal Flux} = -J = \frac{DK_s}{x_{metal}}\left(P_{interface}^{1/2} - P_{Downstream}^{1/2}\right)$$

$$\text{Oxide Flux} = -J = \frac{D_{ox}K_{ox}}{x_{oxide}}\left(P_{upstream}^{1} - P_{interface}^{1}\right)$$

At steady state Metal Flux = Oxide Flux → Solve for P_interface

Solve for P_interface

Let A = $\frac{D_{ox}K_{ox}}{x_{oxide}}$ B = $\frac{DK_s}{x_{metal}}$ and y = $P_{interface}^{1/2}$

$$Ay^2 + By^2 - \left(AP_{upstream} - B\sqrt{P_{downstream}}\right) = 0$$

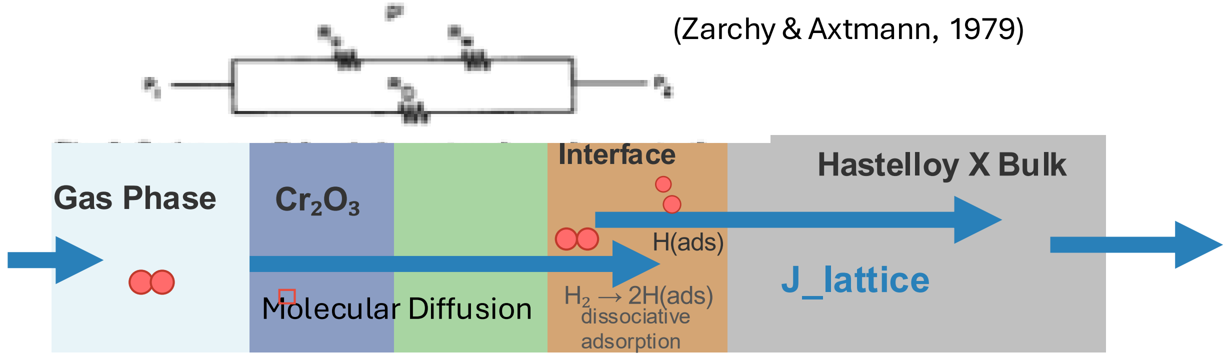
$$y = \sqrt{p_{interface}} = \frac{-B + \sqrt{(B^2 + 4A(AP_{up} + B\sqrt{P_{down}}))}}{2A}$$

$$\boxed{p_{interface} = \left(\frac{-B + \sqrt{(B^2 + 4A(AP_{up} + B\sqrt{P_{down}}))}}{2A}\right)^2}$$

Metal-Oxide Flux matching Condition

Perfect Oxide + Perfect Metal (Series Resistance)

(Zarchy & Axtmann, 1979)



Physics: **Oxide and Metal in series with interface coupling**

At steady state Metal Flux = Oxide Flux → Solve for P_interface

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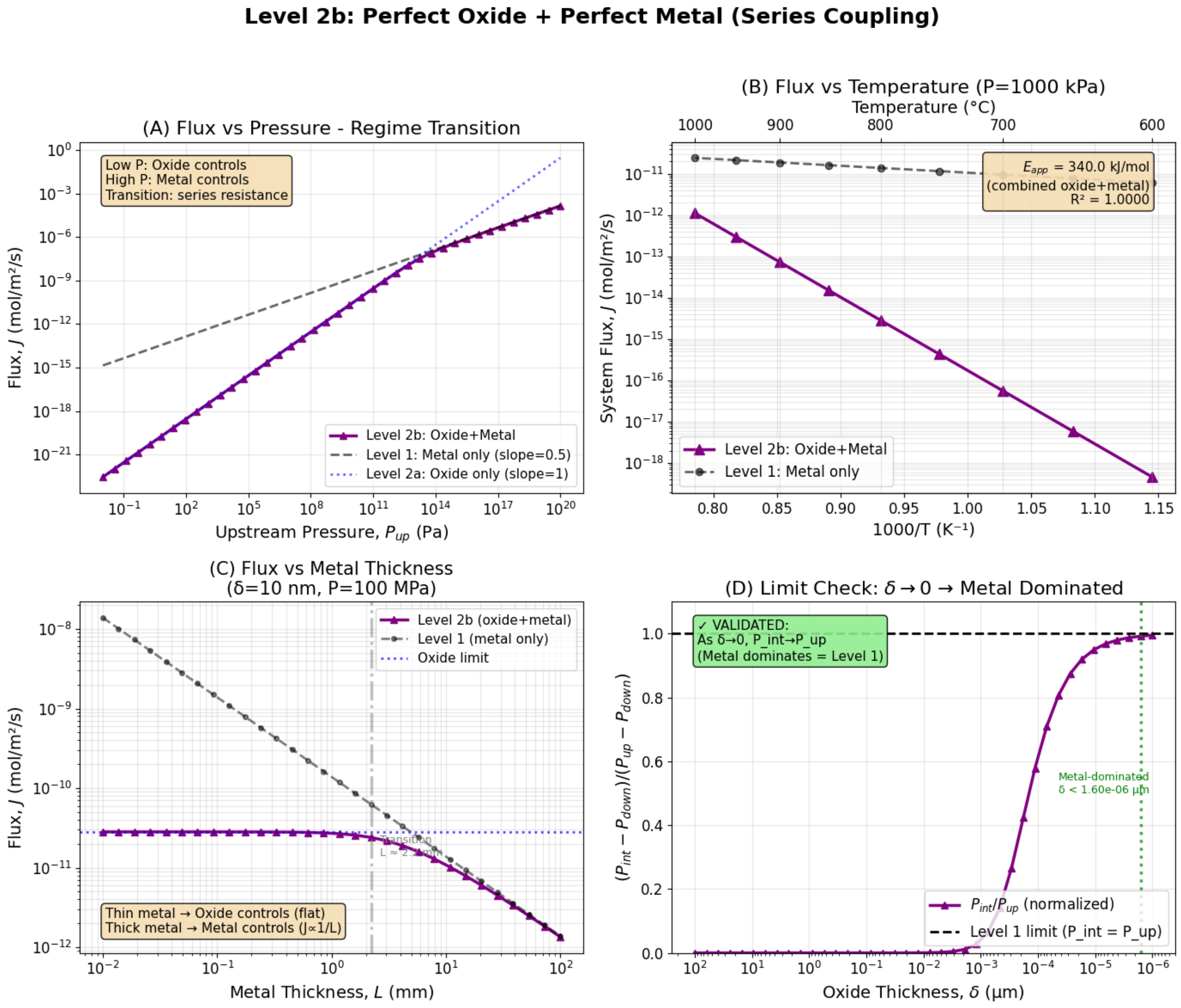
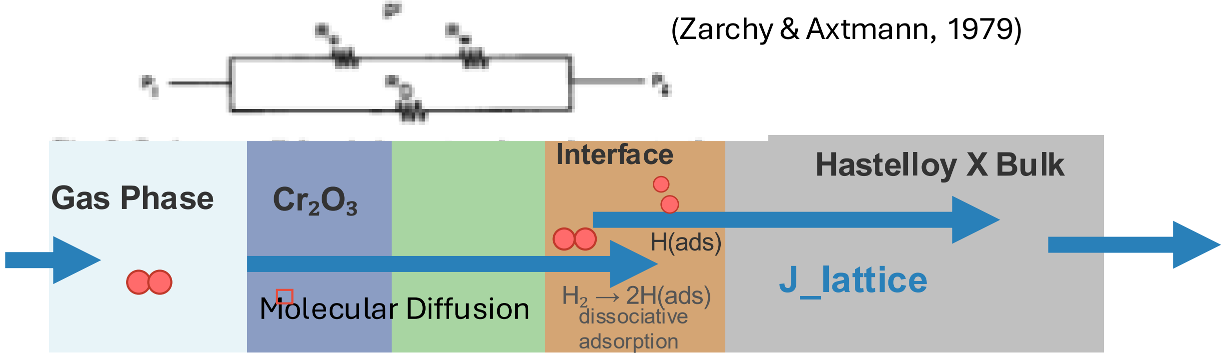


Perfect Oxide + Perfect Metal (Series Resistance)

(Zarchy & Axtmann, 1979)



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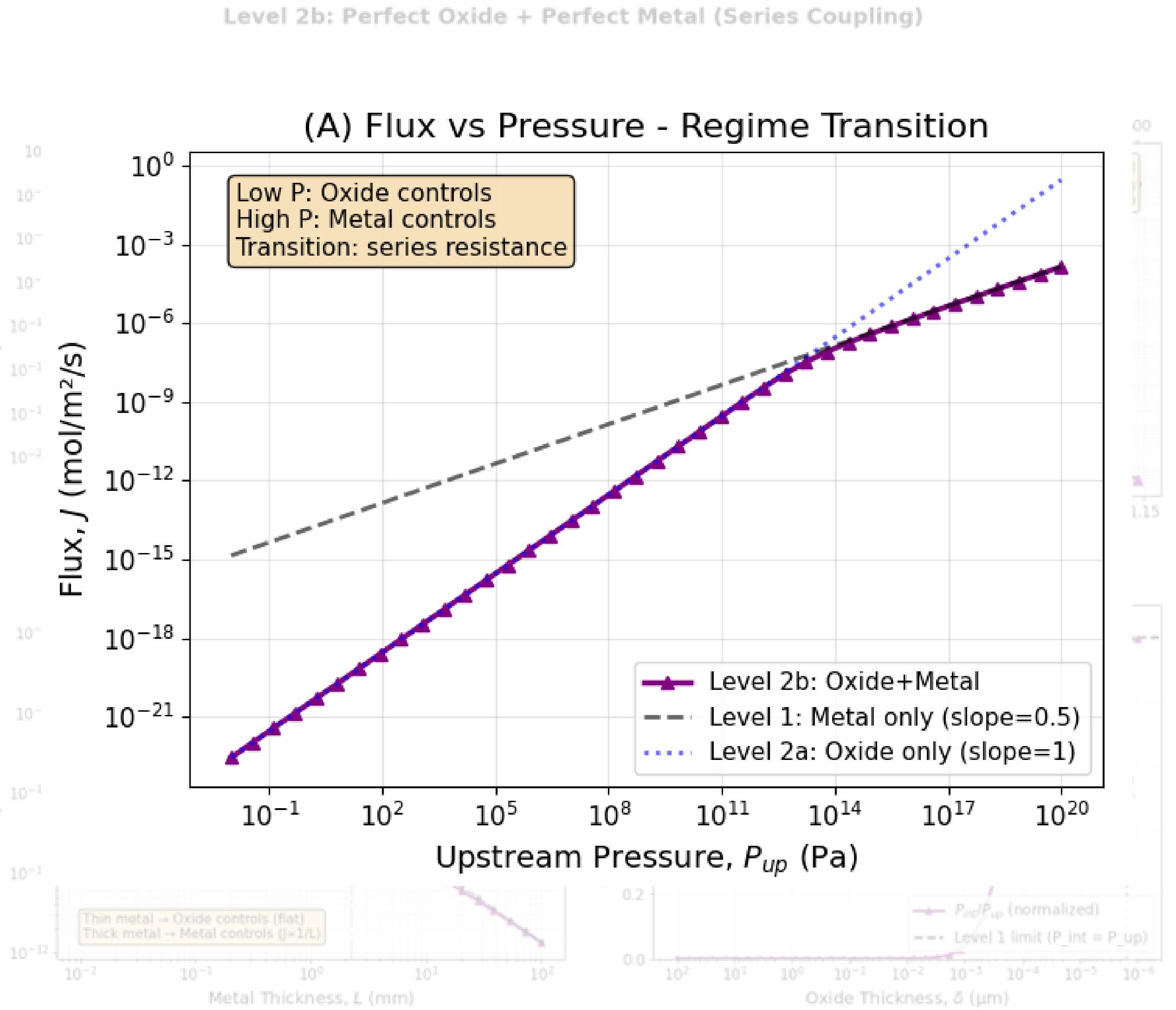

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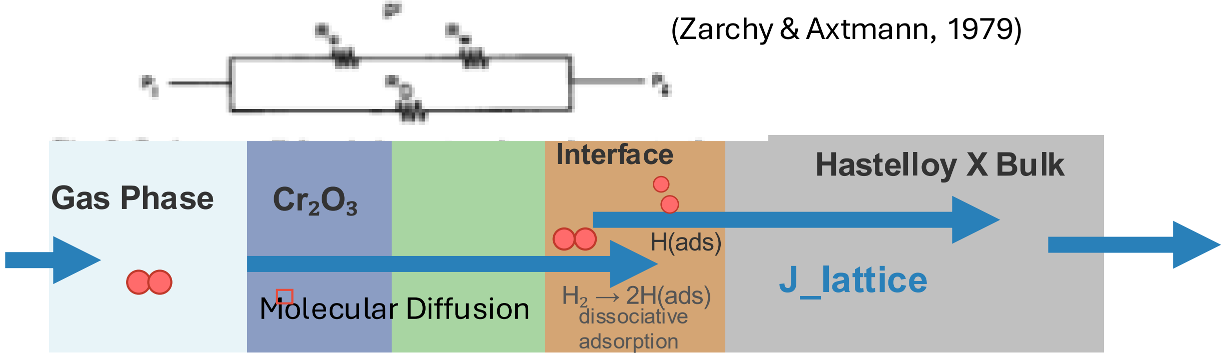

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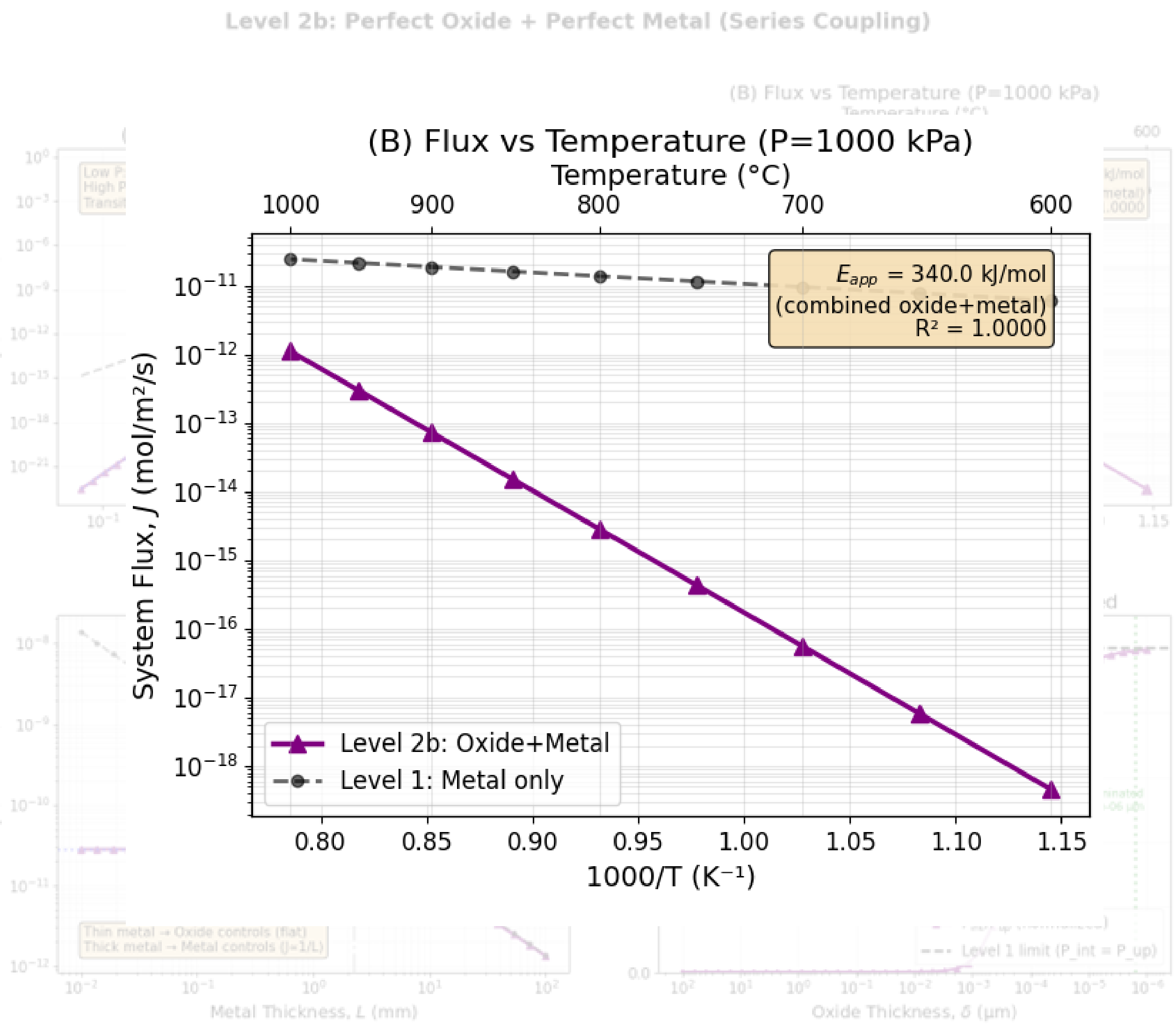
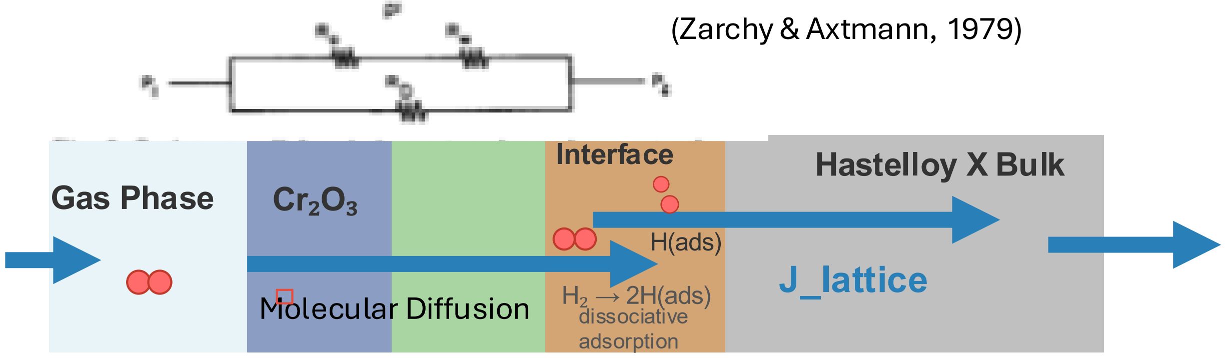


Perfect Oxide + Perfect Metal (Series Resistance)

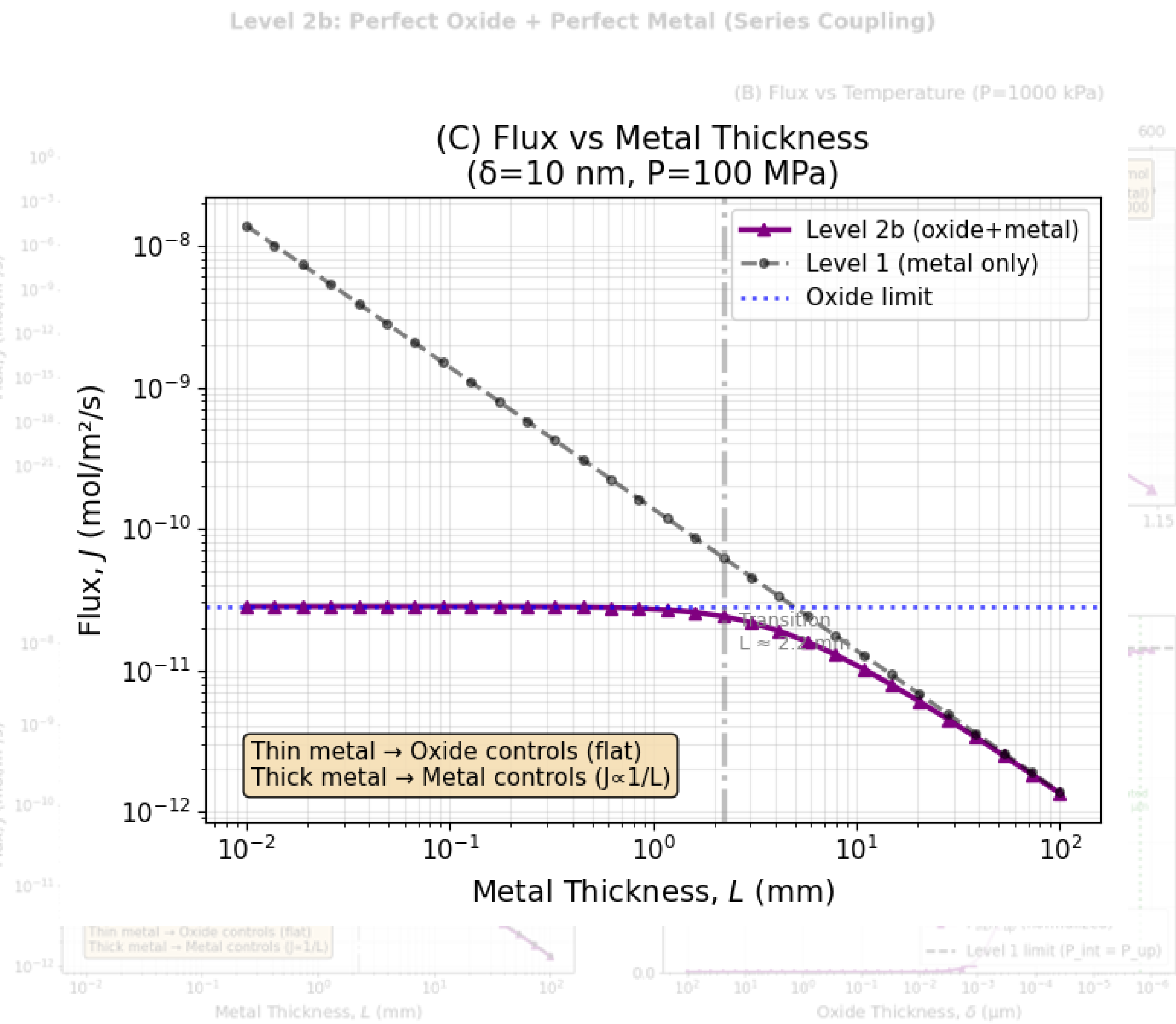
(Zarchy & Axtmann, 1979)



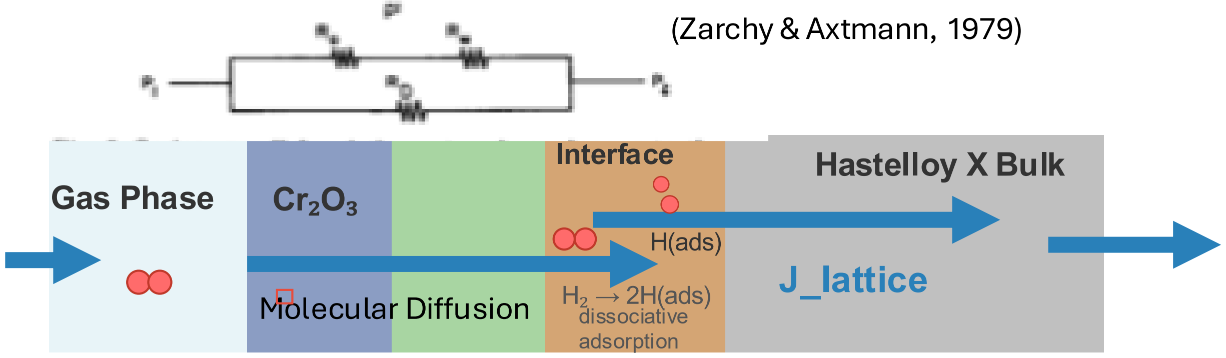
Physics: Oxide and Metal in series with interface coupling

At steady state Metal Flux = Oxide Flux → Solve for P_interface

$$p_{interface} = \left\{ \frac{-B + \sqrt{\left(B^2 + 4A\left(AP_{up} + B\sqrt{P_{down}}\right)\right)}}{2A} \right\}^2$$



Perfect Oxide + Perfect Metal (Series Resistance)



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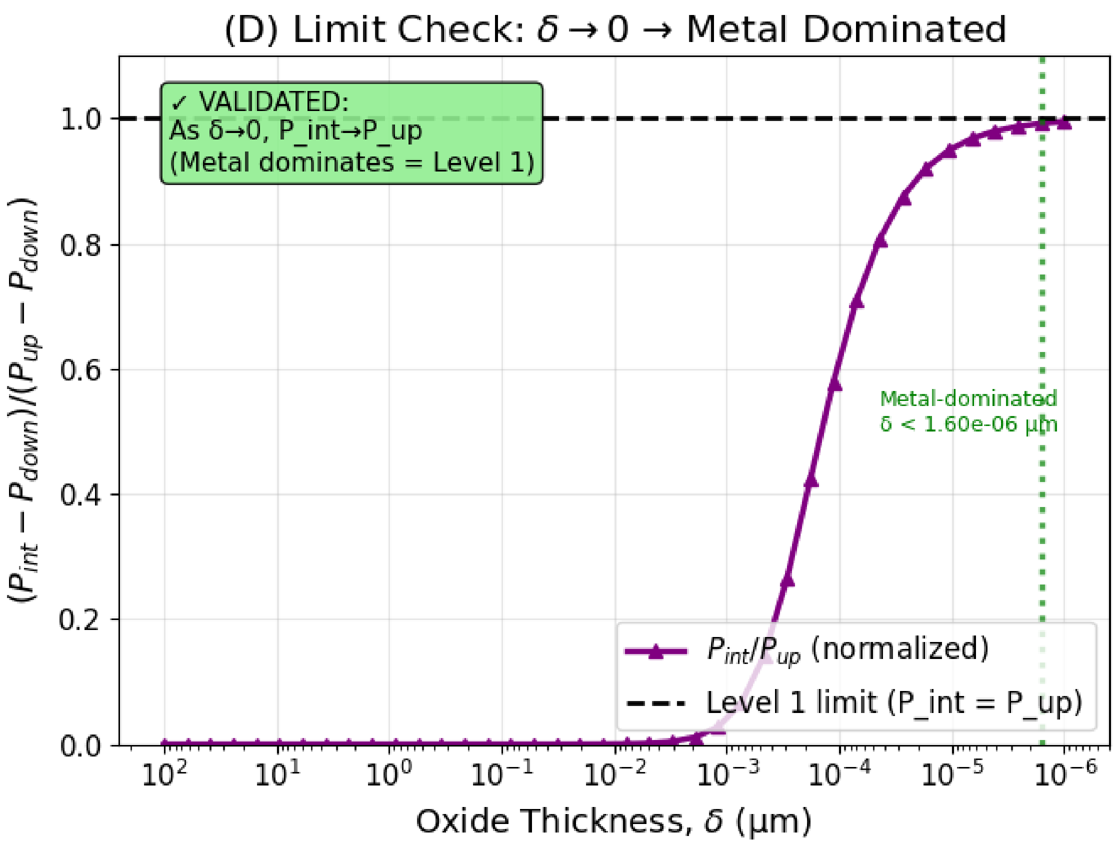
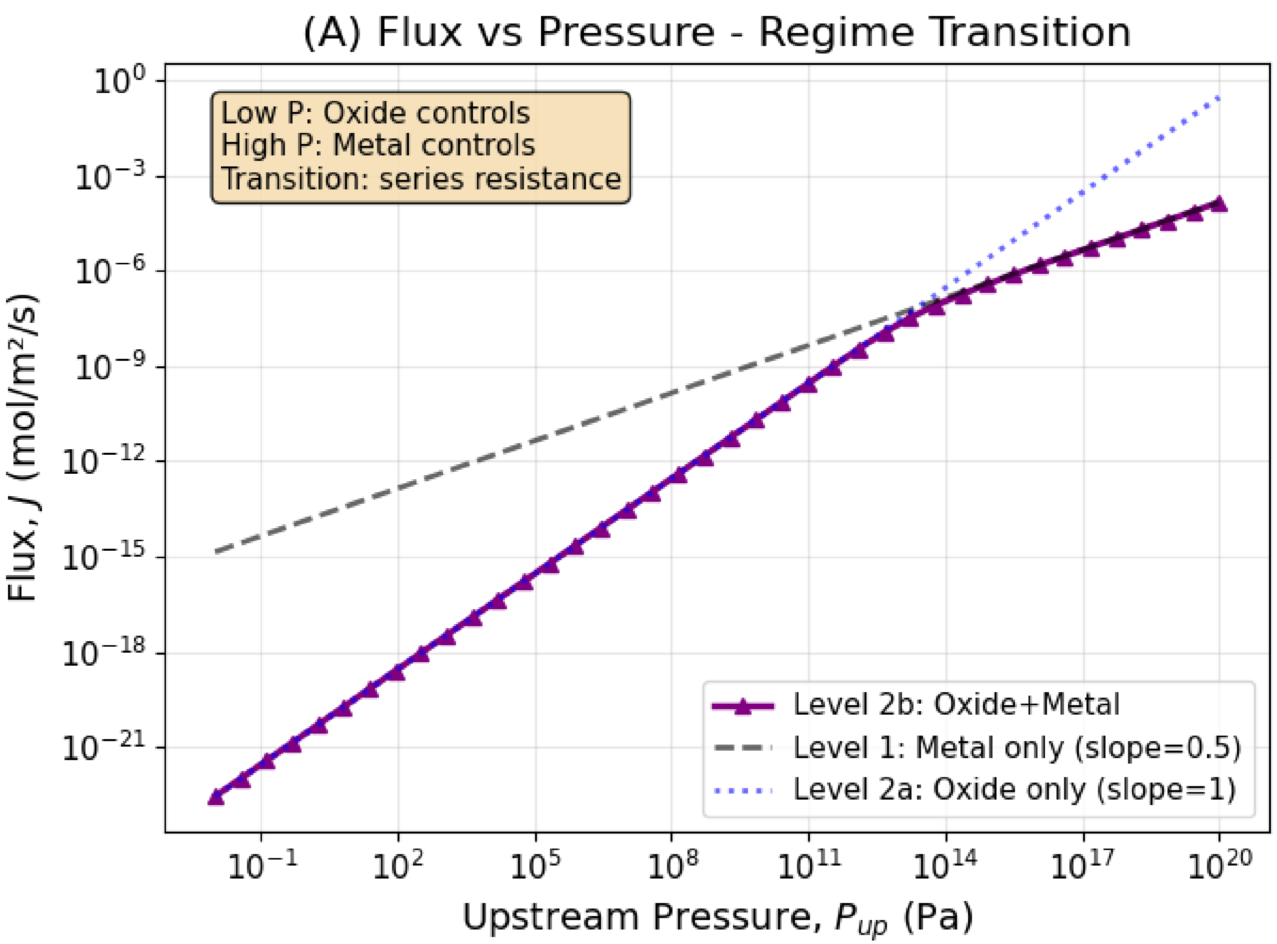
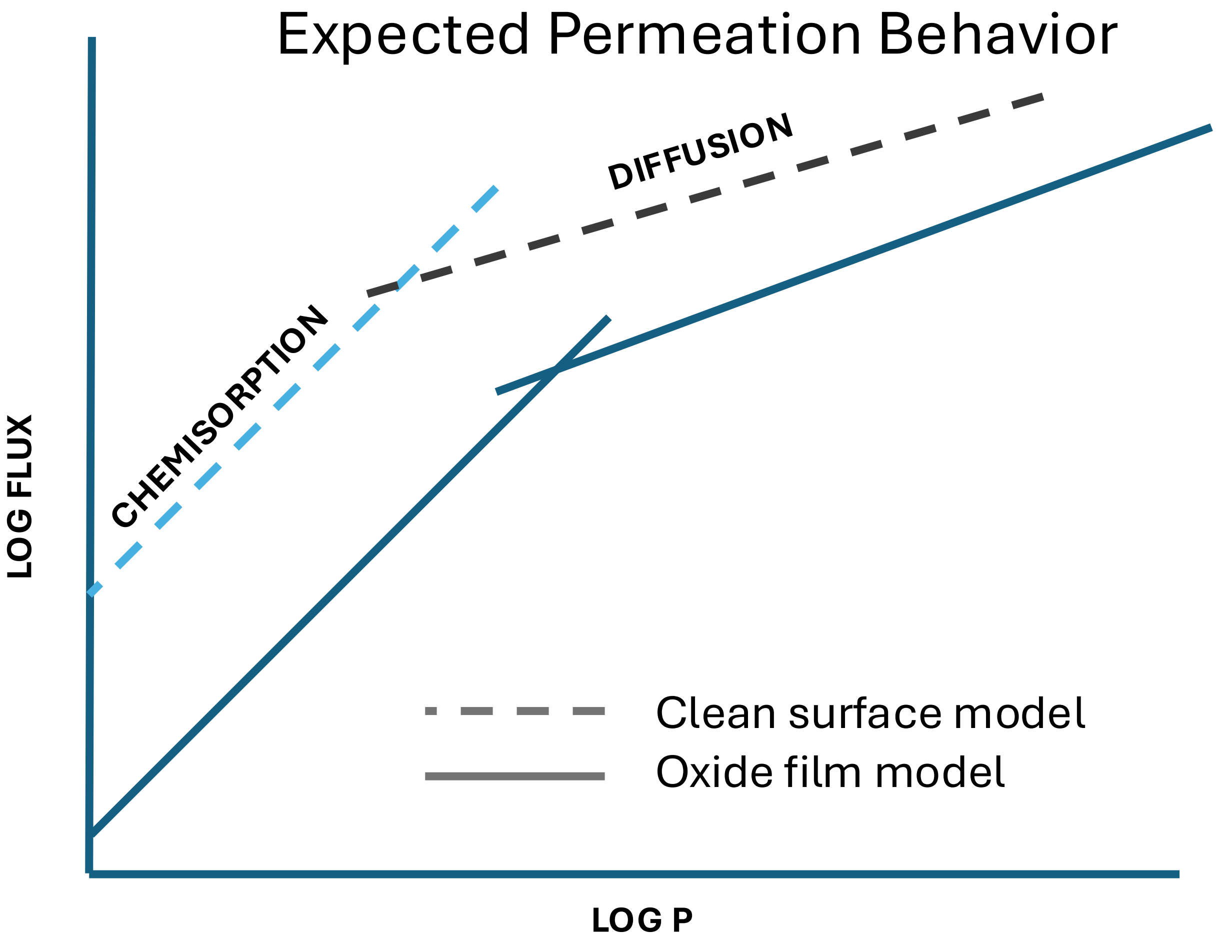
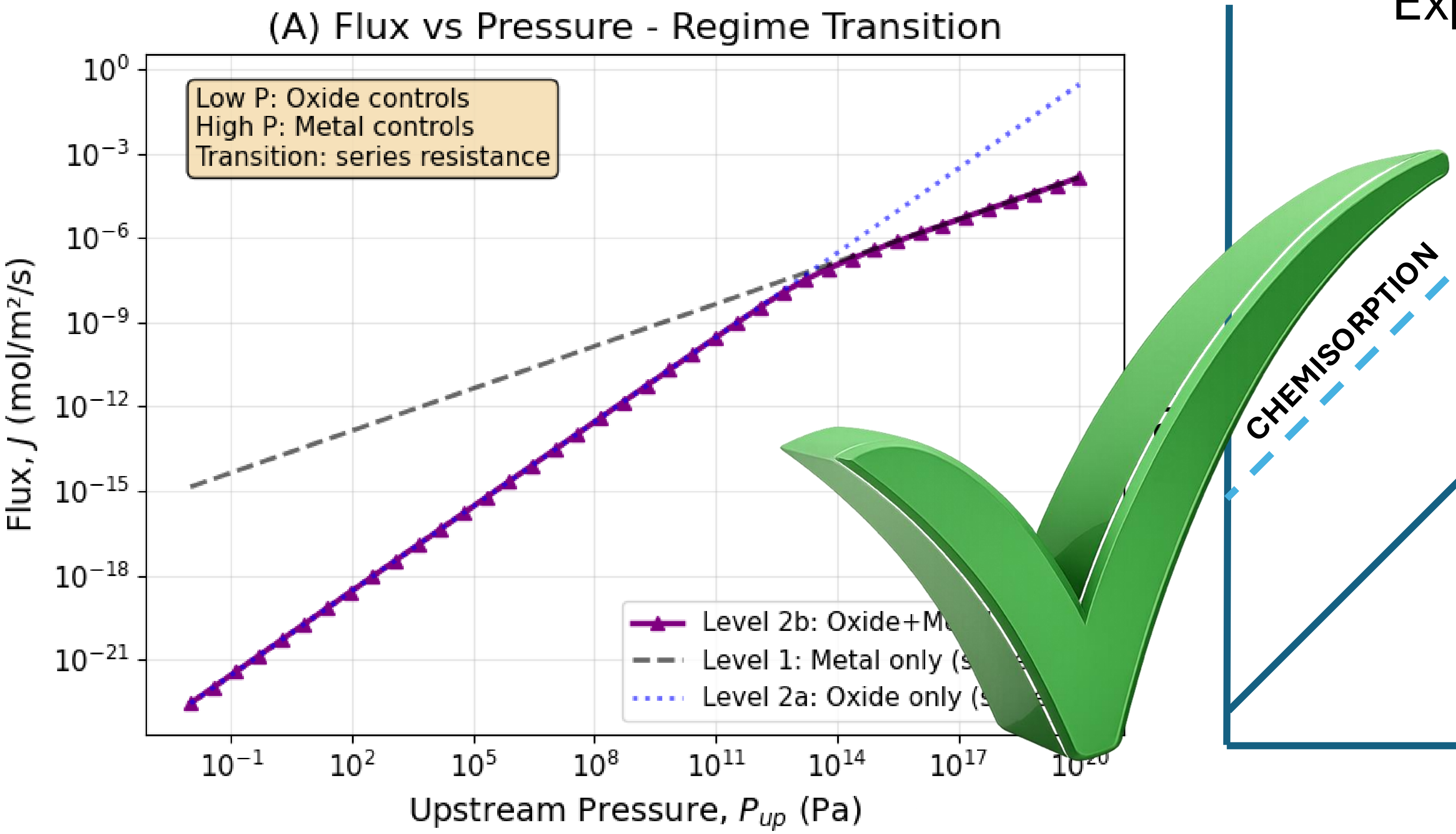


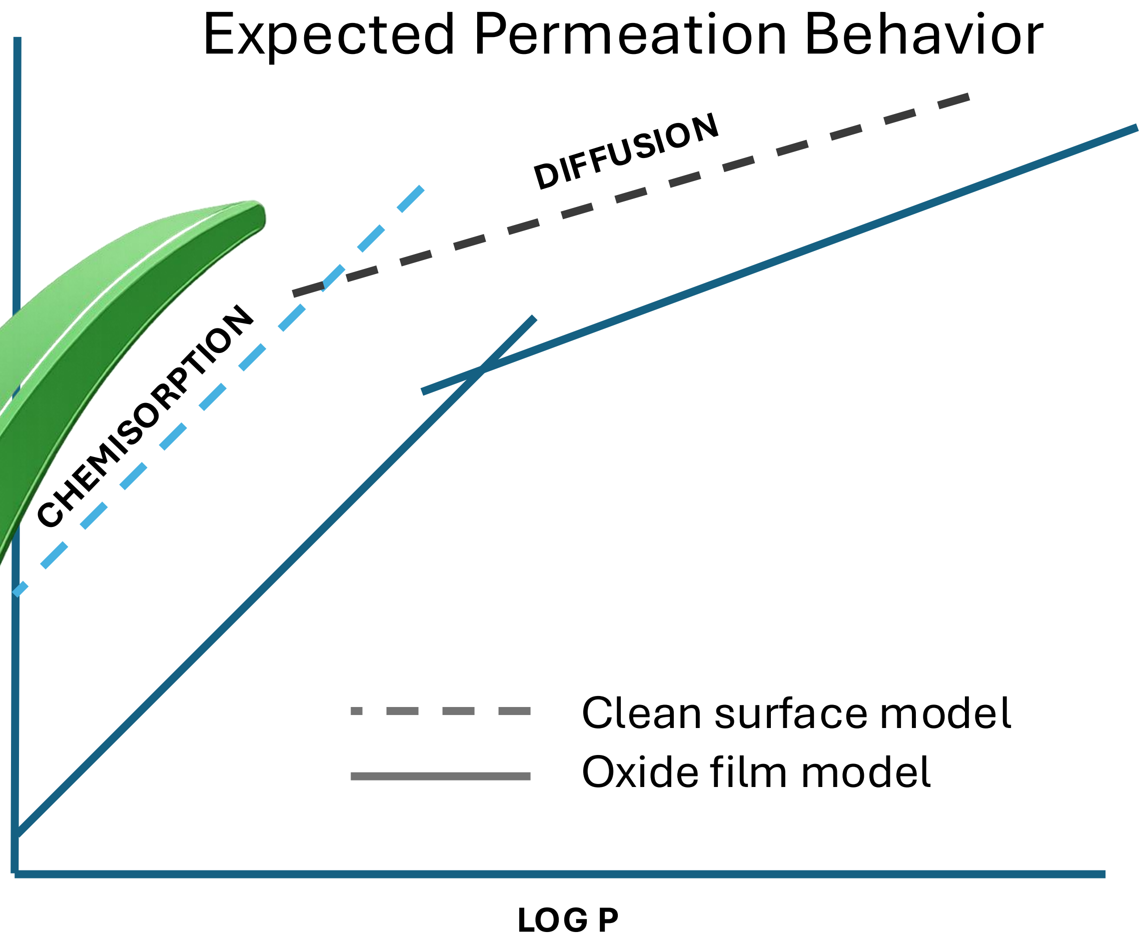
Perfect Oxide + Perfect Metal (Series Resistance)





Perfect Oxide + Perfect Metal (Series Resistance)





Aim 1

Perfect Metal
Atomic Diffusion
(Level 1)

Perfect Oxide
Molecular Diffusion
(Level 2a)

Perfect Oxide
+Perfect Metal
Series Resistance
(Level 2b)

Defective Oxide
+ Perfect Metal
The Parallel Path Model
(Level 3)

Defective Metal
(Level 4)

Defective Oxide
+ Defective Metal
(Level 5)

Defective Oxide + Perfect Metal (The Parallel Path Model)

Classical Modeling Frameworks for Oxide Cracks and Defects

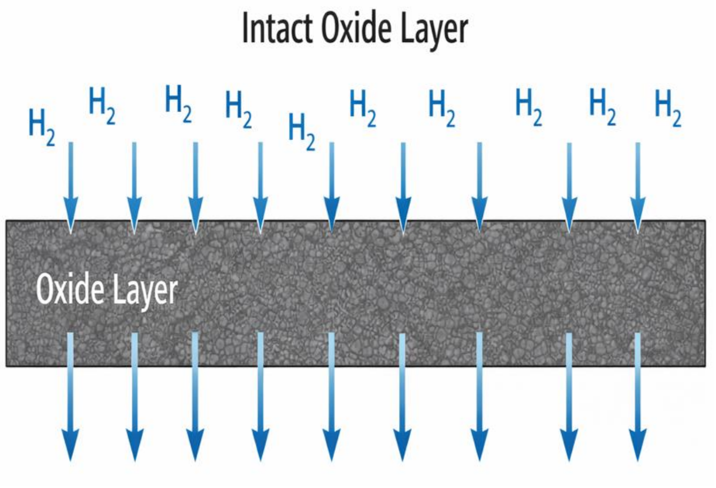
Model Type	Key Features	Mathematical Approach
Parallel Path Model	• Series-parallel resistor network • Intact oxide + defect paths • Explains transition regimes	Network resistance: $\frac{1}{R_{total}} = \frac{1}{R_{oxide}} + \frac{1}{R_{defects}}$
Area-Defect Model	• Defects have effective area • Binary (perfect/defective) • Simple implementation	$J_{total} = J_{oxide}(1 - f_d) + J_{defects}(1 - f_d)$ where f_d = defect fraction
Permeation Reduction Factor (PRF)	• Quantifies barrier effectiveness • Ratio-based metric	$PRF = \frac{\Phi_{metal}}{\Phi_{oxide\_covered}}$

(Zarchy & Axtmann, 1979)

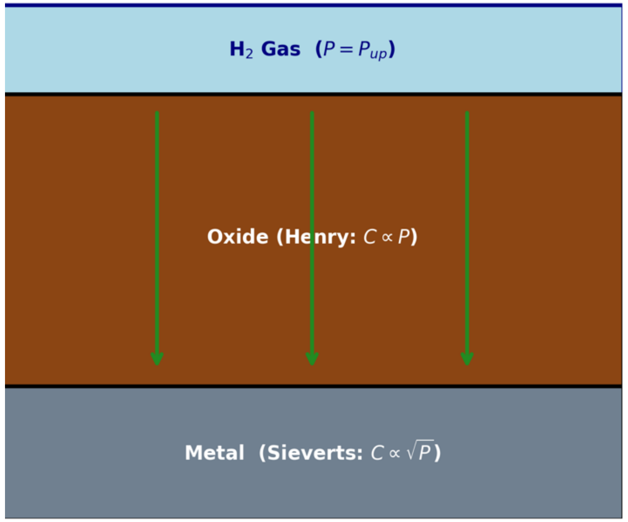
Types of Oxide Defects

- Pinholes (complete oxide absence)
- Crack with thin oxide
- Grain Boundaries in oxide

Defective Oxide + Perfect Metal (The Parallel Path Model)



(A) Intact Oxide



$$J = \left(\frac{D_{ox}K_{ox}}{L_{ox}}\right).\left(P_{up} - P_{down}\right)$$

For Parallel Resistance Analogy:

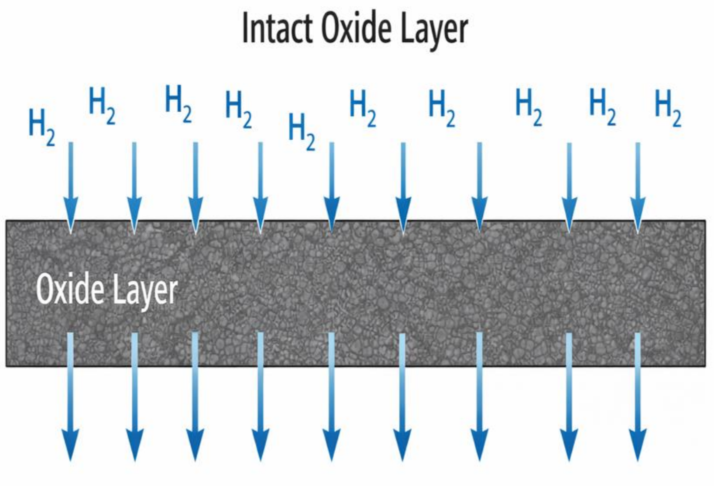
- Parallel resistors: $\frac{1}{R_{total}} = \frac{1}{R_1} + \frac{1}{R_2} + \cdots + \frac{1}{R_n}$
- Total Surface Area: $A_{total} = A_{intact} + A_{defect}$
- Area fractions: $f_{intact} = \frac{A_{intact}}{A_{total}}$; $f_{defect} = \frac{A_{defect}}{A_{total}}$

$$f_{intact} + f_{defect} = 1$$

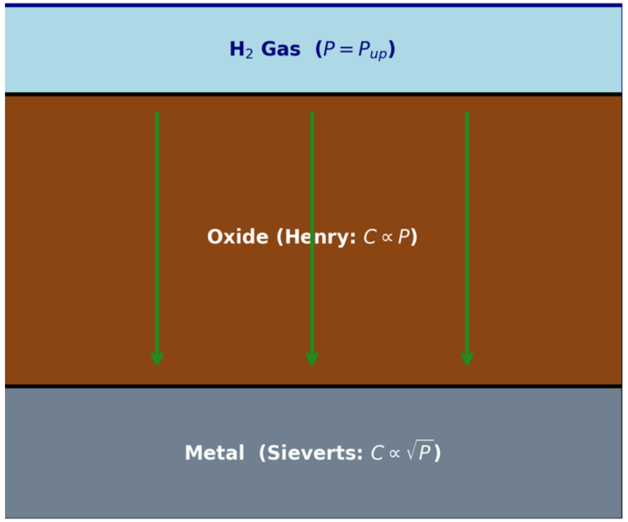
- Flux: $J_{total} = J_{intact} * f_{intact} + J_{defect} * f_{defect}$

$$J_{total} = J_{intact} * (1 - f_{defect}) + J_{defect} * f_{defect}$$

Defective Oxide + Perfect Metal (The Parallel Path Model)



(A) Intact Oxide



$$J = \left(\frac{D_{ox}K_{ox}}{L_{ox}}\right).\left(P_{up} - P_{down}\right)$$

For Parallel Resistance Analogy:

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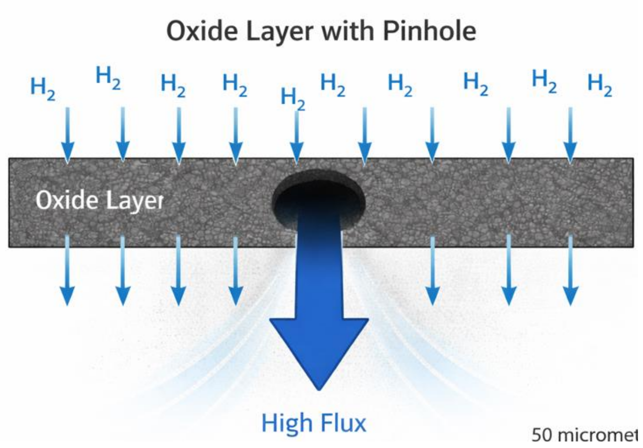
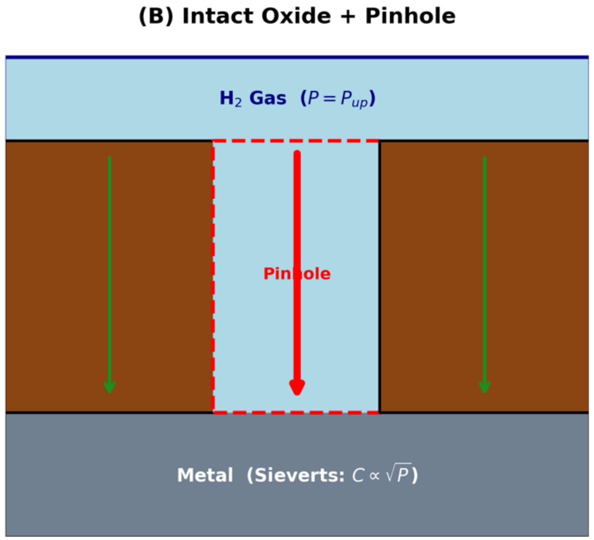
$$f_{intact} + f_{defect} = 1$$

- **Flux:** $J_{total} = J_{intact} * f_{intact} + J_{defect} * f_{defect}$

$$J_{total} = J_{intact} * (1 - f_{defect}) + J_{defect} * f_{defect}$$

Defective Oxide + Perfect Metal (The Parallel Path Model)





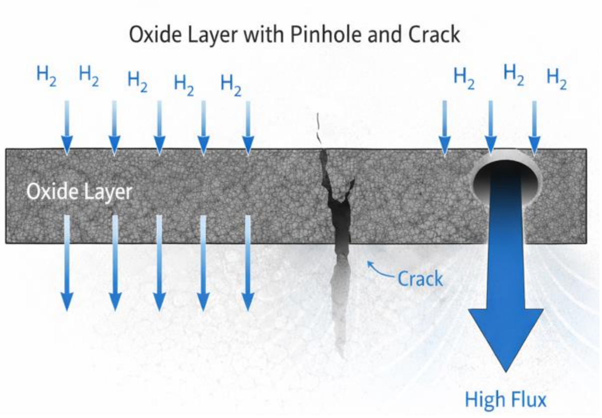
$$J_{total} = J_{intact} * (1 - f_{defect}) + J_{defect} * f_{defect}$$

$$J_{intact} = \left(\frac{D_{ox}K_{ox}}{L_{ox}}\right) . (P_{up} - P_{down})$$

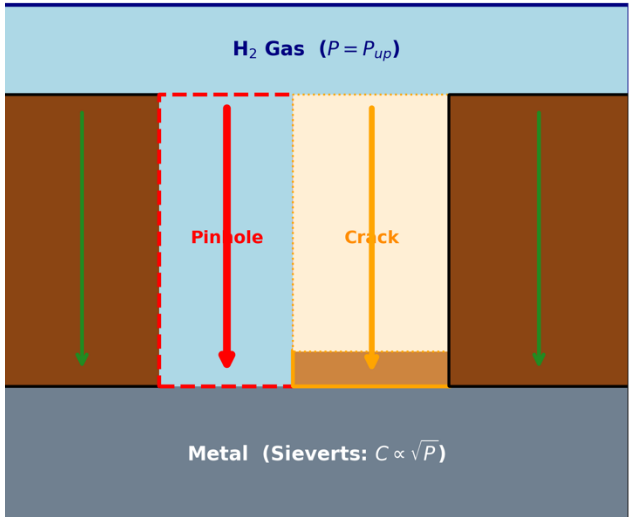
$$J_{defect} = \left(\frac{DK_s}{L}\right) . \left(\sqrt{P_{up}} - \sqrt{P_{down}}\right)$$

Pinholes

Defective Oxide + Perfect Metal (The Parallel Path Model)



(C) Intact Oxide + Pinhole + Crack



$$J_{total} = J_{intact} * (1 - f_{defect}) + J_{defect} * f_{defect}$$

$$J_{intact} = \left(\frac{D_{ox}K_{ox}}{L_{ox}}\right) . (P_{up} - P_{down})$$

$$J_{defect} = f_{pinhole} * J_{pinhole} + f_{crack} * J_{crack}$$

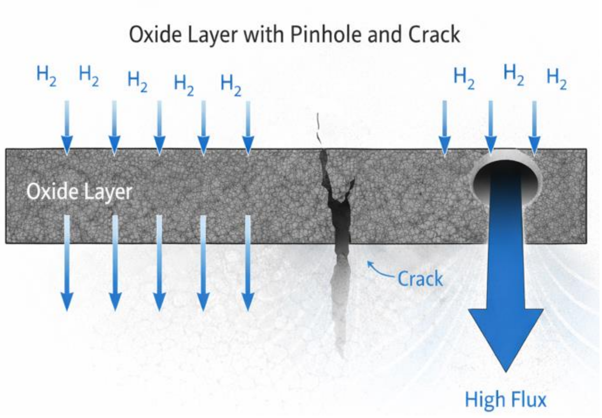
$$J_{pinhole} = \left(\frac{DK_s}{L}\right) . \left(\sqrt{P_{up}} - \sqrt{P_{down}}\right)$$

$$J_{crack} = \left(\frac{D_{ox}K_{ox}}{L_{ox}}\right) . (P_{up} - P_{down})$$

- $L_{crack} = \alpha * L_{oxide} ; \alpha < 1$

$$J_{total} = J_{intact} * (1 - f_{defect}) + f_{pinhole} * J_{pinhole} + f_{crack} * J_{crack}$$

Defective Oxide + Perfect Metal (The Parallel Path Model)



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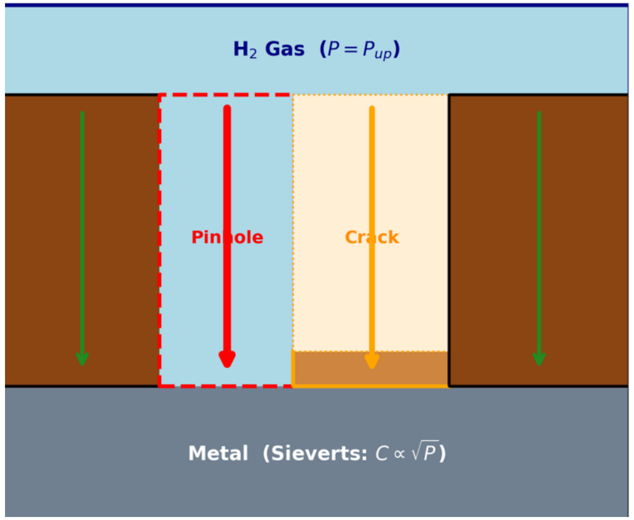


$$J_{total} = J_{intact} * (1 - f_{defect}) + J_{defect} * f_{defect}$$

$$J_{intact} = \left(\frac{D_{ox}K_{ox}}{L_{ox}}\right) . (P_{up} - P_{down})$$

$$J_{defect} = f_{pinhole} * J_{pinhole} + f_{crack} * J_{crack}$$

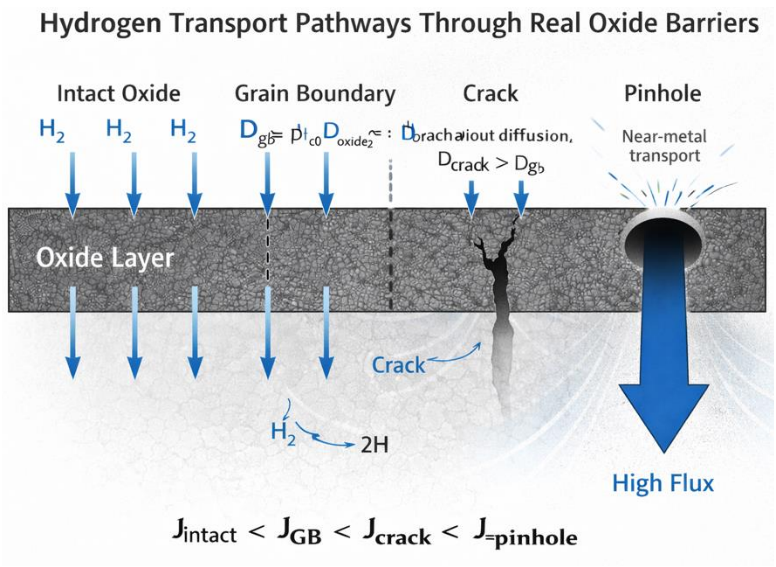
$$J_{pinhole} = \left(\frac{DK_s}{L}\right) . \left(\sqrt{P_{up}} - \sqrt{P_{down}}\right)$$

$$J_{crack} = \left(\frac{D_{ox}K_{ox}}{L_{ox}}\right) . (P_{up} - P_{down})$$

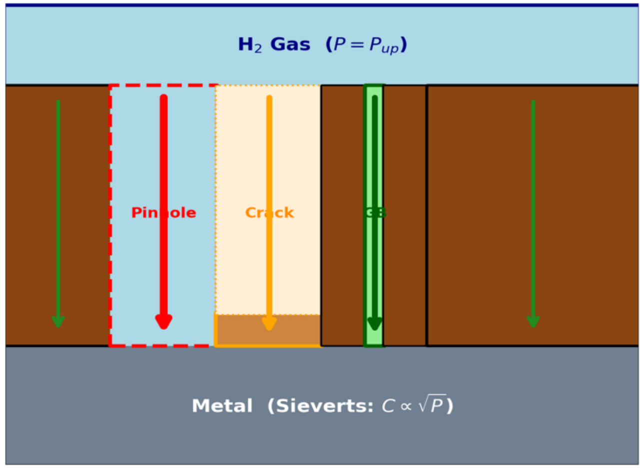
- $L_{crack} = \alpha * L_{oxide}; \alpha < 1$

$$\boxed{J_{total} = J_{intact} * (1 - f_{defect}) + f_{pinhole} * J_{pinhole} + f_{crack} * J_{crack}}$$

Defective Oxide + Perfect Metal (The Parallel Path Model)



(D) Intact Oxide + Pinhole + Crack + GB



$$J_{total} = J_{intact} * (1 - f_{defect}) + J_{defect} * f_{defect}$$

$$J_{intact} = \left(\frac{D_{ox}K_{ox}}{L_{ox}}\right).(P_{up} - P_{down})$$

$$J_{defect} = f_{pinhole} * J_{pinhole} + f_{crack} * J_{crack} + f_{GB} * J_{GB}$$

$$J_{pinhole} = \left(\frac{DK_s}{L}\right).\left(\sqrt{P_{up}} - \sqrt{P_{down}}\right)$$

$$J_{crack} = \left(\frac{D_{ox}K_{ox}}{L_{ox}}\right).(P_{up} - P_{down})$$

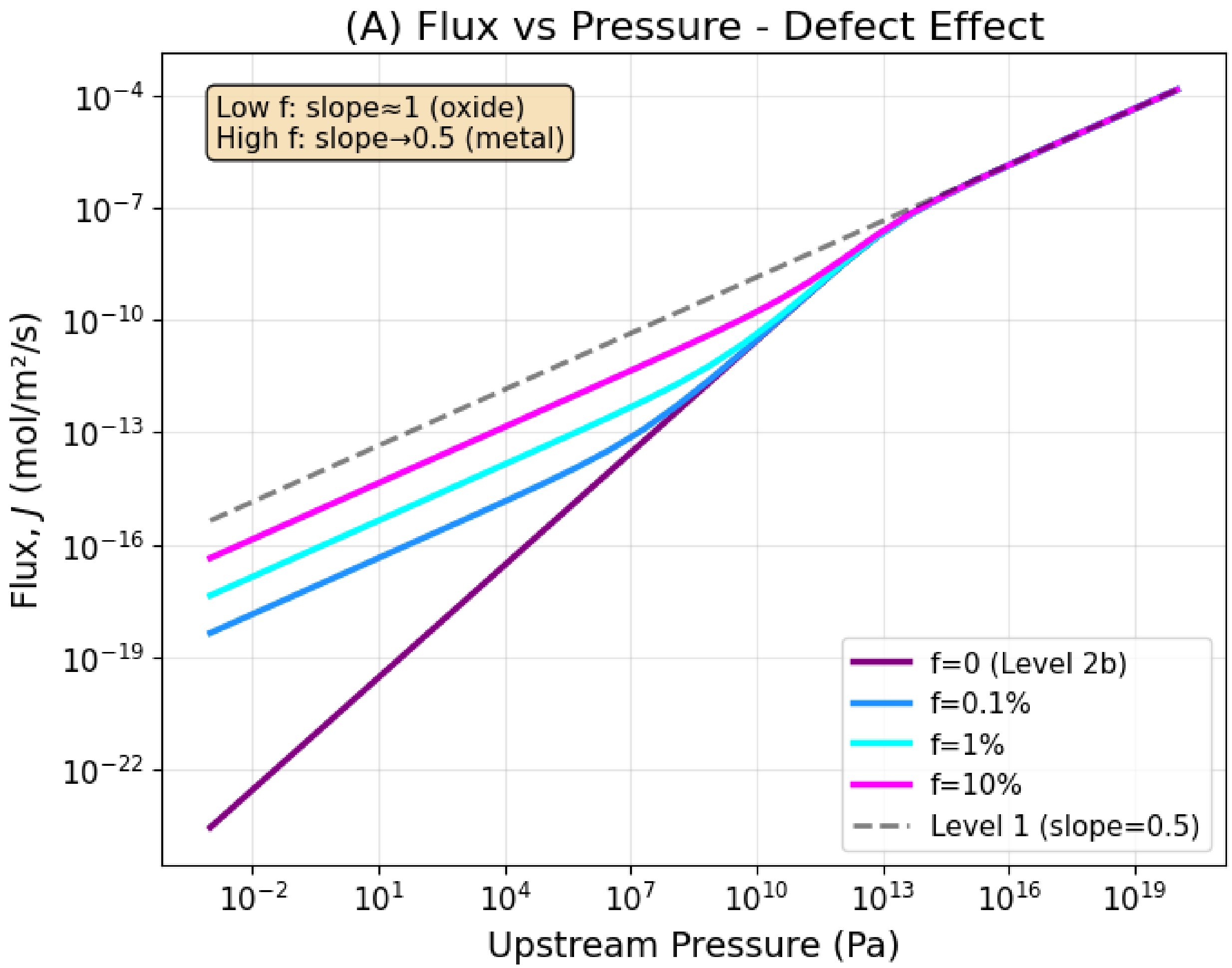
- $L_{crack} = \alpha * L_{oxide}\,;\, \alpha < 1$

$$J_{GB} = \left(\frac{D_{ox}K_{ox}}{L_{ox}}\right).(P_{up} - P_{down})$$

- $D_{gb} = \beta * D_{ox}\,;\, \beta > 1$

$$J_{total} = J_{intact} * (1 - f_{defect}) + f_{pinhole} * J_{pinhole} + f_{crack} * J_{crack} + f_{GB} * J_{GB}$$

Defective Oxide + Perfect Metal (The Parallel Path Model)



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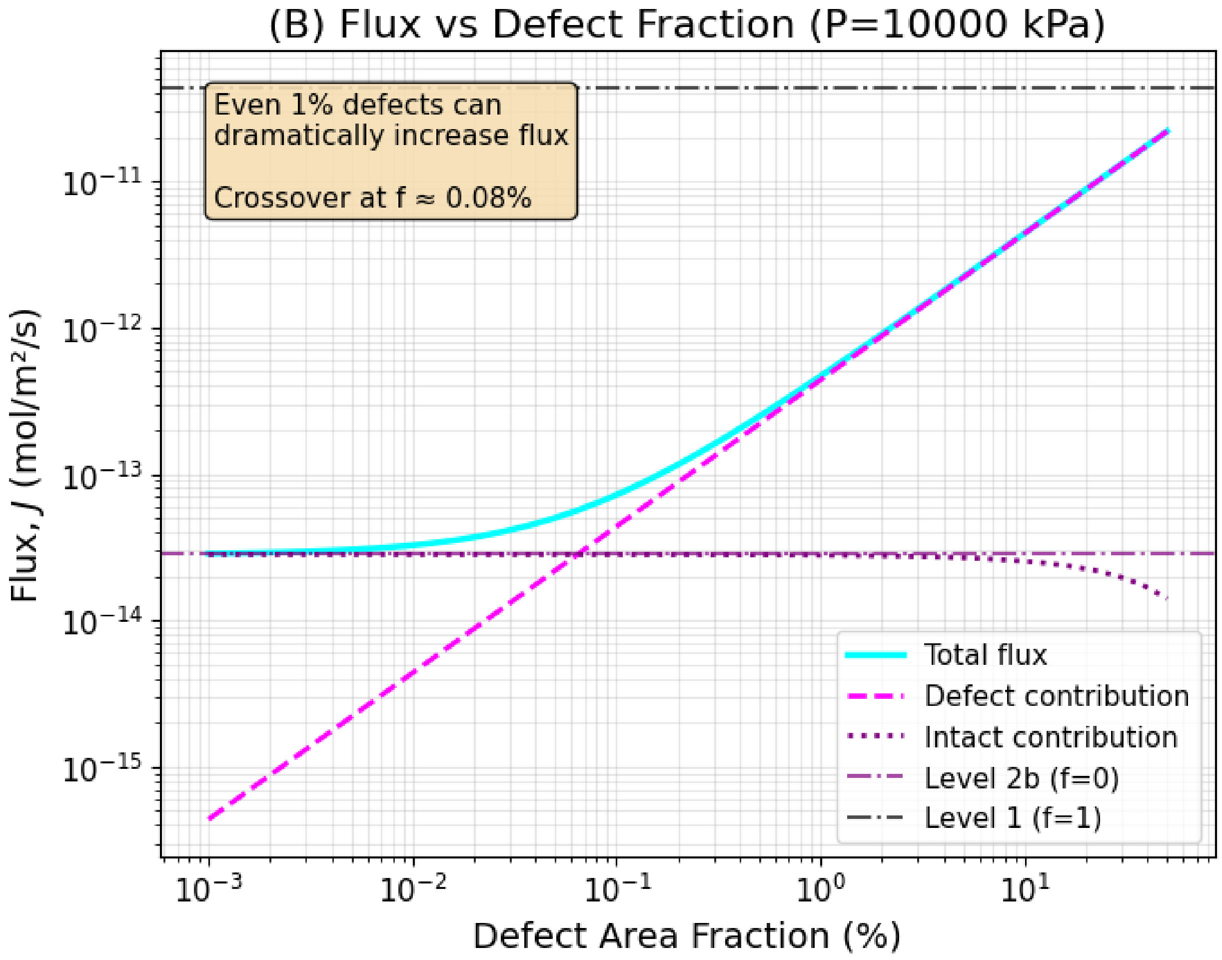

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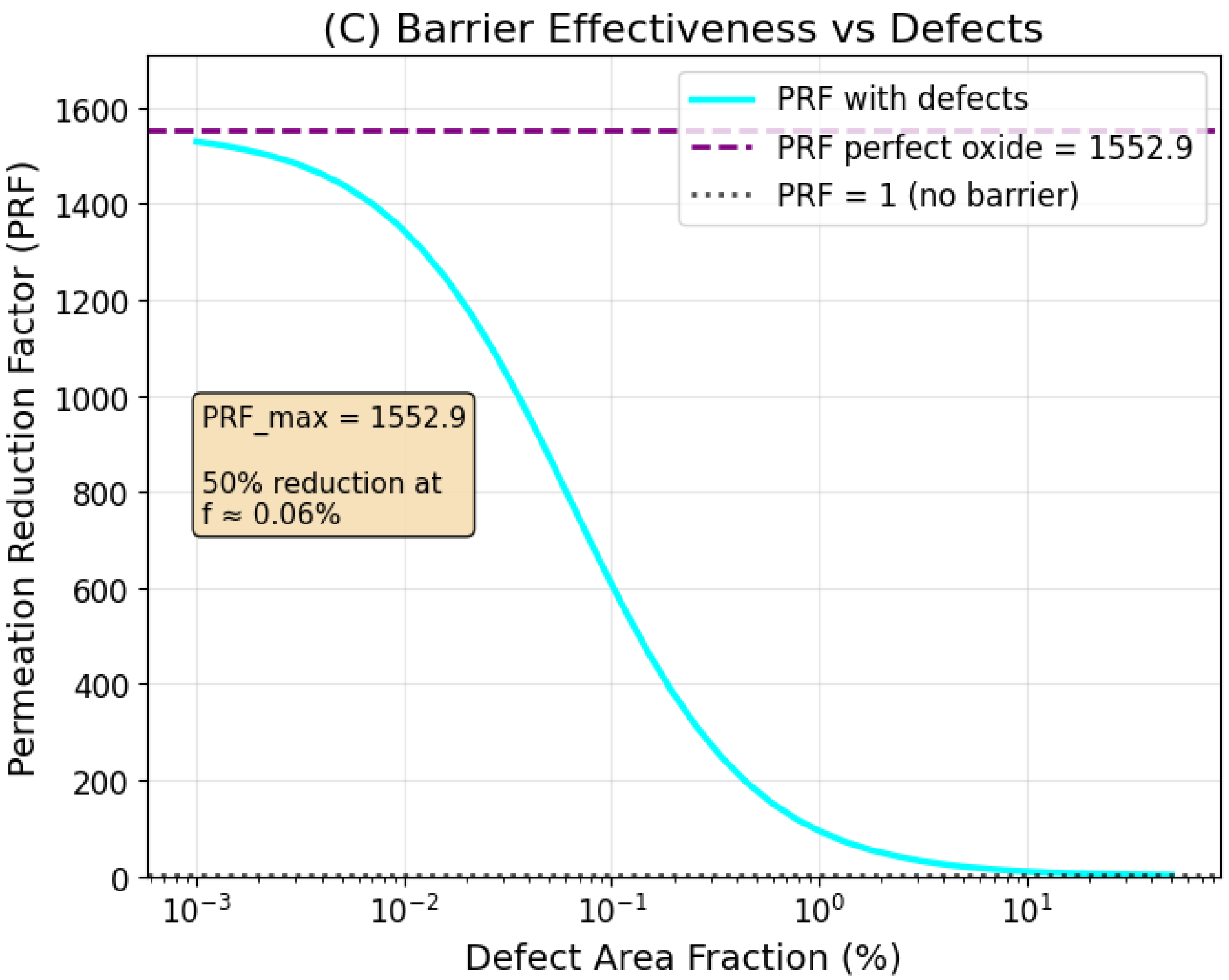

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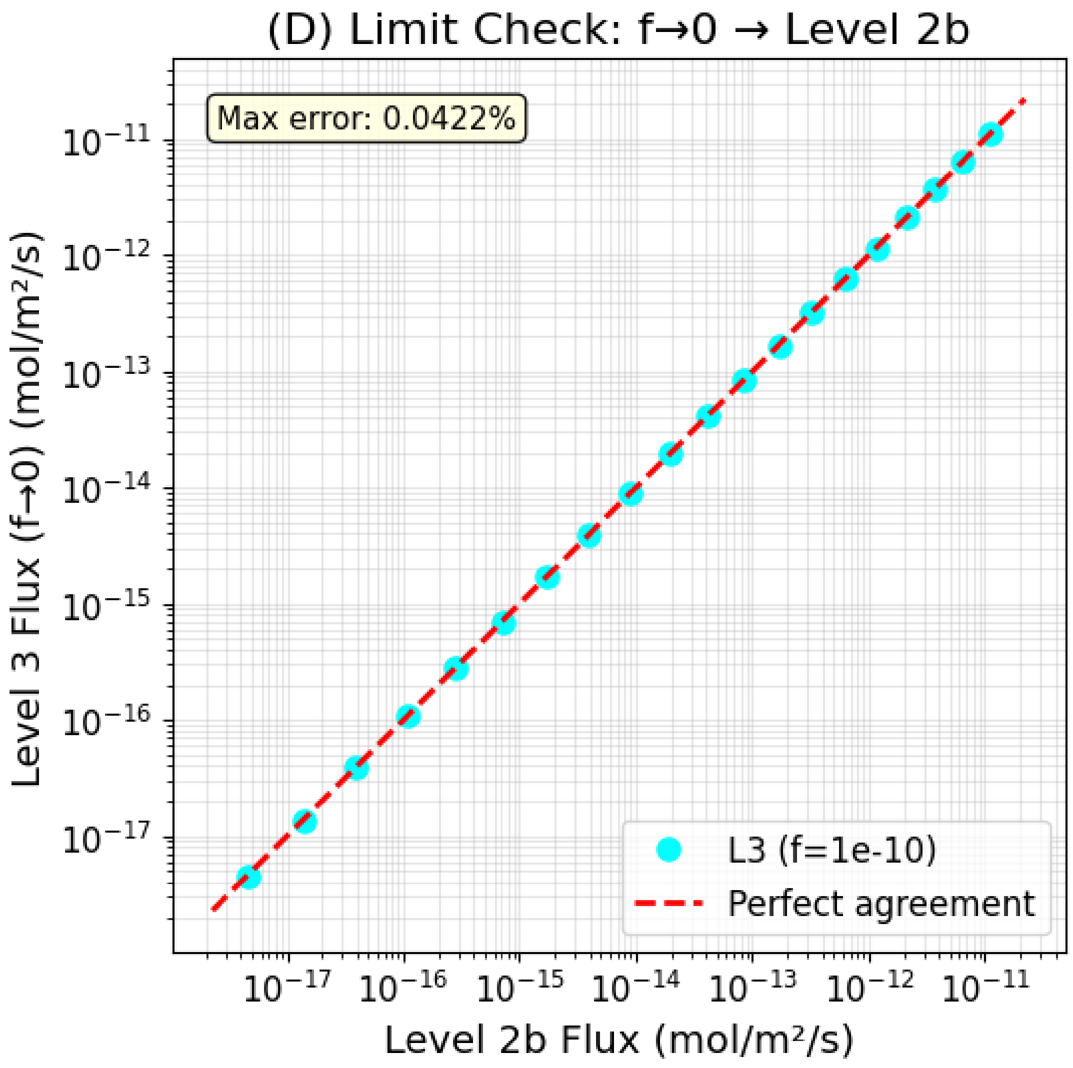
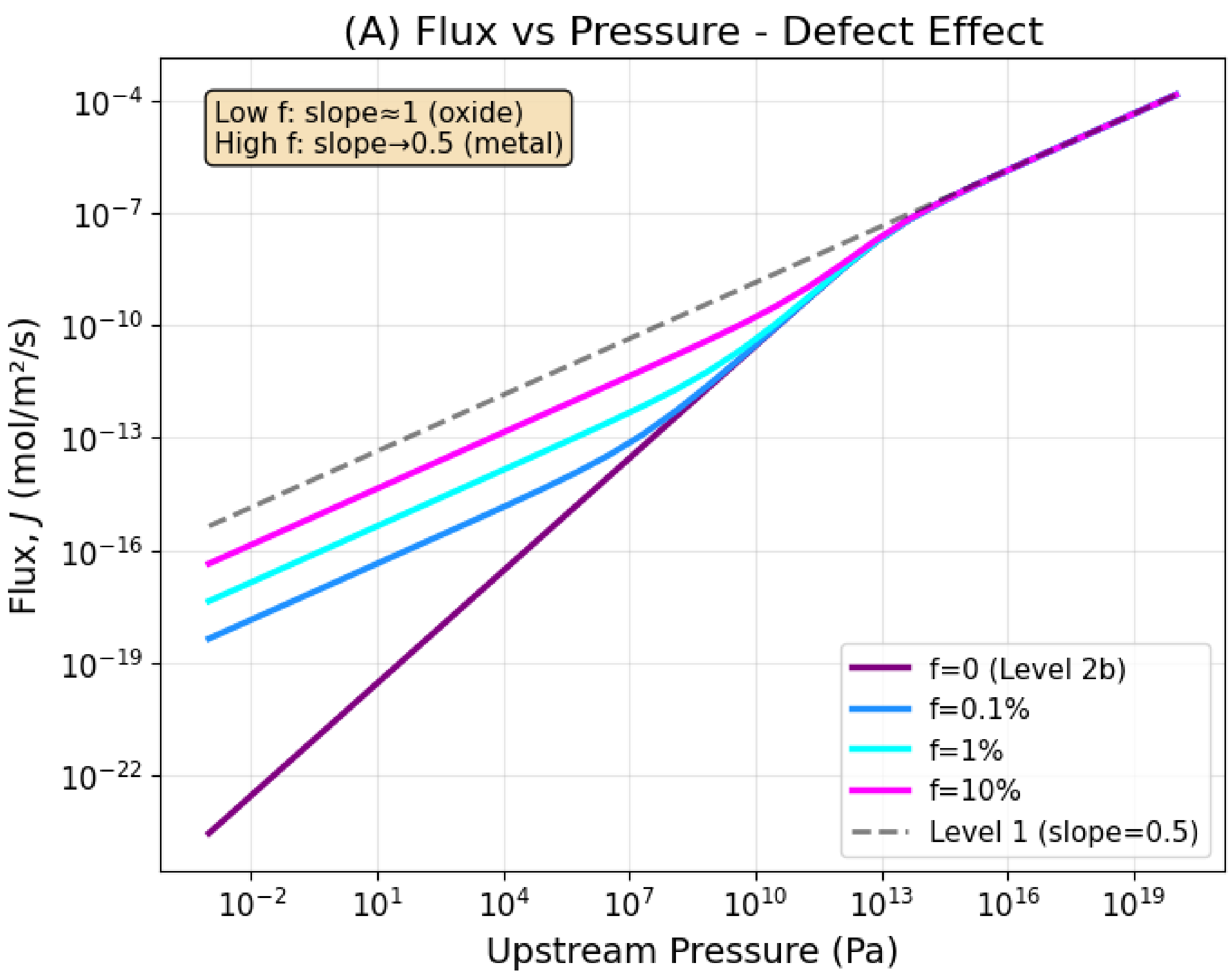
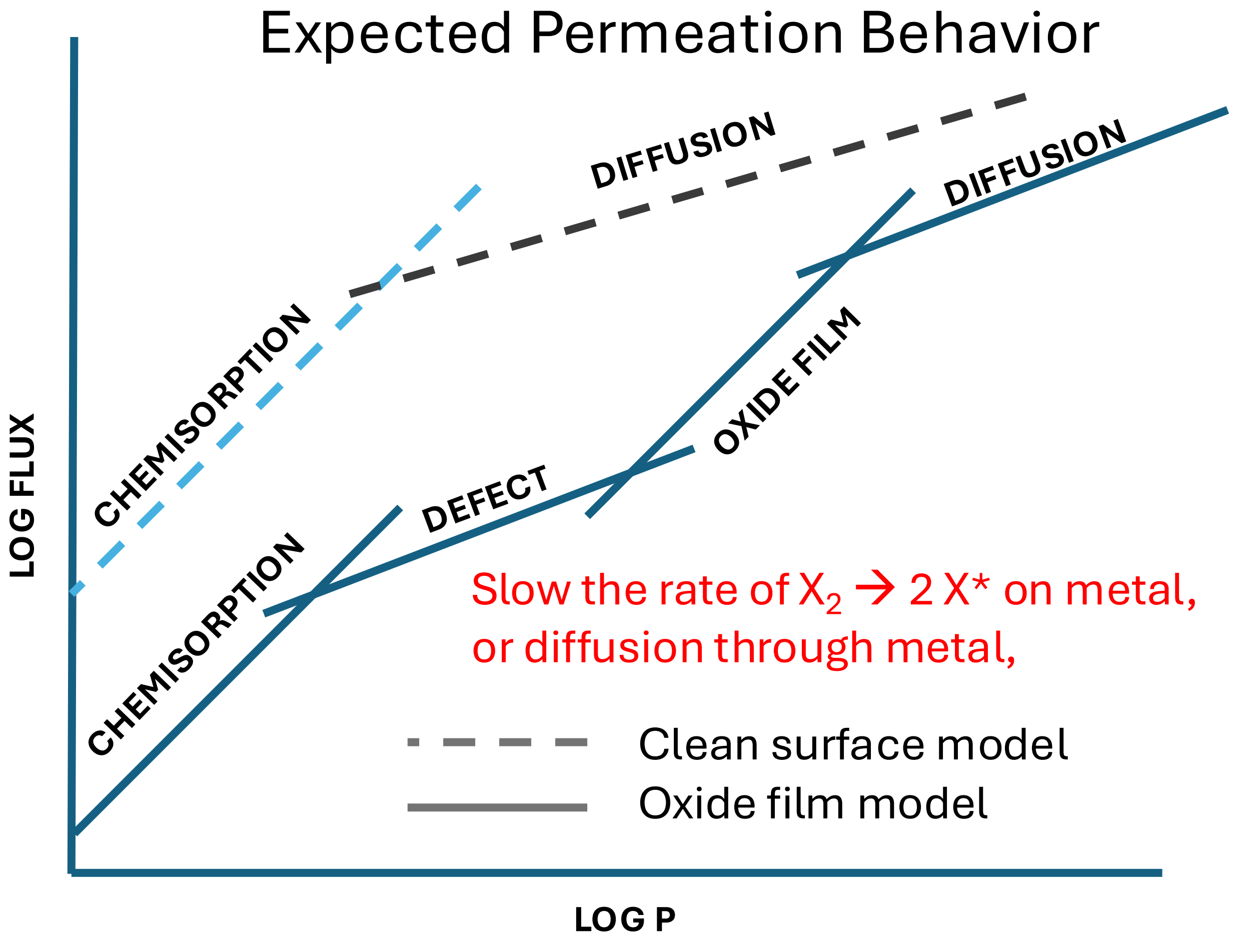
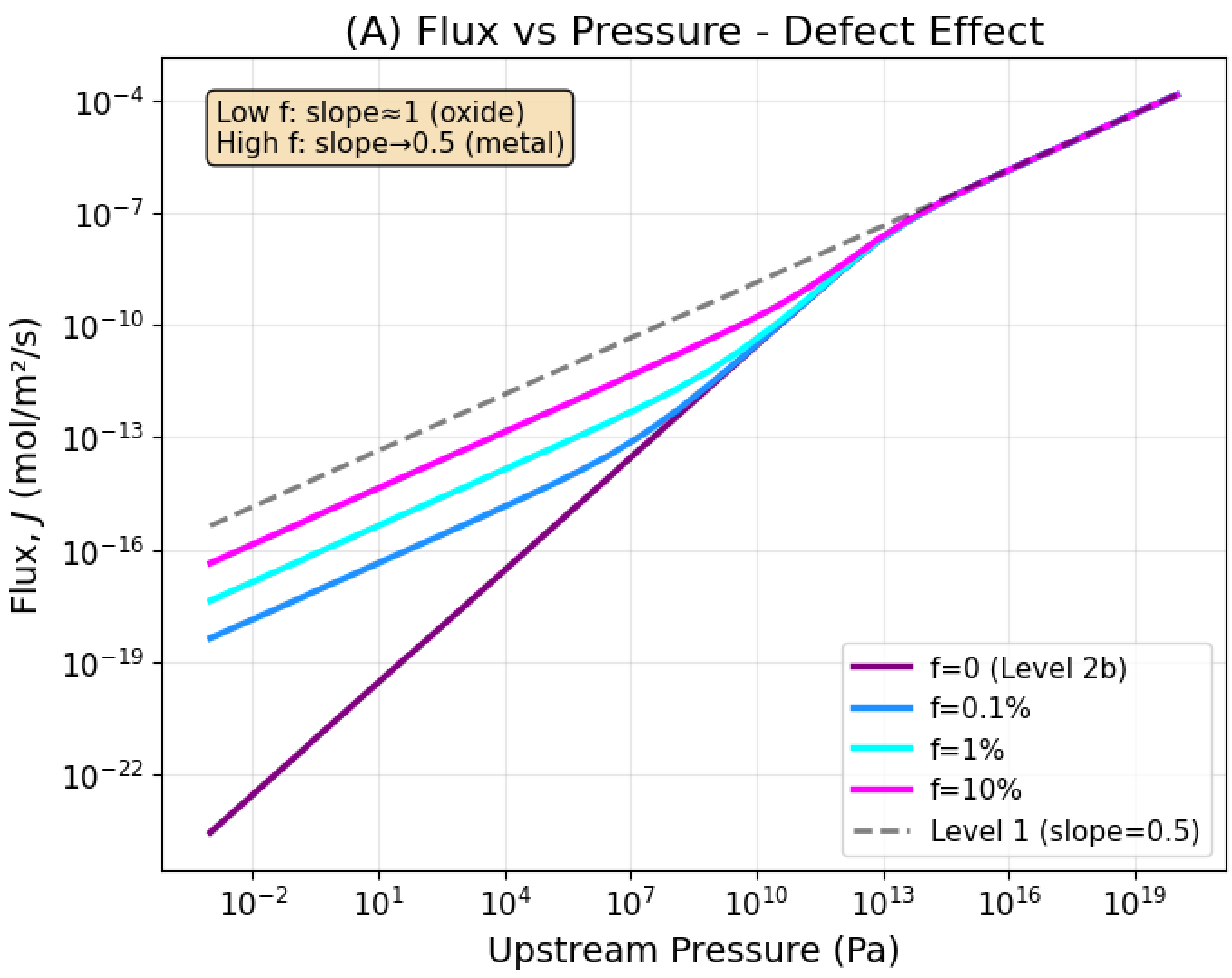


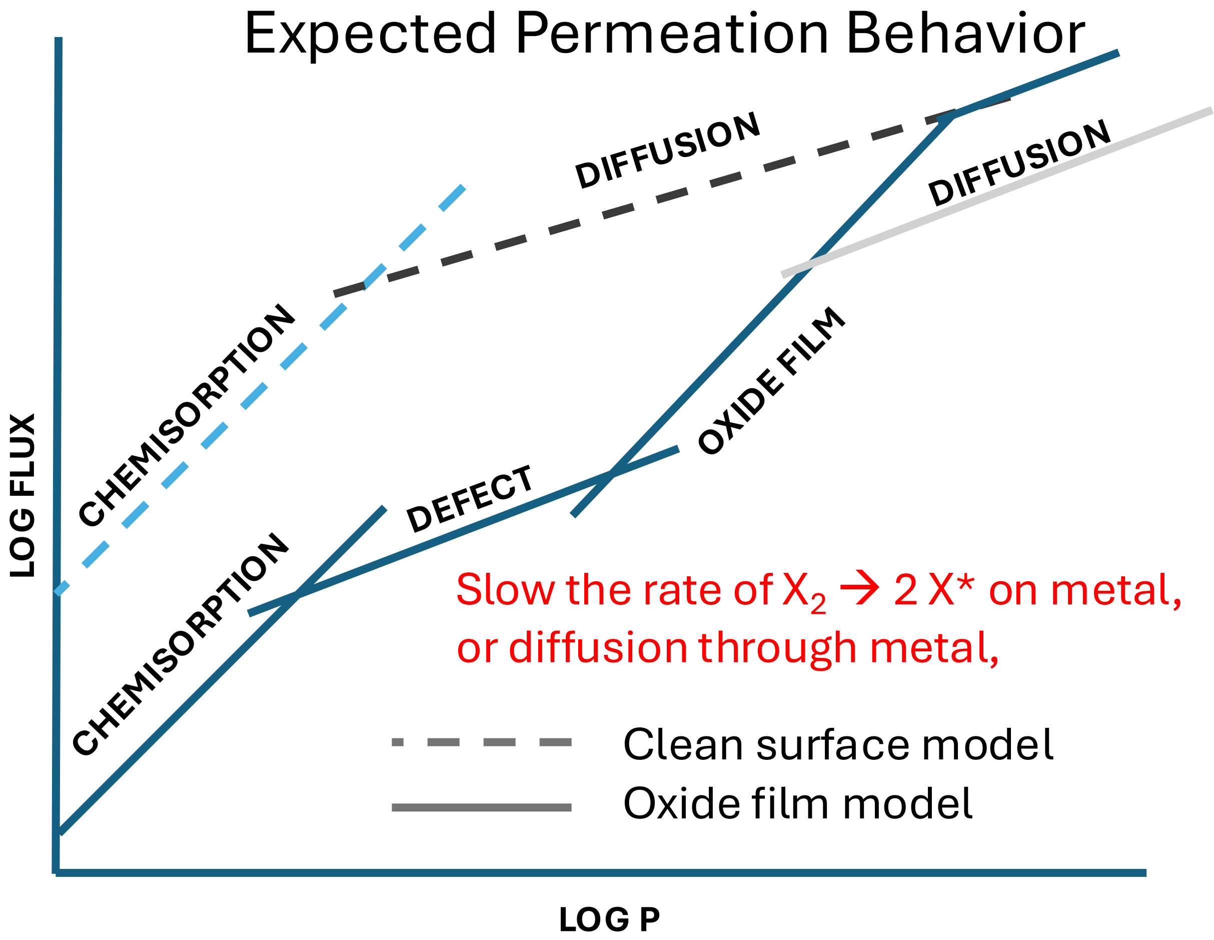
Defective Oxide + Perfect Metal (The Parallel Path Model)



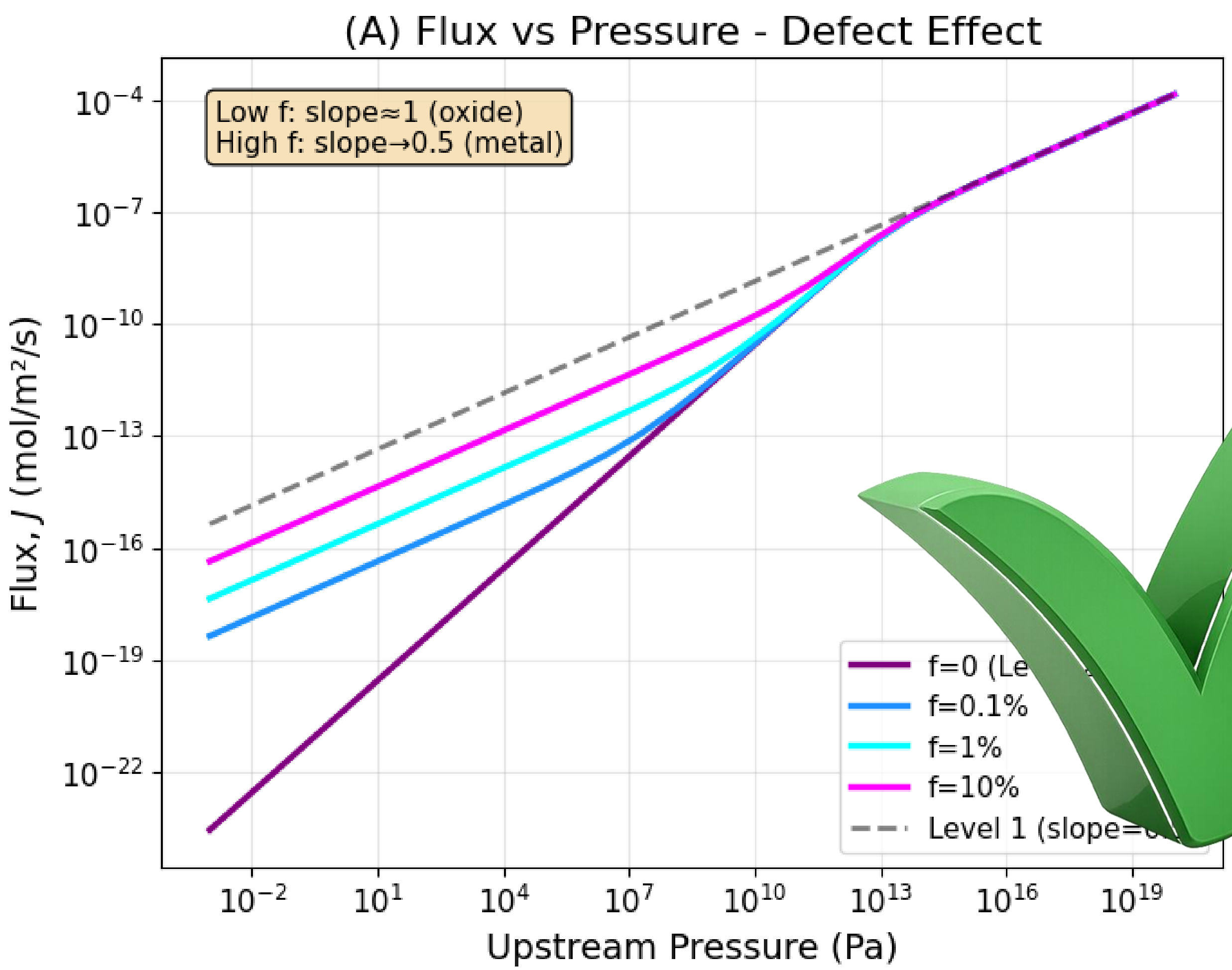


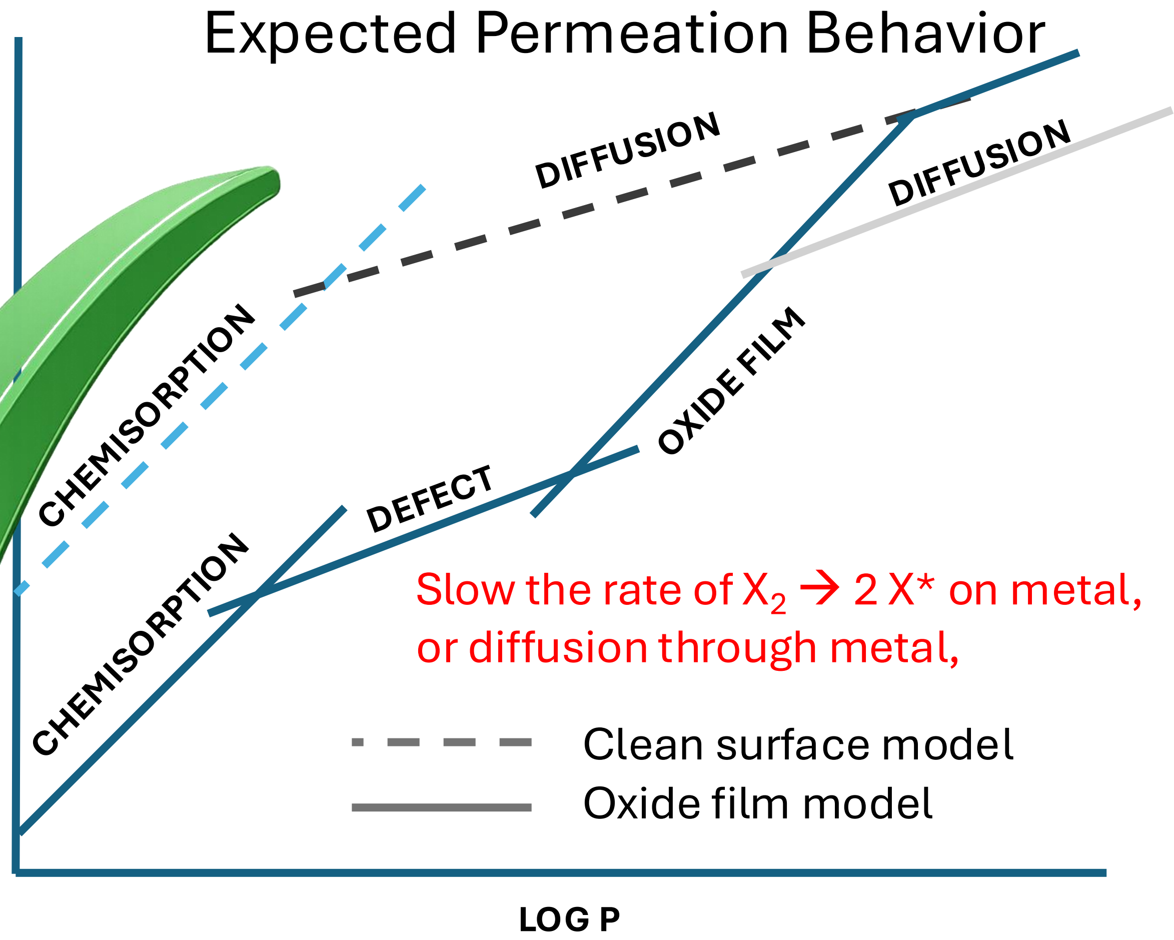
Defective Oxide + Perfect Metal (The Parallel Path Model)





Defective Oxide + Perfect Metal (The Parallel Path Model)





Slow the rate of $X_2 \rightarrow 2X^*$ on metal, or diffusion through metal,

Aim 1

Perfect Metal
Atomic Diffusion
(Level 1)

Perfect Oxide
Molecular Diffusion
(Level 2a)

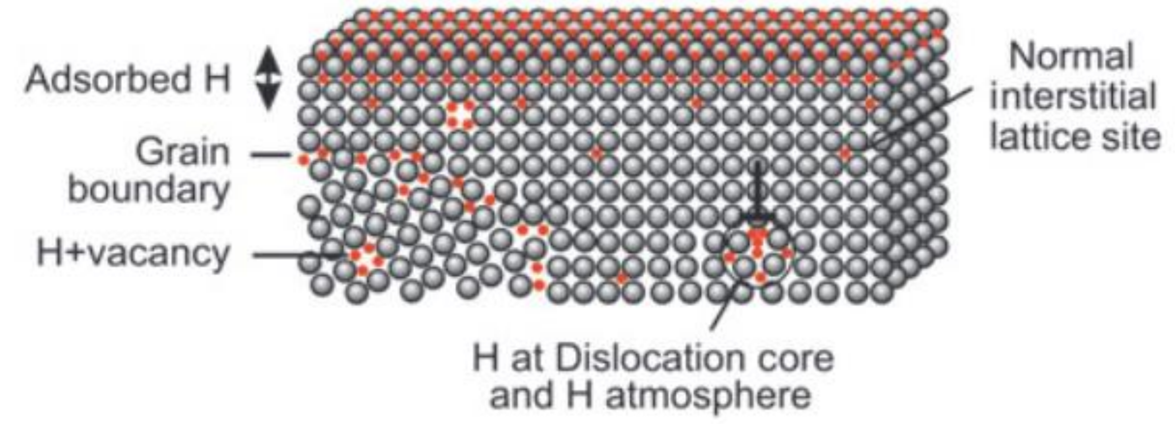
Perfect Oxide
+Perfect Metal
Series Resistance
(Level 2b)

Defective Oxide
+ Perfect Metal
The Parallel Path Model
(Level 3)

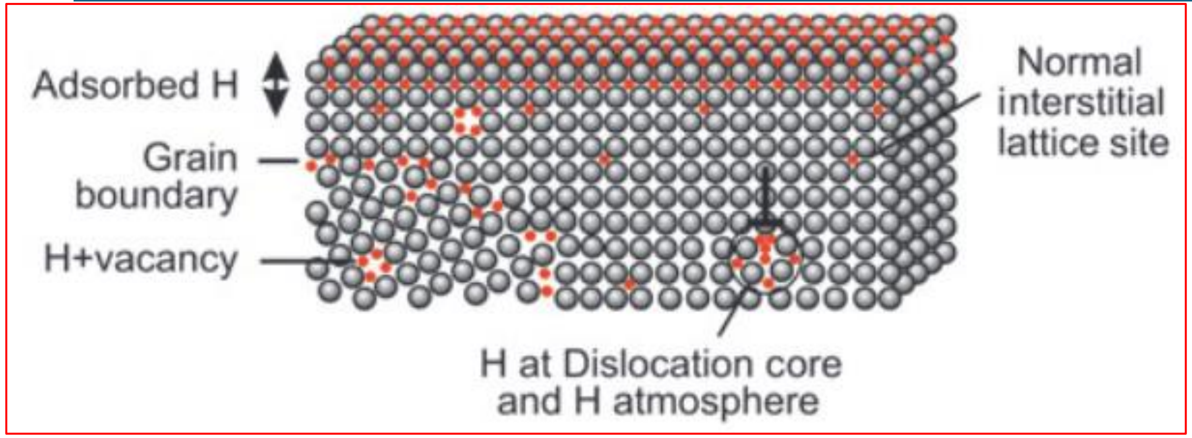
Defective Metal
(Level 4)

Defective Oxide
+ Defective Metal
(Level 5)

Defective Metal Modeling



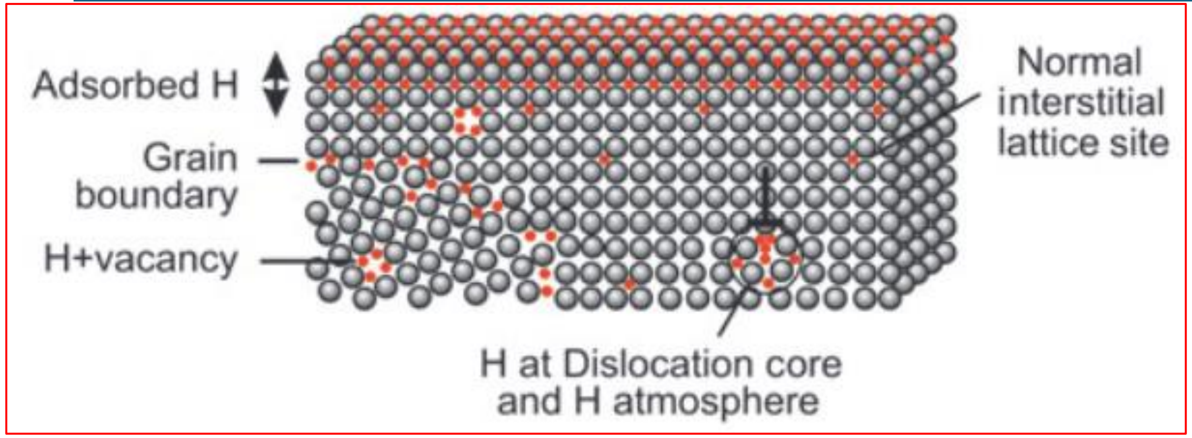
Defective Metal Modeling



Defective Metal

- Lattice
- Grain Boundaries
- Traps
  - Vacancies
  - Dislocations
  - Grain Boundaries
  - Precipitates

Defective Metal Modeling



Defective Metal

- Lattice
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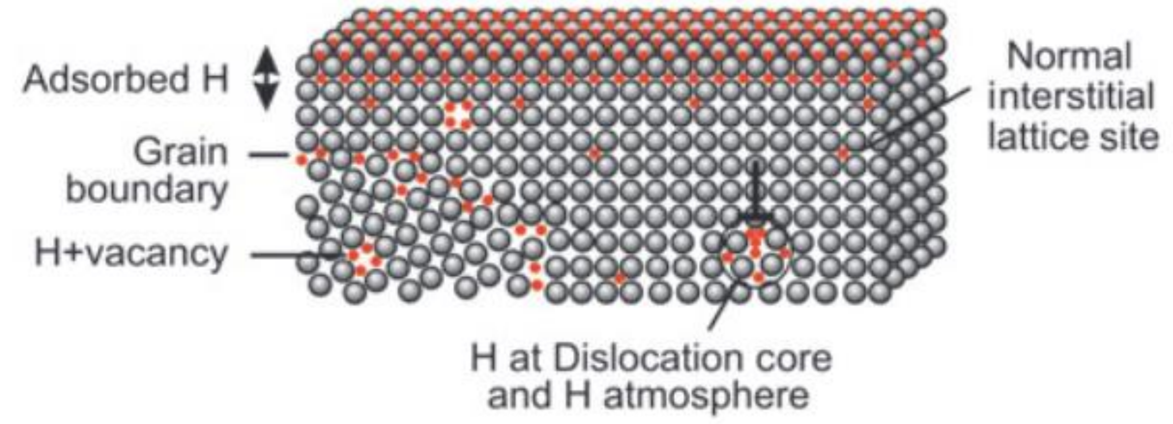
- Traps
  - Vacancies
  - Dislocations
  - Grain Boundaries
  - Precipitates

Lattice

Fick Diffusion

$$Diffusivity = D_{Lattice}$$

Defective Metal Modeling



Defective Metal

- **Lattice**
- **Grain Boundaries**
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  - Vacancies
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Lattice

Fick Diffusion

$$Diffusivity = D_{Lattice}$$

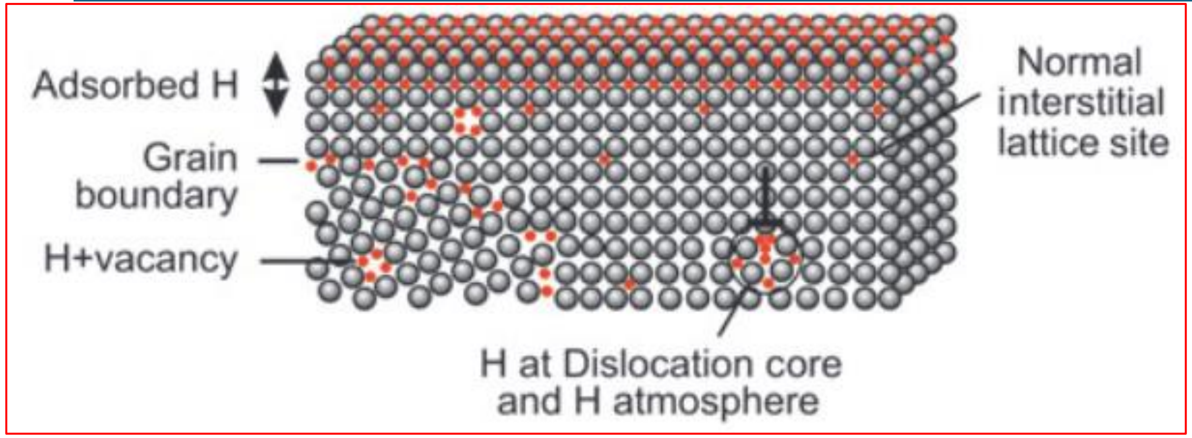
Grain Boundaries

Parallel Path Model (Hart's Equ)

$$D_{eff} = D_{Lattice}(1 - f_{GB}) + D_{GB} f_{GB}$$

$$D_{GB} >> D_{lattice} \qquad f_{GB} = \frac{3 * GB\ thickness}{grain\ size}$$

Defective Metal Modeling



Defective Metal

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Lattice

Fick Diffusion

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Traps

Oriani Equilibrium Model

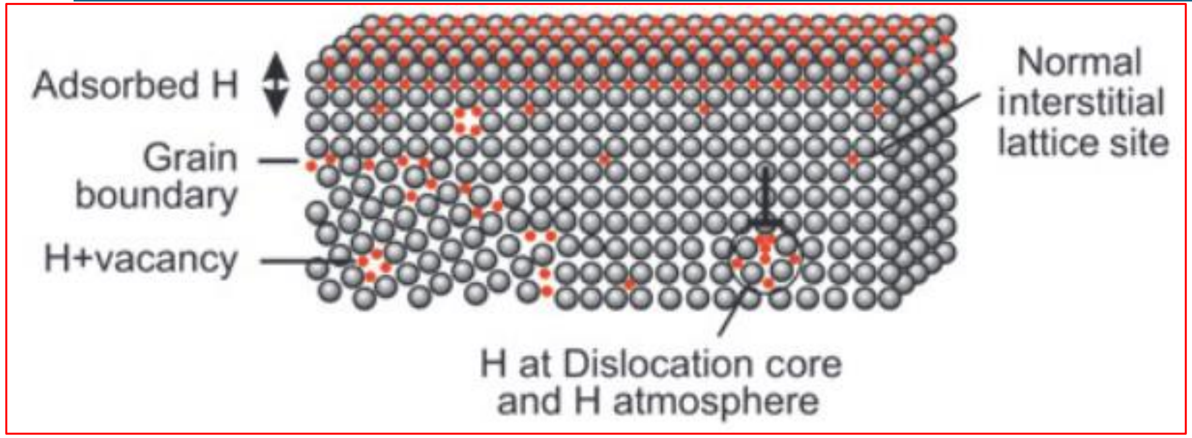
$$D_{eff} = \frac{D_{lattice}}{1 + \sum \frac{N_{T\_i} K_{eq\_i}}{N_L}} \qquad K_{eq\_i} = exp\left(\frac{E_b}{RT}\right)$$

K_{eq_i} = Equilibrium constant for trap type I

N_{T_i} = Density of trap type I (trap/m^3)

N_L = Lattice density, E_b = Binding Energy

Defective Metal Modeling



Defective Metal

- Lattice
- Grain Boundaries
- Traps
  - Vacancies
  - Dislocations
  - Grain Boundaries
  - Precipitates

Lattice — **Fick Diffusion**

$$Diffusivity = D_{Lattice}$$

Grain Boundaries — **Parallel Path Model (Hart's Equ)**

$$D_{eff} = D_{Lattice}(1 - f_{GB}) + D_{GB} f_{GB}$$

$$D_{GB} >> D_{lattice} \qquad f_{GB} = \frac{3 * GB\ thickness}{grain\ size}$$

Traps — **Oriani Equilibrium Model**

$$D_{eff} = \frac{D_{lattice}}{1 + \sum \frac{N_{T\_i} K_{eq\_i}}{N_L}} \qquad K_{eq\_i} = exp\left(\frac{E_b}{RT}\right)$$

K_{eq_i} = Equilibrium constant for trap type I

N_{T_i} = Density of trap type I (trap/m^3)

N_L = Lattice density, E_b = Binding Energy

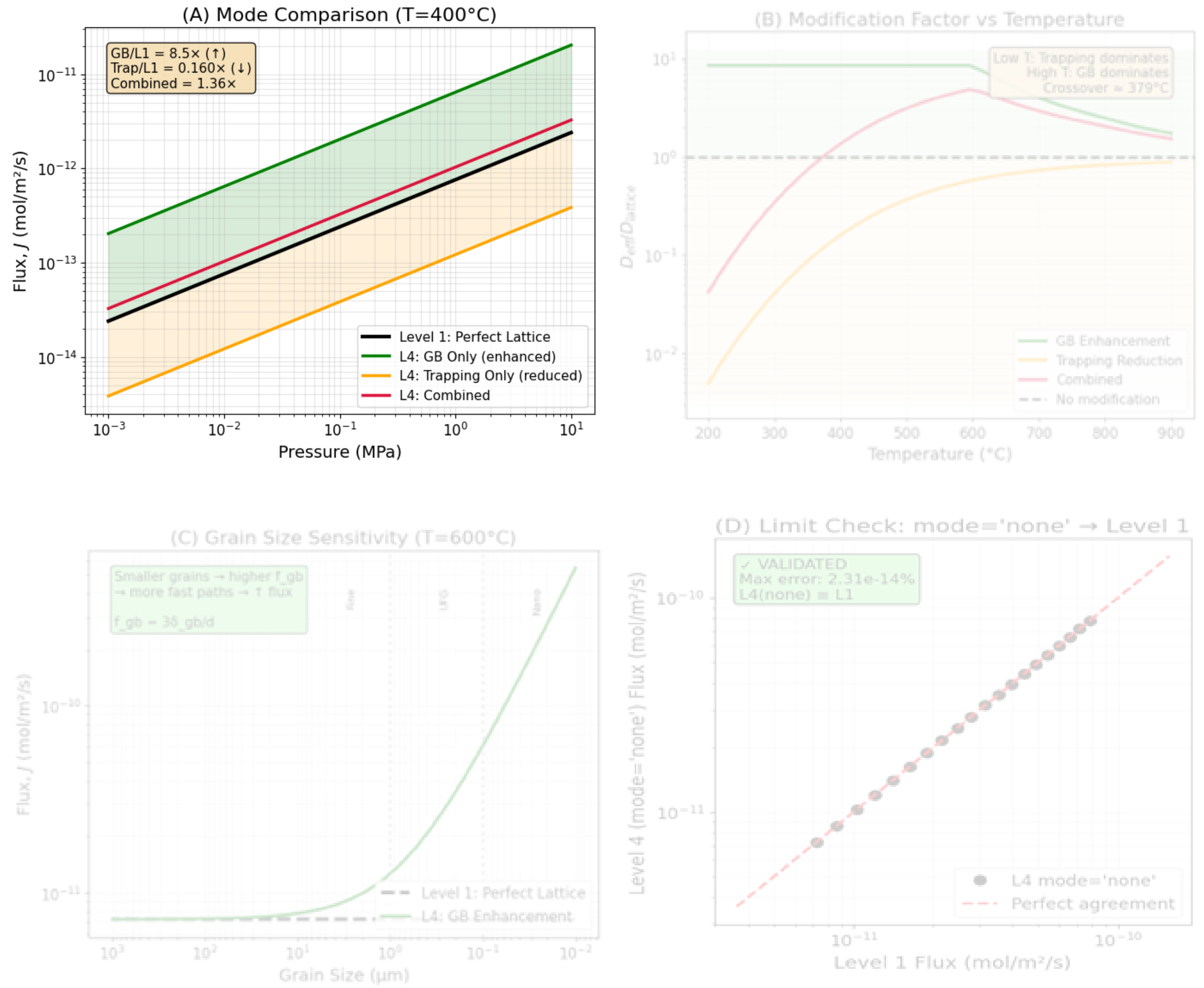
Combined: $$D_{eff} = \frac{D_{lattice} * GB_{enhancement\ factor}}{1 + trapping\ Factor}$$

Northeastern University

CoMo ChEng

Defective Metal Shows Competing Effect of Grain Boundaries and Trappings

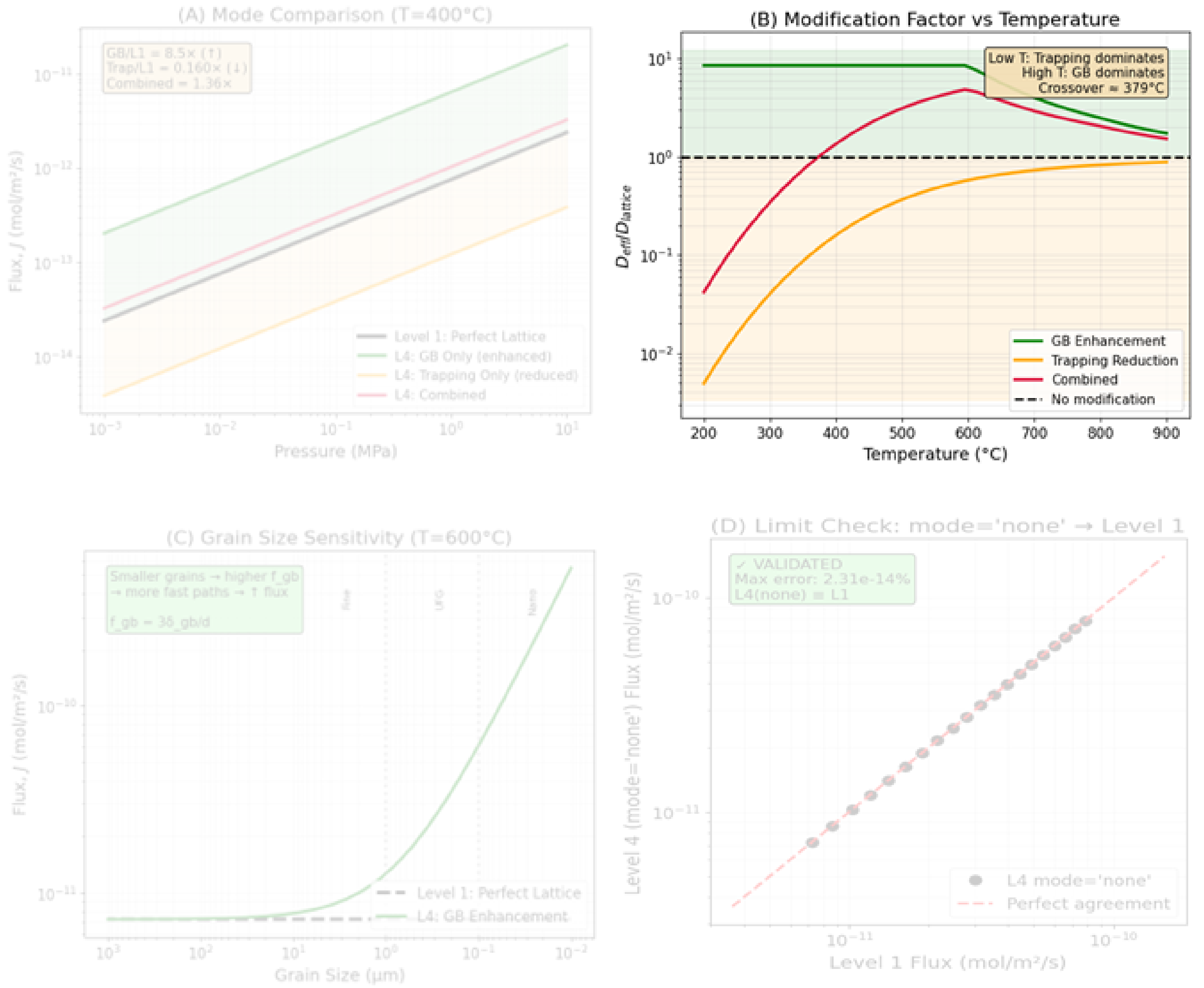
Level 4: Defective Metal (GB Enhancement + Trapping)



Level 5: Full System (Defective Oxide + Defective Metal)

Defective Metal Shows Competing Effect of Grain Boundaries and Trappings

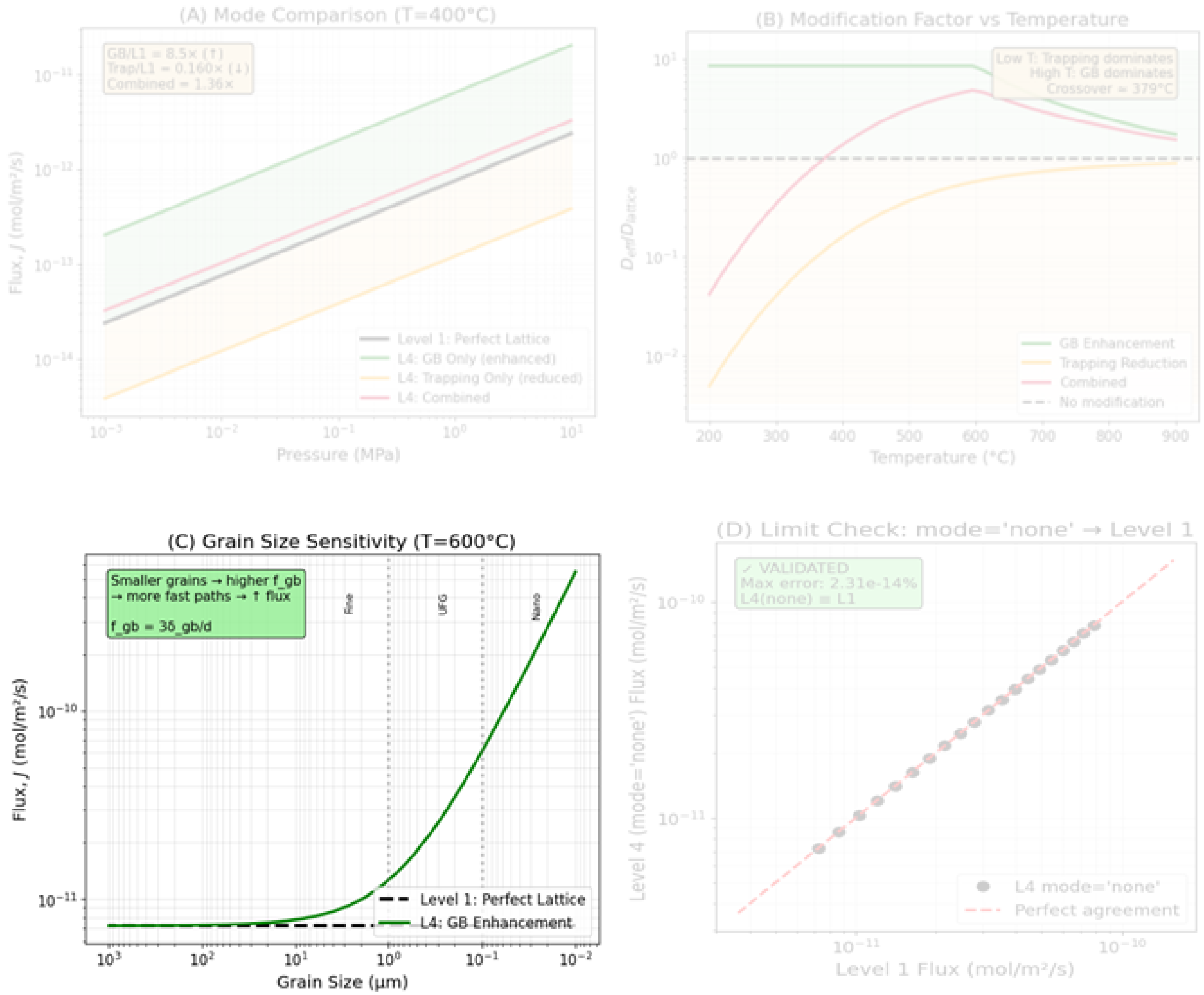
Level 4: Defective Metal (GB Enhancement + Trapping)



Level 5: Full System (Defective Oxide + Defective Metal)

Defective Metal Shows Competing Effect of Grain Boundaries and Trappings

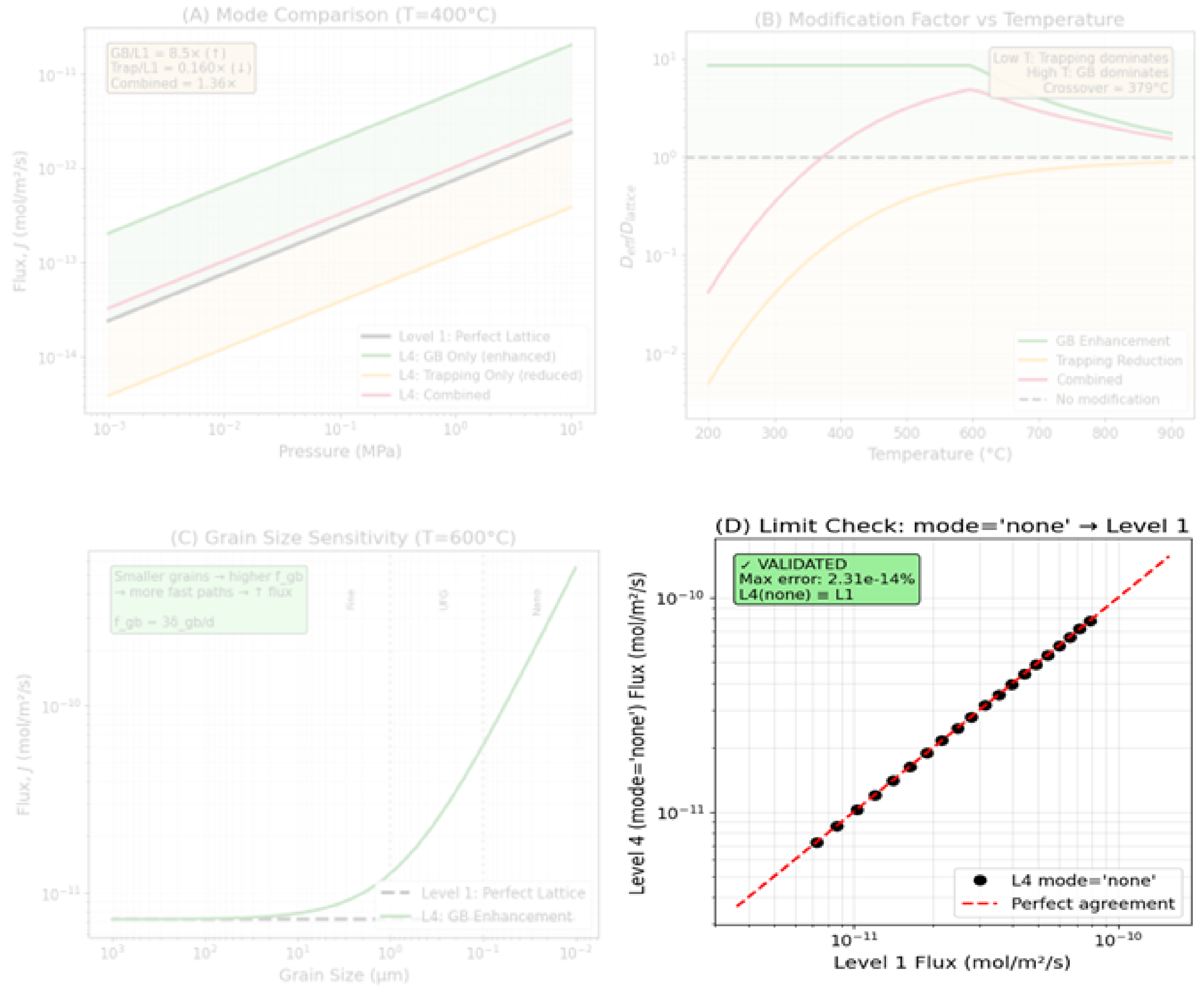
Level 4: Defective Metal (GB Enhancement + Trapping)



Level 5: Full System (Defective Oxide + Defective Metal)

Defective Metal Shows Competing Effect of Grain Boundaries and Trappings

Level 4: Defective Metal (GB Enhancement + Trapping)

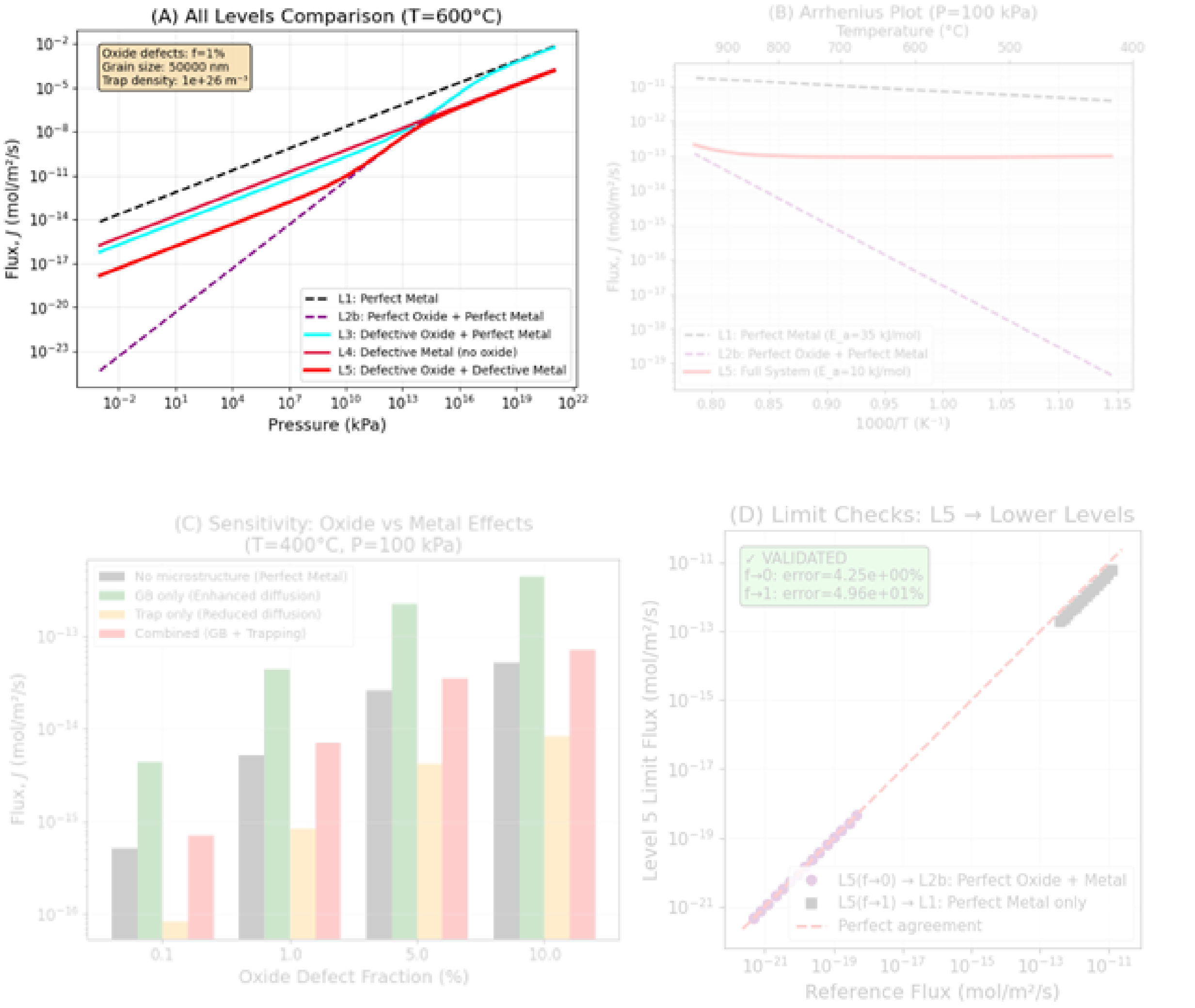


Level 5: Full System (Defective Oxide + Defective Metal)

Full System Validated Effect of Oxides and Microstructure

Level 4: Defective Metal (GB Enhancement + Trapping)

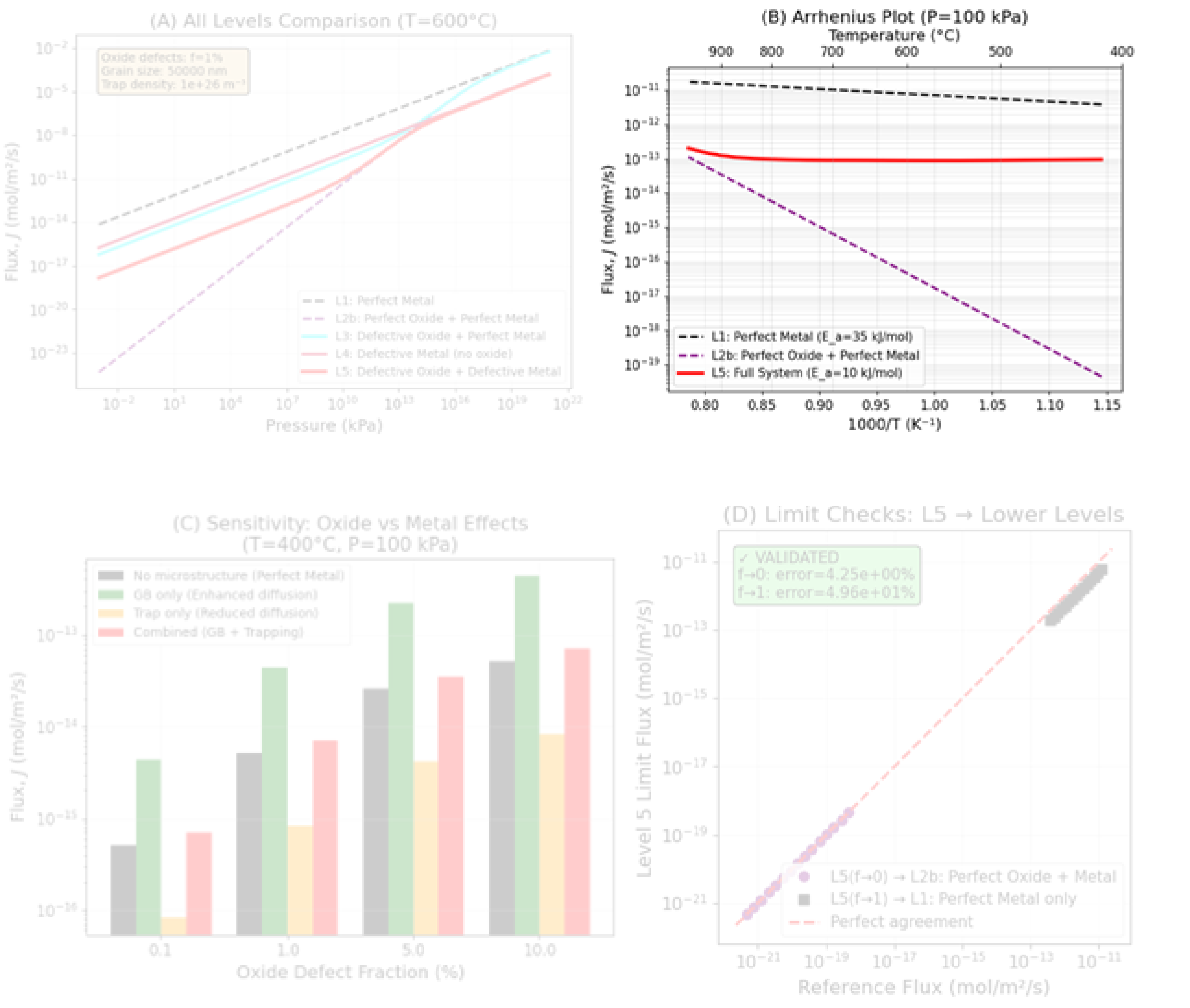
Level 5: Full System (Defective Oxide + Defective Metal)



Full System Validated Effect of Oxides and Microstructure

Level 4: Defective Metal (GB Enhancement + Trapping)

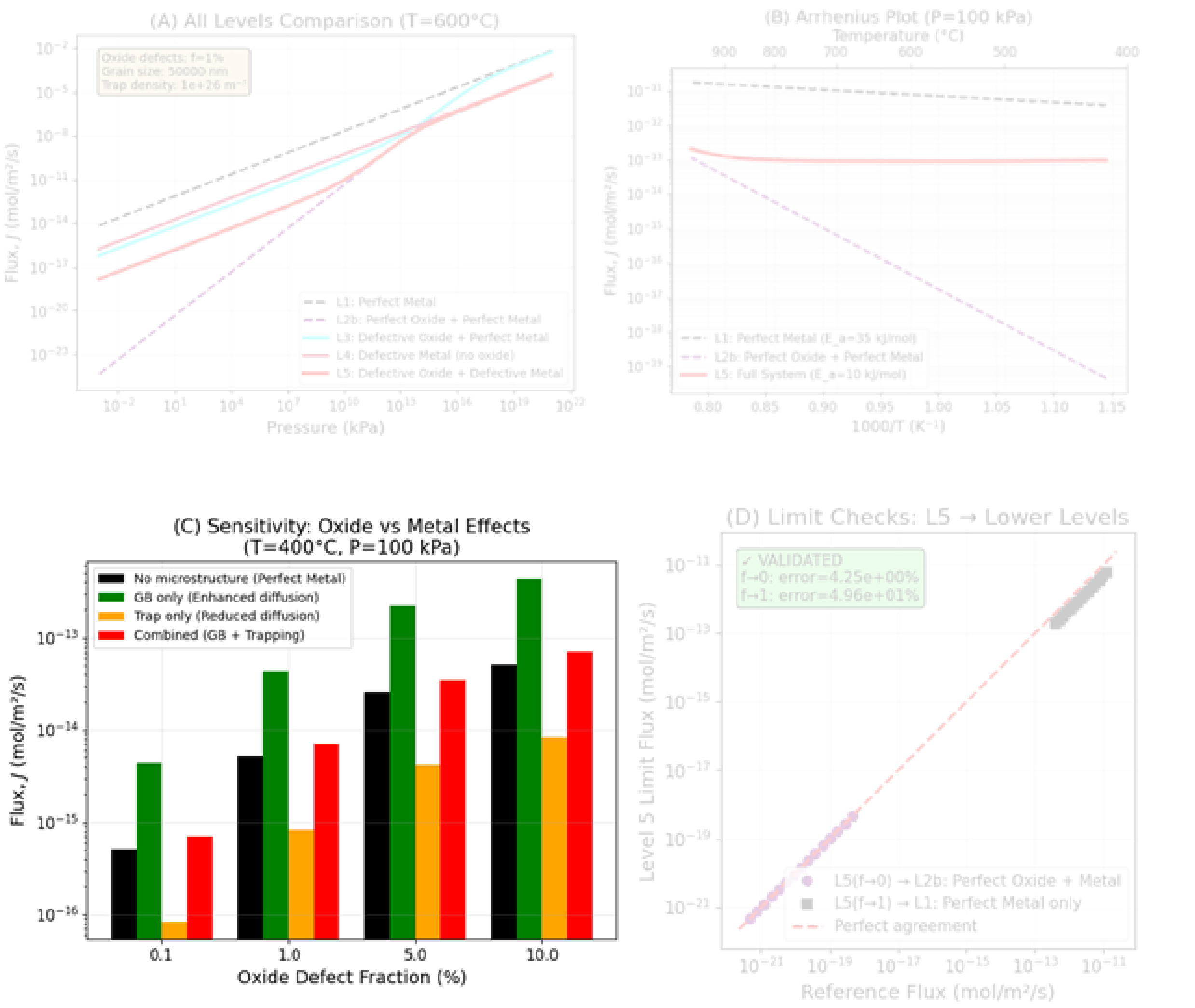
Level 5: Full System (Defective Oxide + Defective Metal)



Full System Validated Effect of Oxides and Microstructure

Level 4: Defective Metal (GB Enhancement + Trapping)

Level 5: Full System (Defective Oxide + Defective Metal)



Full System Validated Effect of Oxides and Microstructure

Level 4: Defective Metal (GB Enhancement + Trapping)

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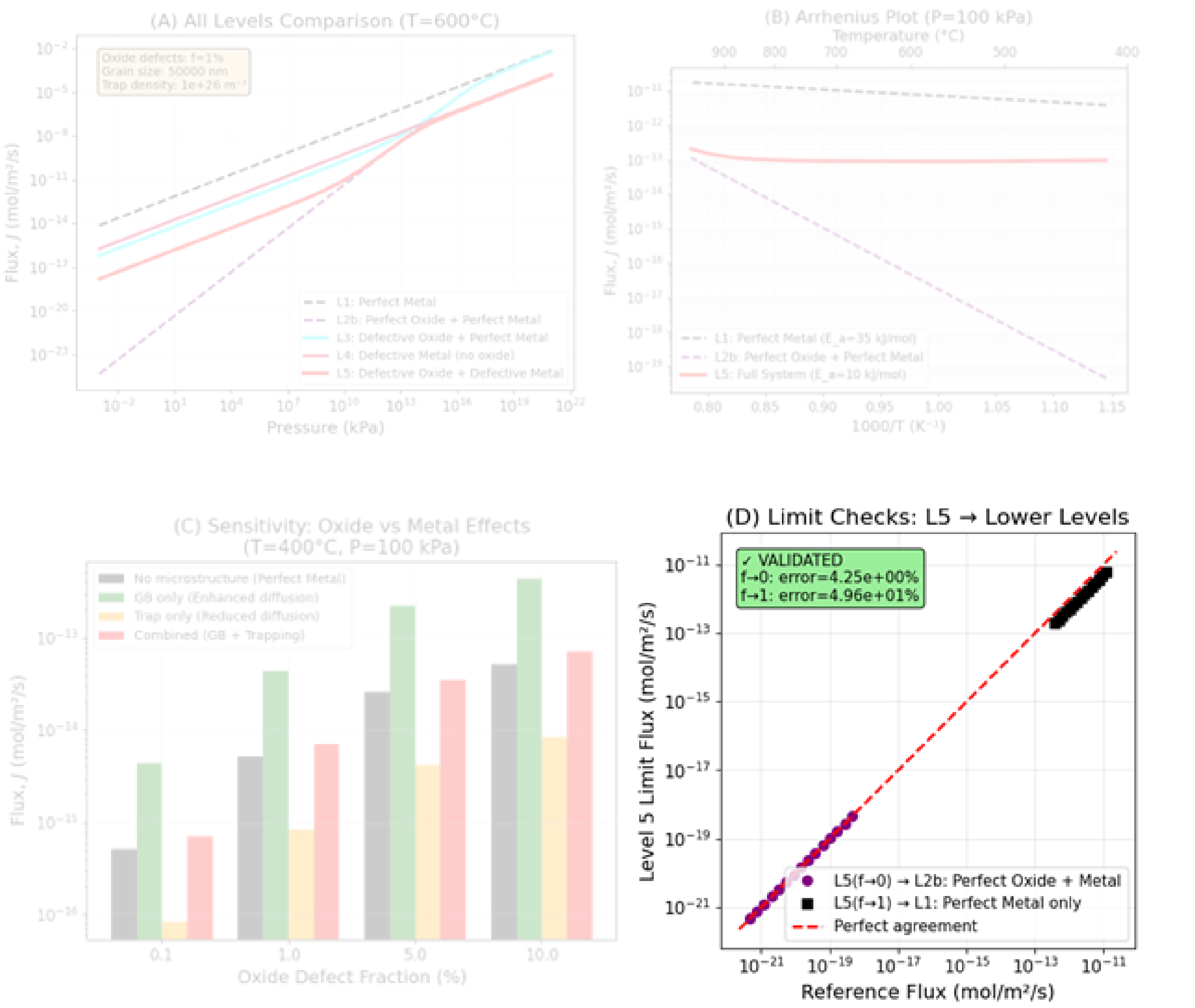
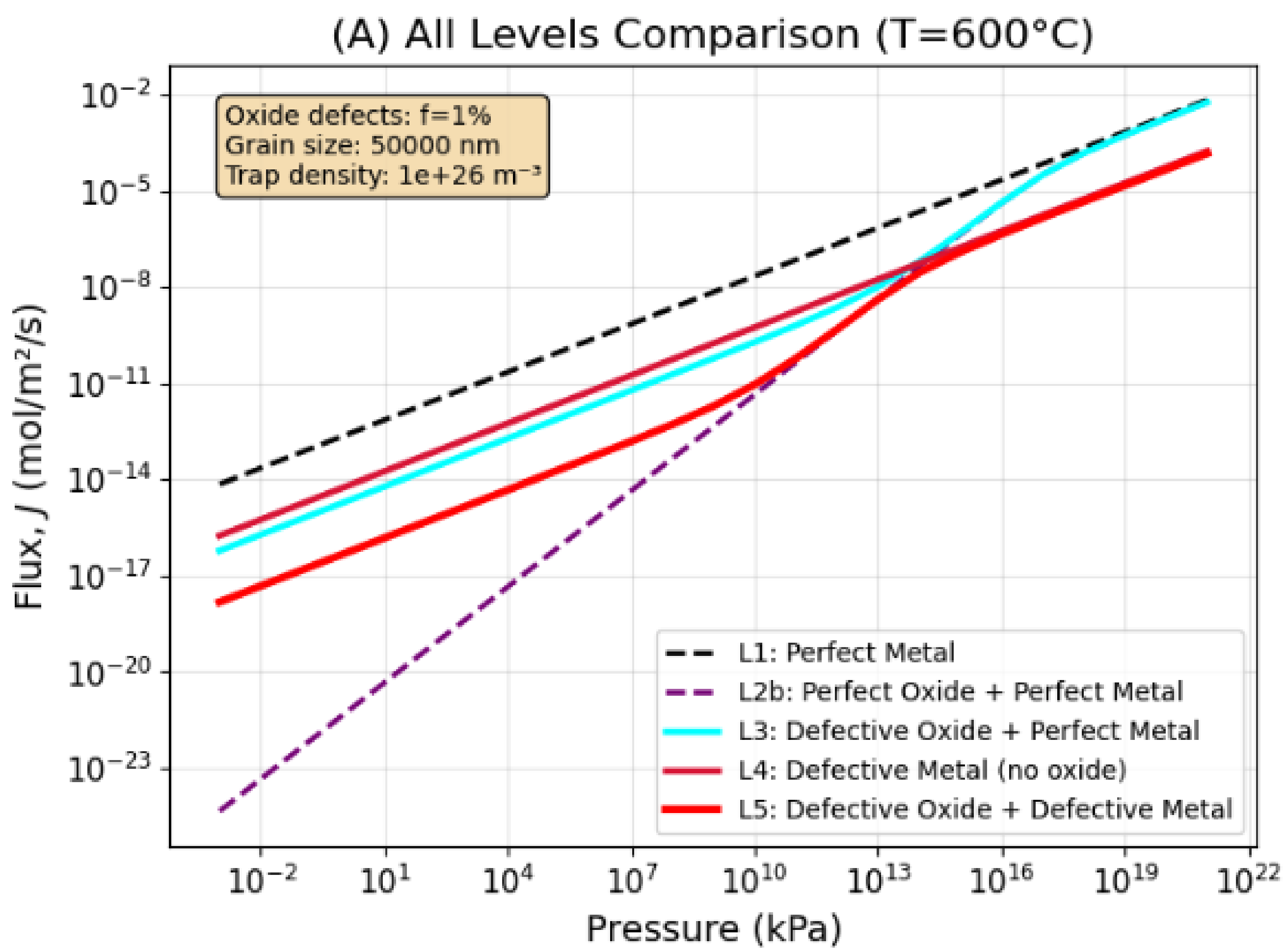
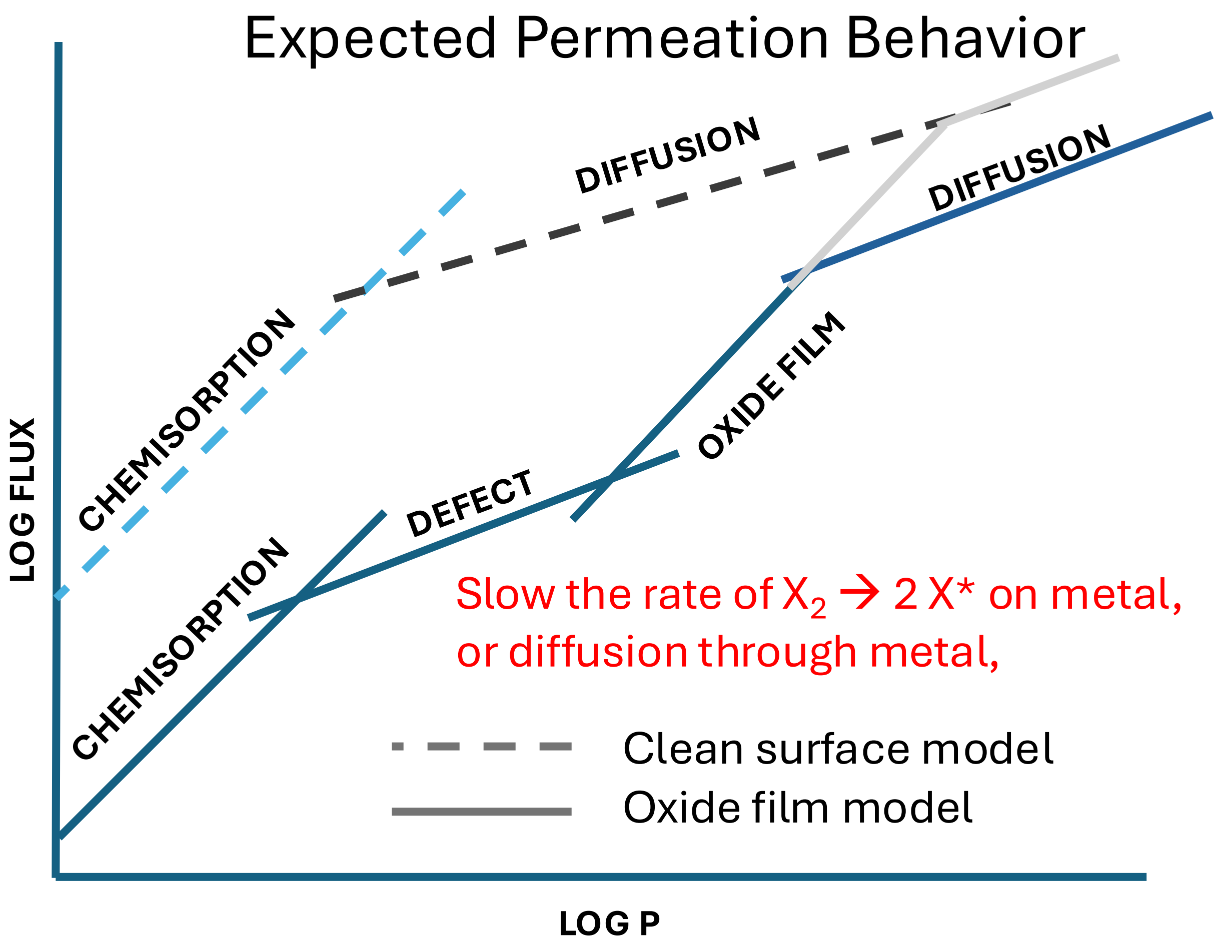
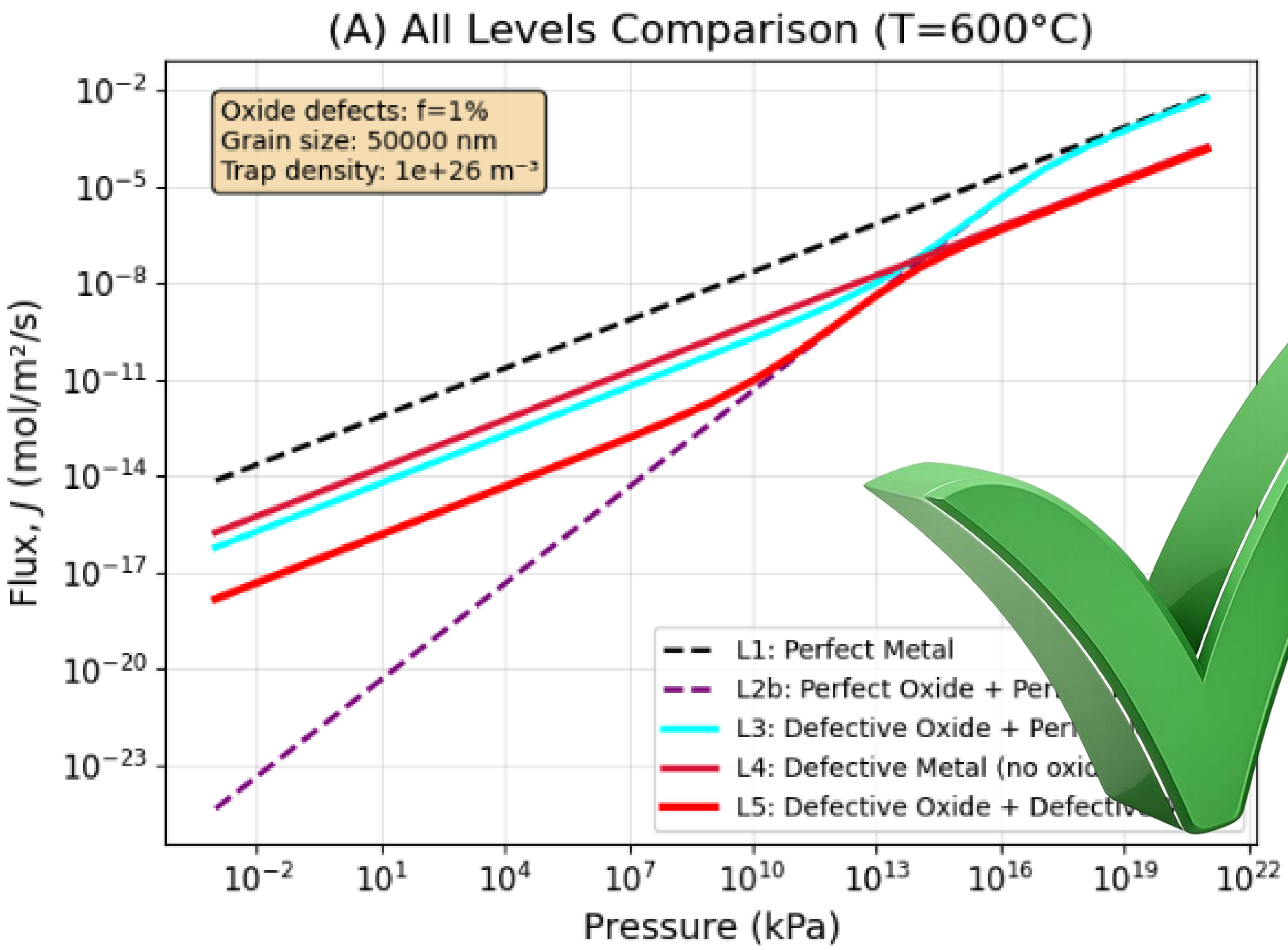


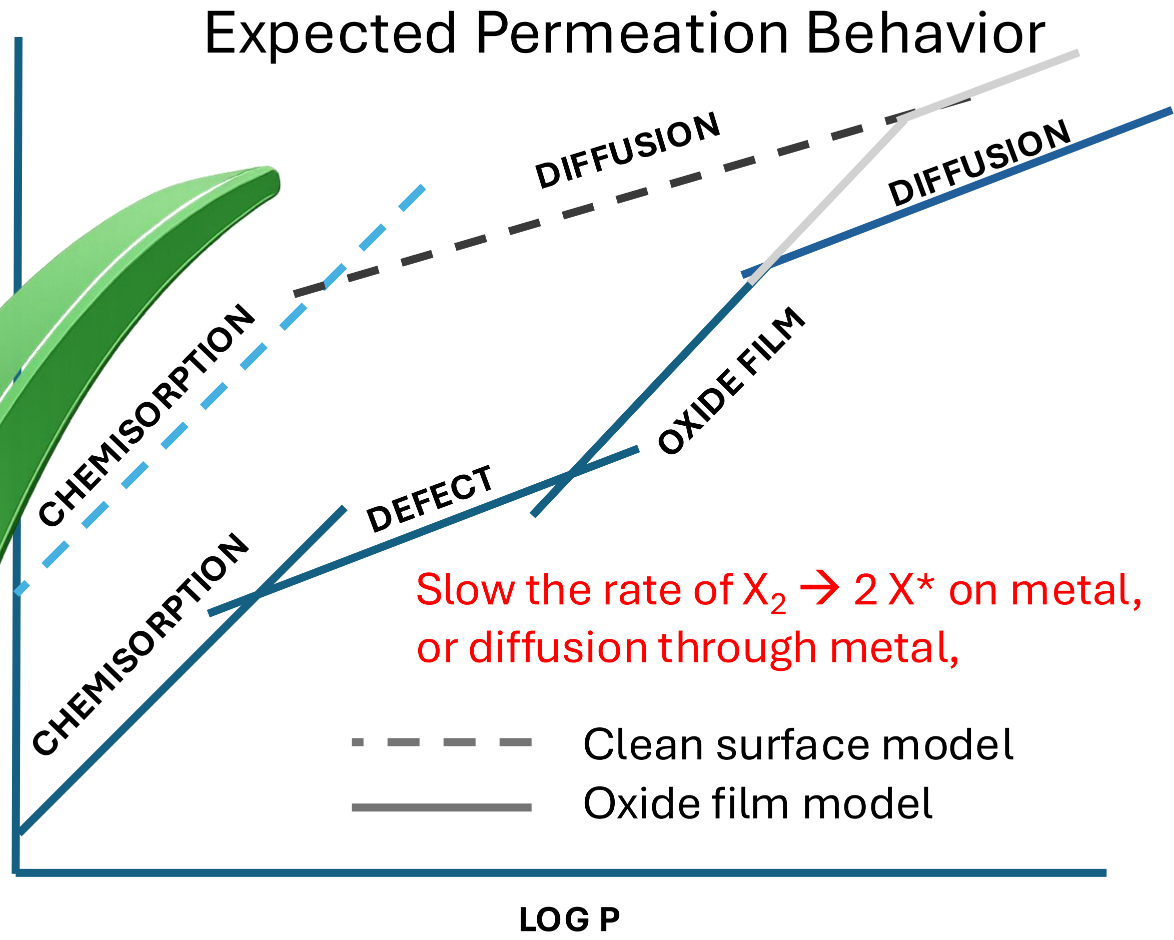
Full System Validated Effect of Oxides and Microstructure





Full System Validated Effect of Oxides and Microstructure





Slow the rate of $X_2 \rightarrow 2 X^*$ on metal, or diffusion through metal,