Exploring the Role of Bulk Hydrogen Diffusion in Vacuum Power Flow

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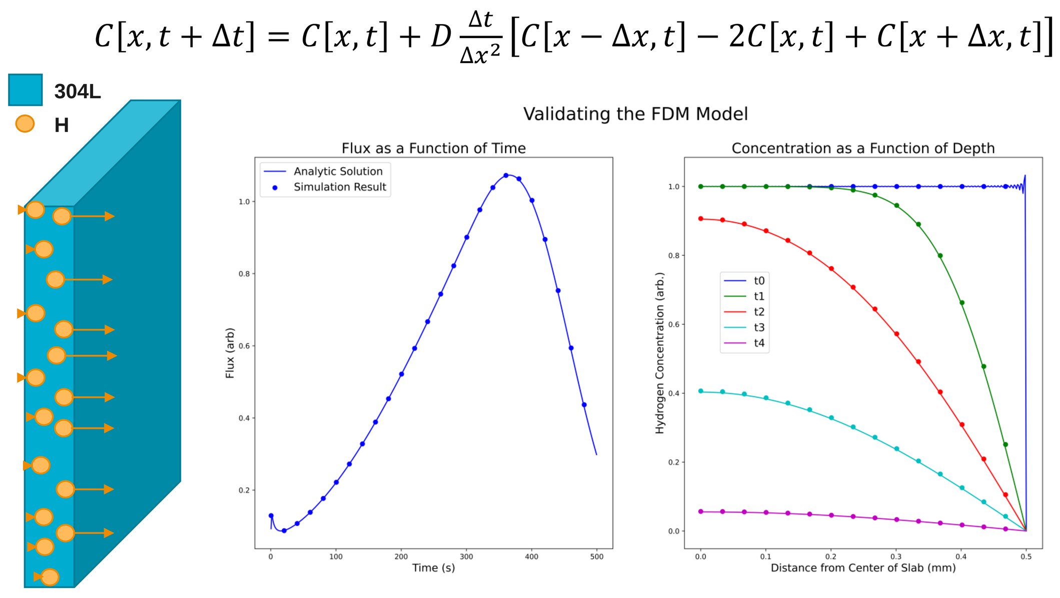
Abstract

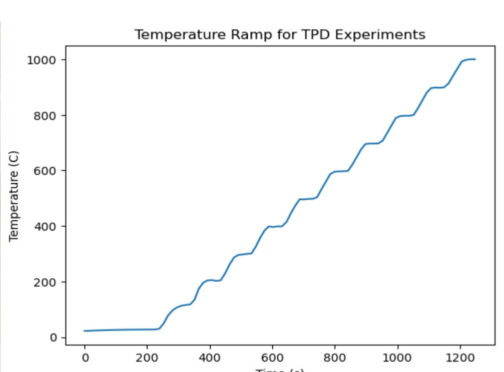
- High current pulses conducted through stainless steel magnetically insulated transmission lines (MITLs) increase the temperature of the material which releases neutral gasses into the anode-cathode gap. These neutral gasses may then be ionized by the extreme electric fields or collisions and accelerated across the gap resulting in current loss [1]. Recently, interest in improving power flow has been growing and many researchers are working to mitigate these losses [2]. Hydrogen is of particular interest because it is known to cause much of the observed losses due to its it low mass, allowing for a sufficient acceleration to cross the gap on pulsed power timescales. To better understand the underlying processes that cause these losses, we have been studying the diffusion and desorption of hydrogen from stainless steel.

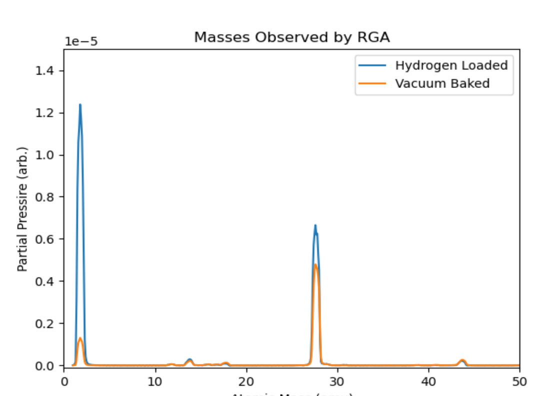
Modeling Diffusion

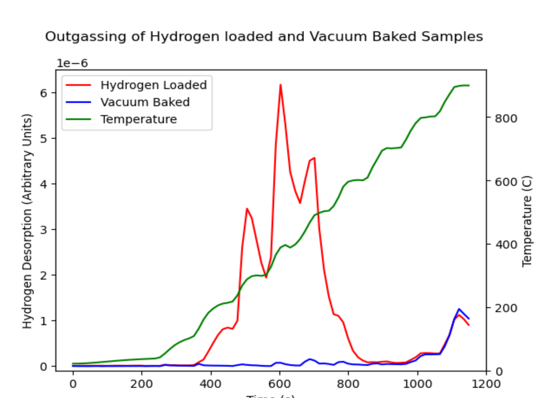
- Fick's Law in 1D:
  $\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2}$ with $D = D_0 \exp\left(\frac{-E_a}{RT}\right)$
- Analytical Solution
  $C(x,t) = \frac{4C_0}{\pi}\sum_{n=0}^{\infty}\frac{(-1)^n}{2n+1}\cos\left(\frac{(2n+1)\pi}{2L}x\right)\exp\left[-\left(\frac{(2n+1)\pi}{2L}\right)^2\int_0^t D(t)dt\right]$
- Discretized form used in numerical finite difference method (FDM) model
  $C[x,t+\Delta t] = C[x,t] + D\frac{\Delta t}{\Delta x^2}\left[C[x-\Delta x,t] - 2C[x,t] + C[x+\Delta x,t]\right]$



Slow Temperature Programmed Diffusion (TPD) Experiments

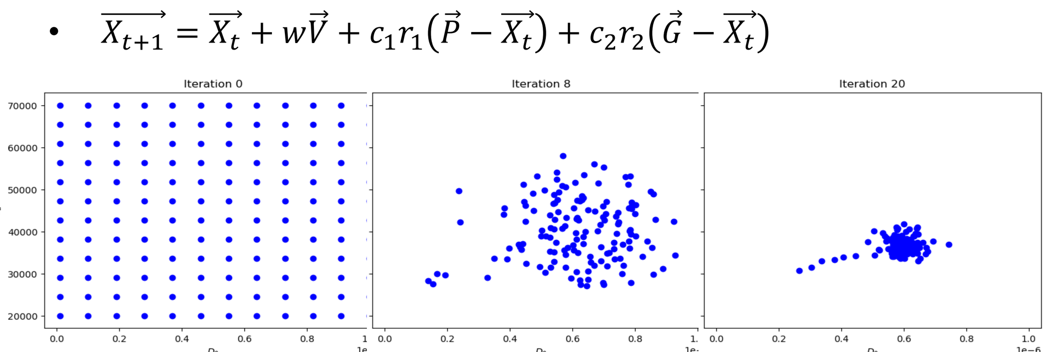






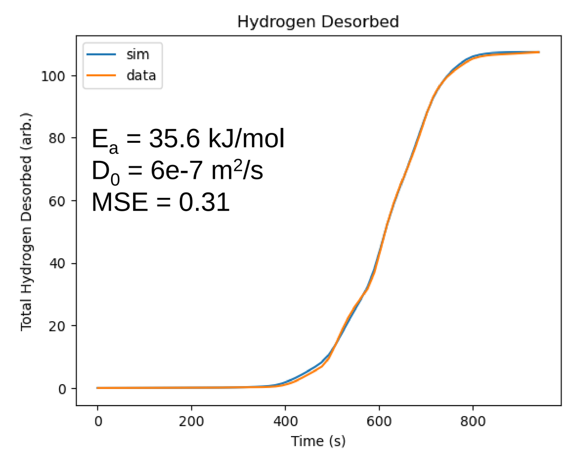
Optimization to Experimental Data

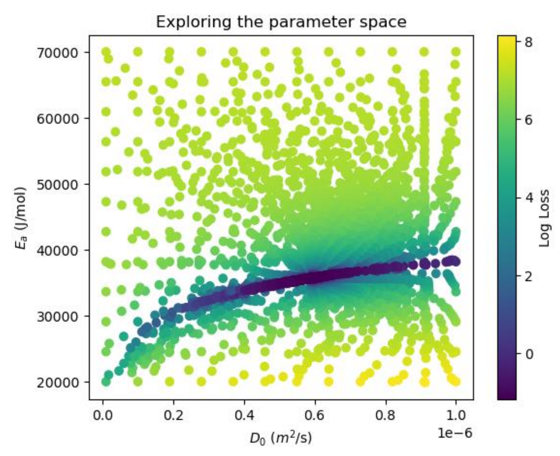
- The FDM simulation was optimized to experimental data using Particle Swarm optimization
  - $\overrightarrow{X_{t+1}} = \overrightarrow{X_t} + w\vec{V} + c_1 r_1(\vec{P} - \overrightarrow{X_t}) + c_2 r_2(\vec{G} - \overrightarrow{X_t})$



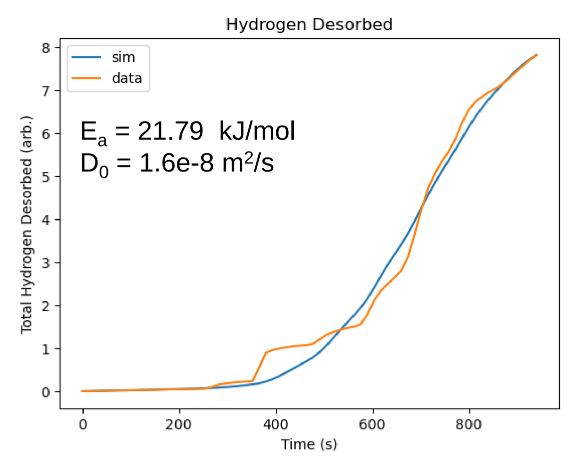
Optimization Results

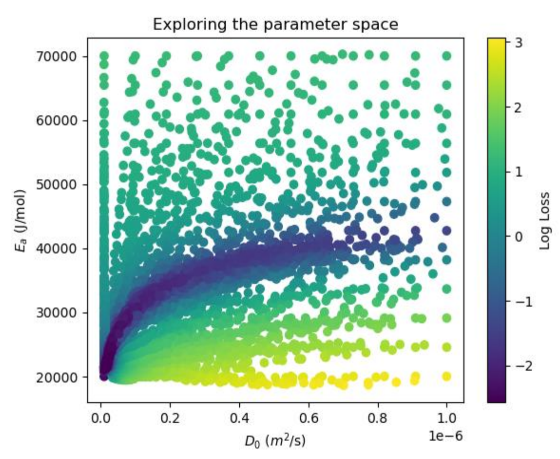
- Hydrogen Loaded





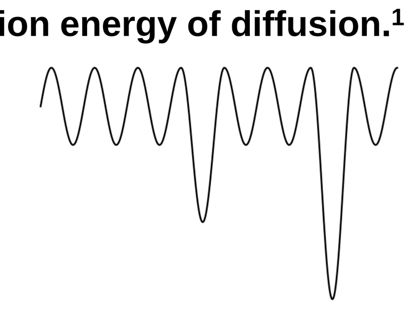
- Vacuum Baked





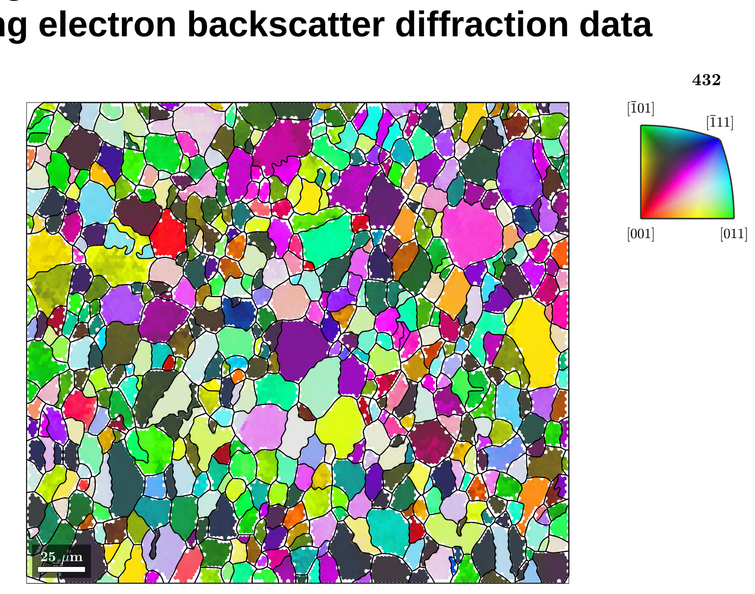
Hydrogen Trapping Models

- Fick's laws do not capture all the relevant physics of hydrogen diffusion through stainless steel because not all the sites have the same activation energy of diffusion.[1]



- $\frac{\partial C_L}{\partial t} + \frac{\partial C_T}{\partial t} - D\frac{d^2 C_L}{dx^2} = 0$
- $\frac{dC_T}{dt} = f(x, t, T, C_i, N_i, E_i \ldots)$

- The density of lattice sites can be determined from the density and molar mass of the material.[1]
  - $N_L = \frac{N_A \beta \rho}{M} = \frac{6.022e23\frac{\text{atom}}{\text{mol}} * 1\frac{\text{site}}{\text{atom}} * 8000\frac{\text{kg}}{\text{m}^3}}{0.0558\frac{kg}{mol}} = 8.74e28\frac{\text{sites}}{\text{m}^3}$
  - $N_L[\text{ppmw}] = 1e6\frac{N_L[\text{m}^{-3}]}{1000\rho N_A} = 18149 \text{ ppmw}$
- The density of trap sites can be estimated from properties of the grain boundaries and dislocations and Burger's vector using electron backscatter diffraction data



Dislocations due to Grain Boundaries

Model	Equation	220 um Sample
Song[2]	$N_T = 2N_L S_V b$	2e25
Liu[3]	$N_T = N_L\frac{b}{d}$	1e23
Turk[4]	$N_T = \frac{3}{db^2}$	2e23

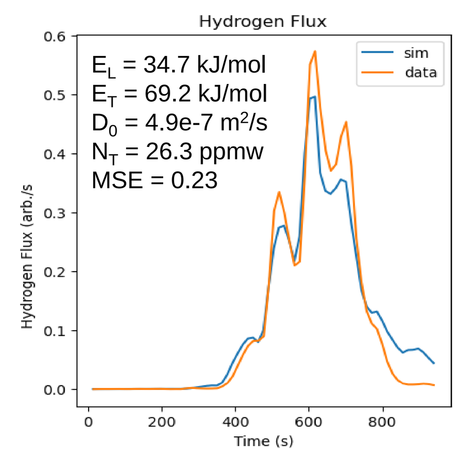
Dislocations due to Dislocations

Model	Equation	220 um Sample
Krom[1]	$N_T = \frac{\sqrt{\lambda}\rho}{a}$	1e24
Song[2]	$N_T = N_L \pi b^2 \rho$	2e24
Turk[4]	$N_T = 25 N_L \pi b^2 \rho$	1e26

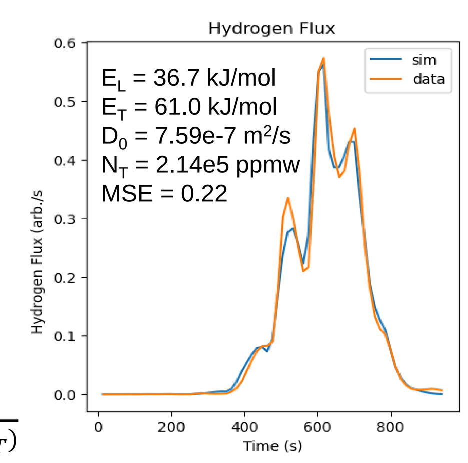
Modeling Trapping Phenomena

- To model more complex phenomena, the FDM code was expanded to include lattice sites and trap sites, and the particle swarm optimization algorithm was expanded to train any arbitrary number of parameters

- **Oriani Local Equilibrium Model[5]**
- $\mu_i = \mu_i^0 - RT\ln\frac{\theta_i}{1-\theta_i}$
- Assume 1 trap type and $\mu_L = \mu_T$
- $\frac{\theta_L(1-\theta_T)}{\theta_T(1-\theta_L)} = \exp\left(\frac{\mu_L^0 - \mu_T^0}{RT}\right) = \exp\left(\frac{E_b}{RT}\right)$
- $D_{eff} = D_L\frac{dC_L}{dC_T} = D_L\frac{C_L}{C_L + C_T(1-\theta_T)}$



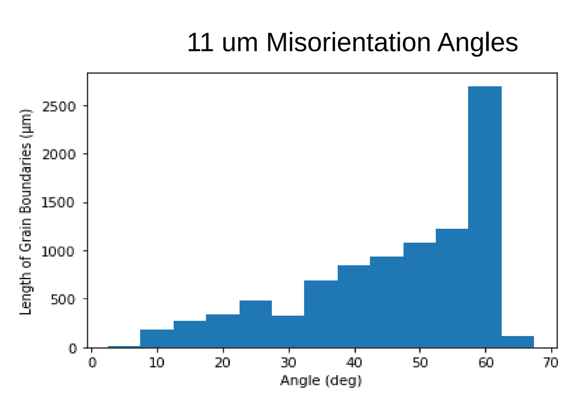
- **Optimize to Krom Trapping Model[1]**
- $\frac{\partial C_T}{\partial t} = \frac{\partial C_T}{\partial t}\Big|_{L\to T} - \frac{\partial C_T}{\partial t}\Big|_{T\to L}$
- $\frac{\partial C_T}{\partial t}\Big|_{L\to T} = \nu C_L \exp\left(\frac{-E_L}{RT}\right)\frac{N_T - C_T}{(N_L - C_L) + (N_T - C_T)}$
- $\frac{\partial C_T}{\partial t}\Big|_{T\to L} = \nu C_T \exp\left(\frac{-E_T}{RT}\right)\frac{N_L - C_L}{(N_L - C_L) + (N_T - C_T)}$
- $\frac{\partial C_L}{\partial t} = D\frac{d^2 C_L}{dx^2} - \nu C_L \exp\left(\frac{-E_L}{RT}\right)\frac{N_T - C_T}{(N_L - C_L) + (N_T - C_T)} + \nu C_T \exp\left(\frac{-E_T}{RT}\right)\frac{N_L - C_L}{(N_L - C_L) + (N_T - C_T)}$

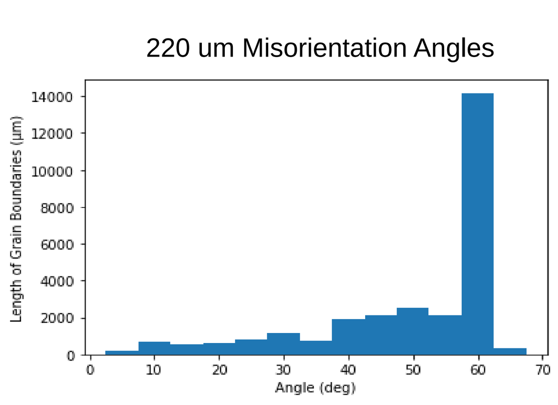


Next Steps

- Correlate Trapping Energy Distribution to dislocation and grain boundary misorientation distribution

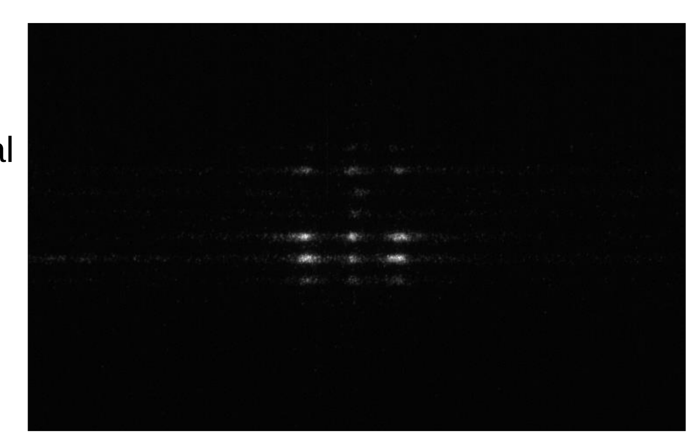
$$\Delta\theta \leq 15°\Sigma^{-\frac{5}{6}}$$





- Short timescale heating experiments
- Pulsed Power Experiments

Plasma density can be estimated from the Zeeman splitting of hydrogen spectral lines. In addition to out short-timescale heating experiments, we have pulsed power experiments planned to test against our diffusion model



References and Acknowledgment

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