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Sensitivity and response time of Pd nanowire H sensors

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Approach

- Phenomenological model for H absorption into Pd
- Fit parameters to reproduce experimental results
- Simulate diffusion into Pd nanowire
- Compute change in resistance

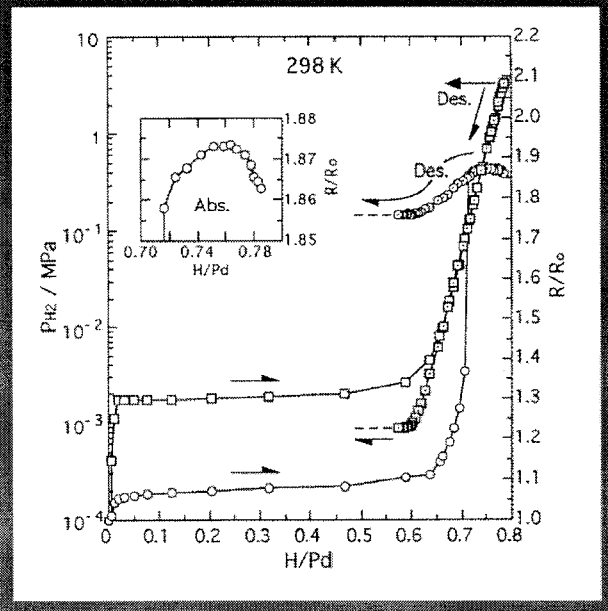
Results

- Sensitivity does not depend on nanowire diameter
- Response time increases with diameter

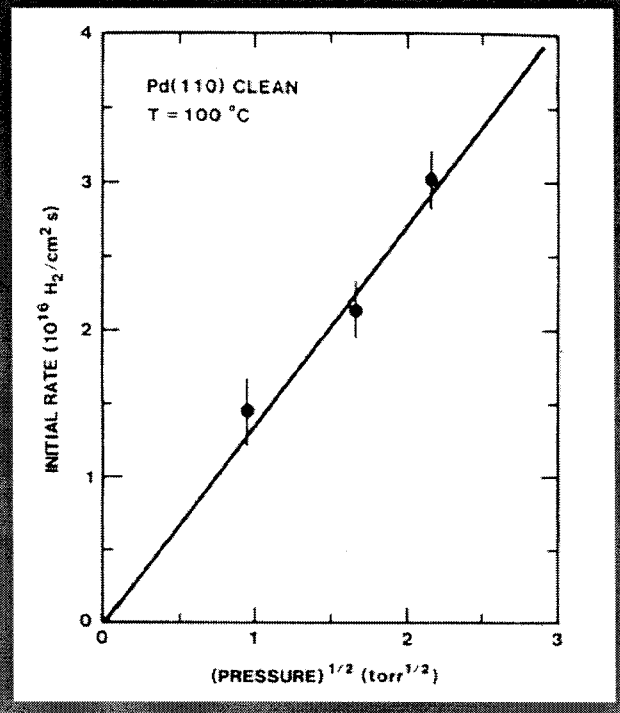
Funding from JPL Research and Technology Development

H absorption into Pd: Experiments

Phase diagram



Kinetics



Phase transition

- Phase α: fcc a=0.3891 nm
- Phase β: fcc a=0.4026 nm
- Miscibility gap β_{min}-α_{max}

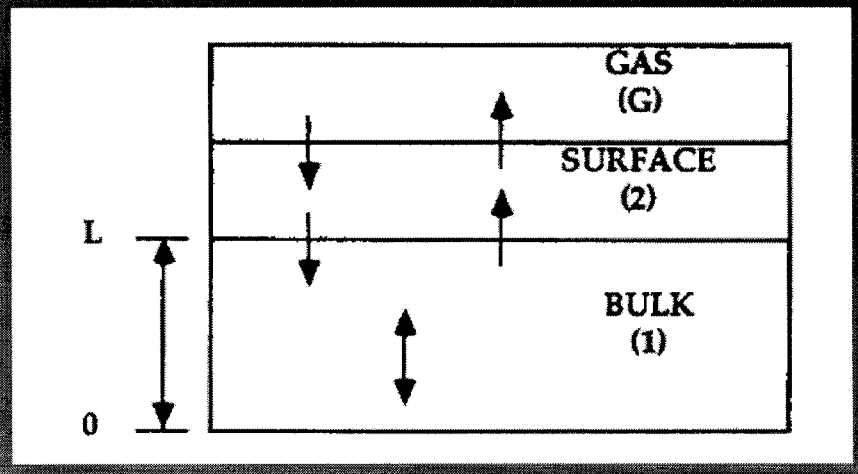
Resistance change

Additional scattering centers

Initial absorption rate R_0

- ∝ P: absorption bound
- ∝ √P: diffusion bound

H absorption into Pd nanowire



Absorption model

- Two interfaces
- Dissociative absorption
- Activated desorption
- Diffusion in bulk Pd

$$\frac{d\tilde{\theta}}{dt} = R_{12}\tilde{\rho}\left(1-\tilde{\theta}\right) - R_{21}\tilde{\theta}\left(1-\tilde{\rho}\right) + R_a \frac{2}{\theta_s}\left(1-\tilde{\theta}\right)^2 - R_d\tilde{\theta}^2\theta_s$$

Rate equation

$$R_a = \frac{SP}{\sqrt{2\pi M k_B T}} \qquad R_d = F_{2G}e^{-\beta E_{2G}}$$

Absorption and desorption rates

$$\frac{d\rho}{dt} = \frac{1}{r}\frac{d}{dr}\left(rD(r)\frac{d\rho}{dr}\right)$$

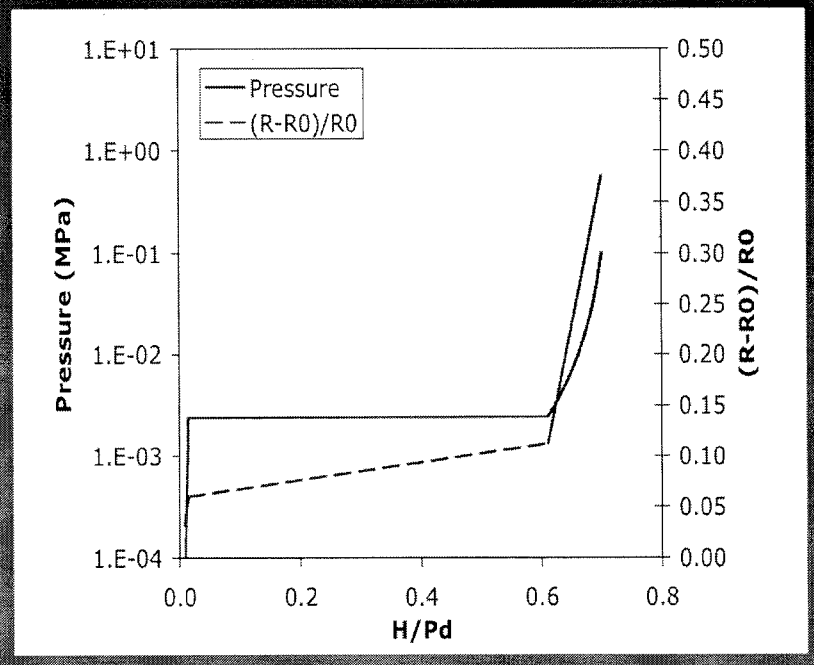
Diffusion equation

$$J(R) = -D\frac{d\rho(R)}{dr} = R_{21}\theta\left(1-\tilde{\rho}\right) - R_{12}\tilde{\rho}\theta_S\left(1-\tilde{\theta}\right)$$

Boundary condition

Fitting to experiment

Phase diagram



Stationary solution

$$J(R)=0 \longrightarrow R_a \frac{2}{\theta_s}\left(1-\tilde{\theta}\right)^2 - R_d \tilde{\theta}^2 \theta_s = 0$$

$$\tilde{\theta}_\infty = \frac{1}{1+\theta_S\sqrt{\frac{R_d}{2R_a}}}$$

Surface coverage

$$\tilde{\rho}_\infty = \frac{R_{21}\tilde{\theta}_\infty}{R_{21}\tilde{\theta}_\infty + R_{12}\left(1-\tilde{\theta}_\infty\right)}\frac{\rho_S}{\rho_{Pd}}$$

Density

(1) $\rho_s^\alpha = \rho_s^\beta = \rho_s \le \rho_{Pd}$

(2) $R_d^\alpha\left(\theta_s^\alpha\right)^2 = R_d^\beta\left(\theta_s^\beta\right)^2 = D$

(3), (4) $\dfrac{R_{12}^\alpha}{R_{21}^\alpha} \neq \dfrac{R_{12}^\beta}{R_{21}^\beta}$

$\theta_s^\alpha = \theta_s^\beta = \theta_s = \theta_{Pd}$

Phase α

(1) $\tilde{\rho}_\infty(P_0) = \alpha_{\max} = 0.015$

(2) $\tilde{\rho}_\infty(P) \propto \sqrt{P}$

$R_0 = B\sqrt{P} \longrightarrow R_{12}^\alpha$

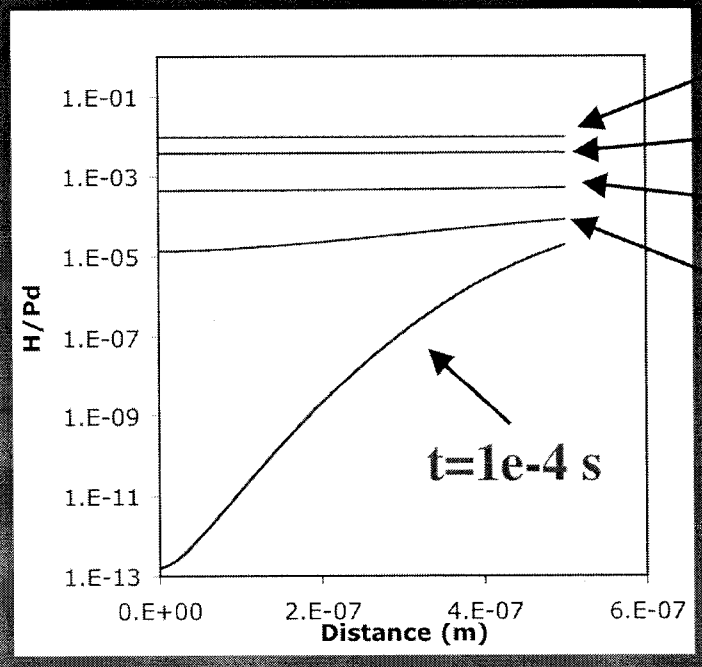
Phase β

(3) $\tilde{\rho}_\infty(P_0) = \beta_{\min} = 0.61$

(4) $\tilde{\rho}_\infty(P_1) = \beta_1 = 0.7$

Results for nanowire

Dynamics of H diffusion

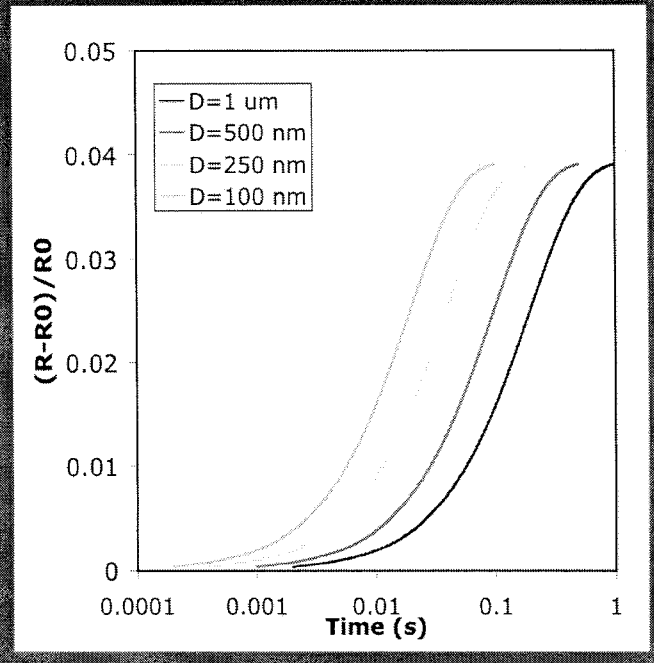


t=1 s
t=1e-1 s
t=1e-2 s
t=1e-3 s

Numerical solution (time and space)

- Rate equation
- Diffusion equation

Dynamics of resistance variation



Conclusion

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