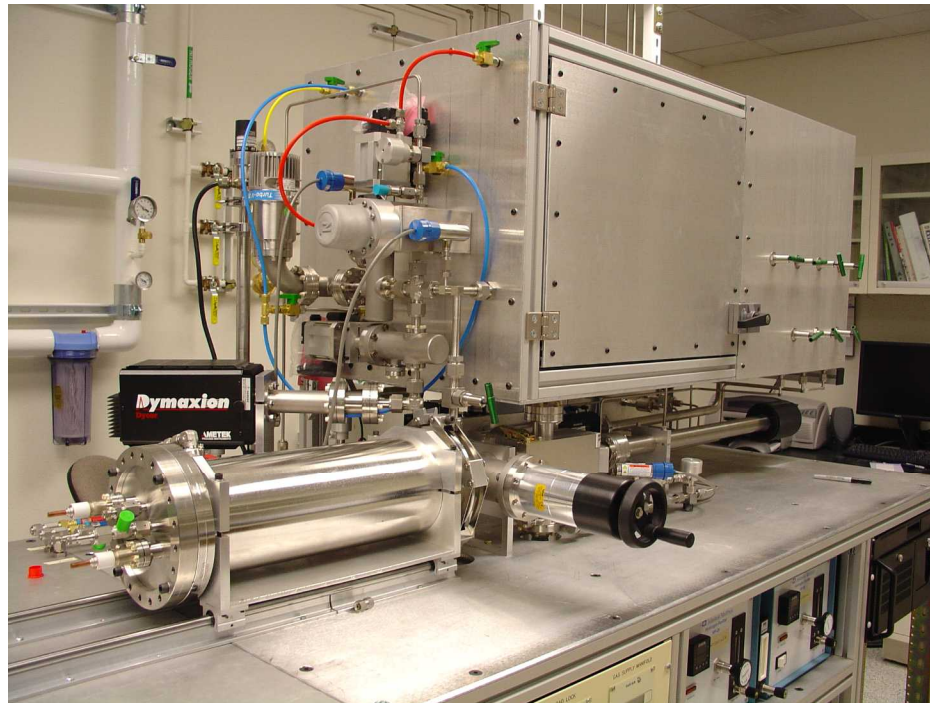


PCT Study: Erbium-Hydrogen System (Preliminary Results)

SAND2008-0748C

Rob Ferrizz, Tom Louck, Loren Espada, Dan Kammler, Clark Snow



Hydrogen and Helium Isotopes in
Materials Conference, February 2008



Acknowledgements

Metal Hydrides Team

Loren Espada, Clark Snow, Dan Kammler, Tom Louck, Barry Ritchey,
Elaine Boespflug, David Hawn, Garry Simmons

PCT Apparatus – Previous Owners

Saskia King, Craig Tewell

Inspiration in the Literature

Intro to Rare Earth Hydrides

- Vajda, P., Hydrogen In Rare-Earth Metals, Including RH_{2+x} Phases. *Handbook on the Physics and Chemistry of Rare Earths* **20**, 207-291 (1995).

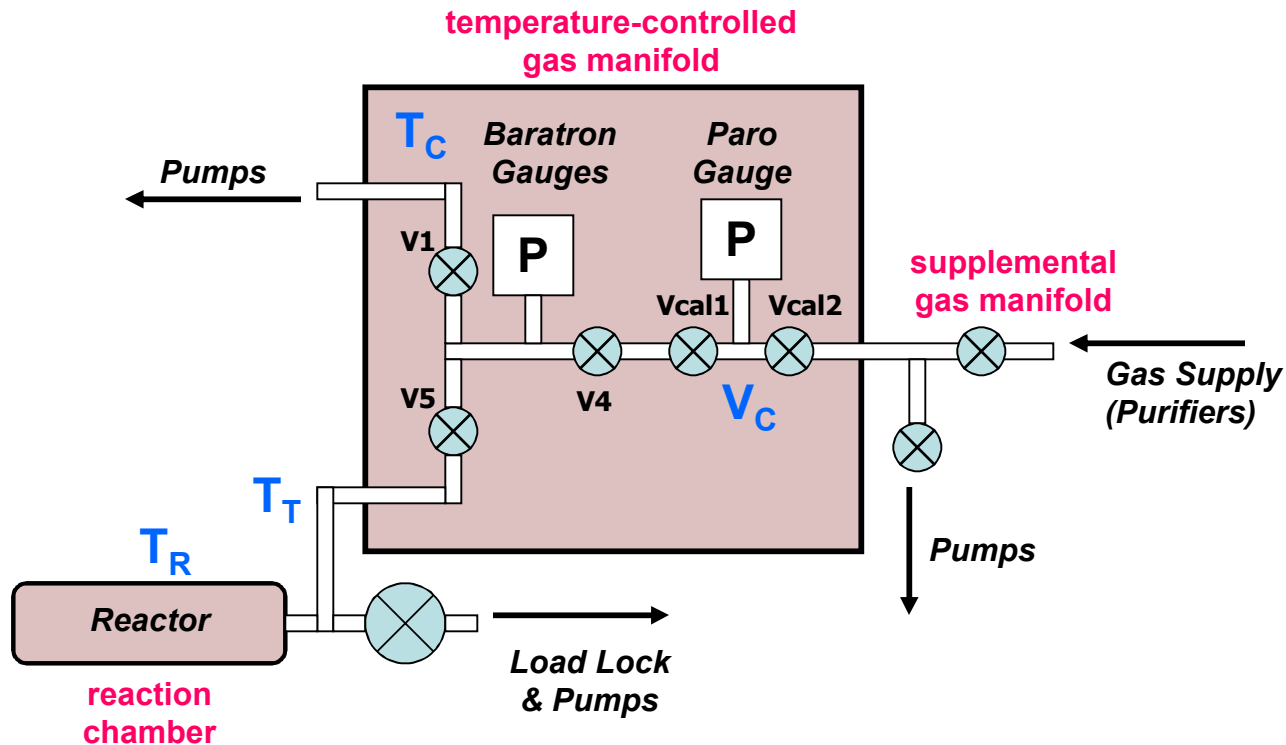
Erbium-Hydrogen Isotherms

- Lundin, C. E., The erbium-hydrogen system. *Transactions of the Metallurgical Society of AIME* **242**, 903-907 (1968).

Intro to Kinetics & Hydrides

- Bloch, J., Kinetics and mechanisms of metal hydrides formation – a review. *Journal of Alloys and Compounds* **253-254**, 529-541 (1997).
- Luo, W., Gross, K. J., A kinetics model of hydrogen absorption and desorption in Ti-doped $NaAlH_4$. *Journal of Alloys and Compounds* **385**, 224-231 (2004).

PCT Apparatus



Outline of Presentation:

1. H/D Loader

“Routine Operation”

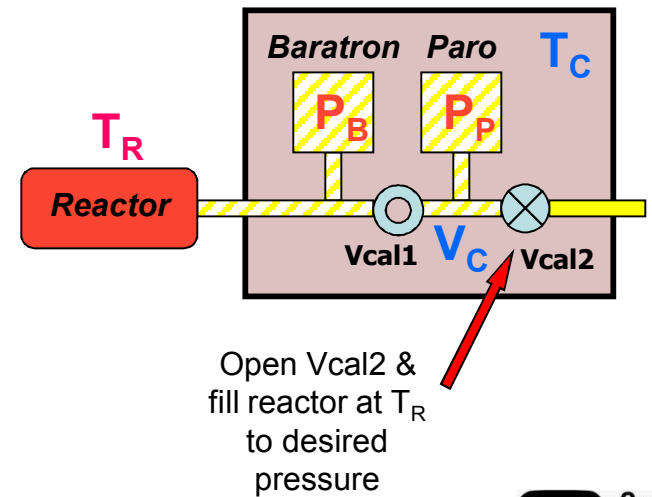
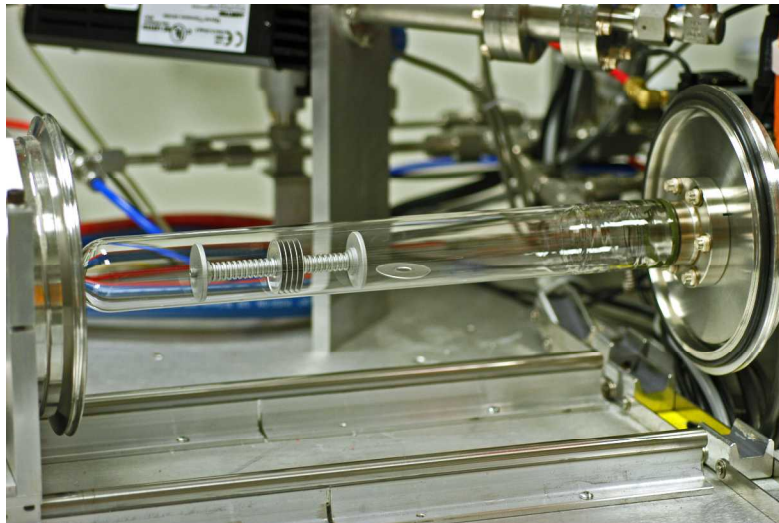
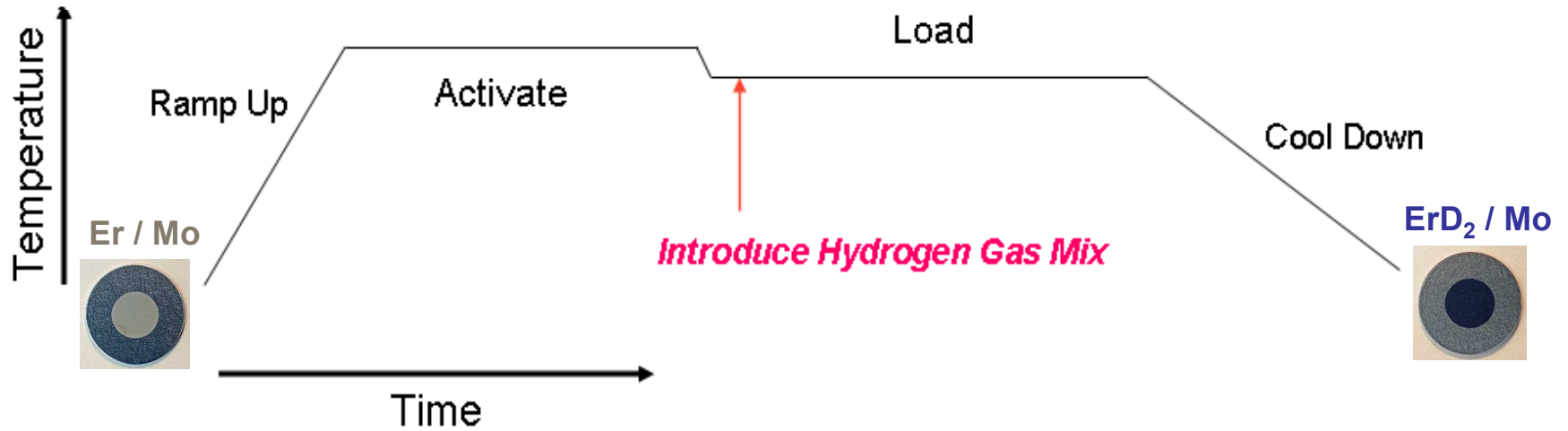
2. Thermodynamics (Isotherms)

“Primary Application”

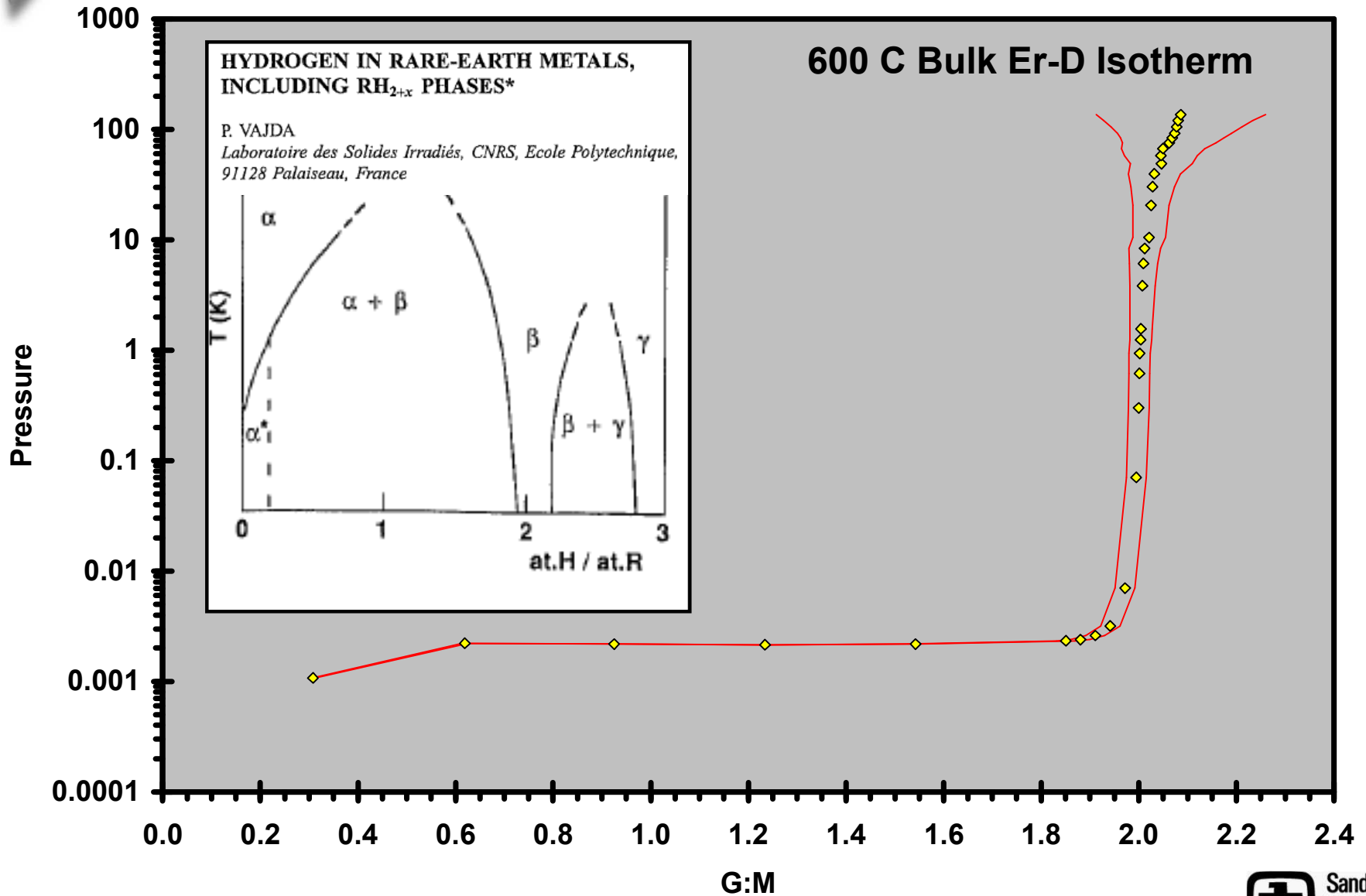
3. Kinetics

“Future Focus”

H/D Loader



Thermodynamics (Isotherms)



Experimental Approach

Step 1.) Open Vcal2

Fill V_C at T_C to P_A

Step 2.) Close Vcal2

Record P_A

Calculate molar aliquot $n_A = (P_A \times V_C) / (R \times T_C)$

Step 3.) Open Vcal1

Expand Gas into Reactor at T_R

Allow system to equilibrate

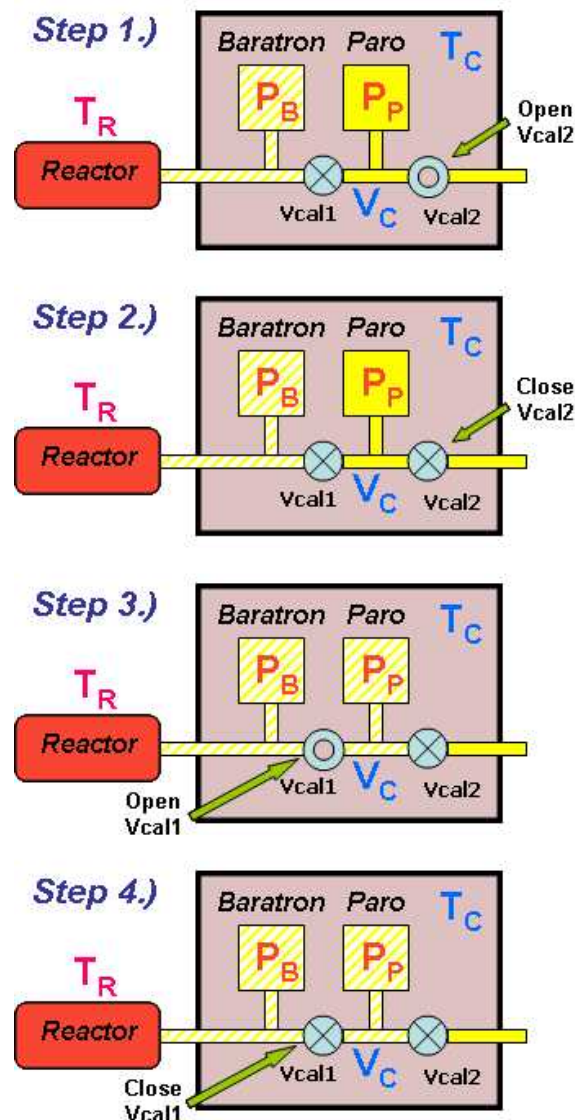
Record equilibrium pressure vs. time $P_{EQ_i}(t)$

Calculate gas phase moles $n_G = f(P_{EQ_i})$ ['mole meter']

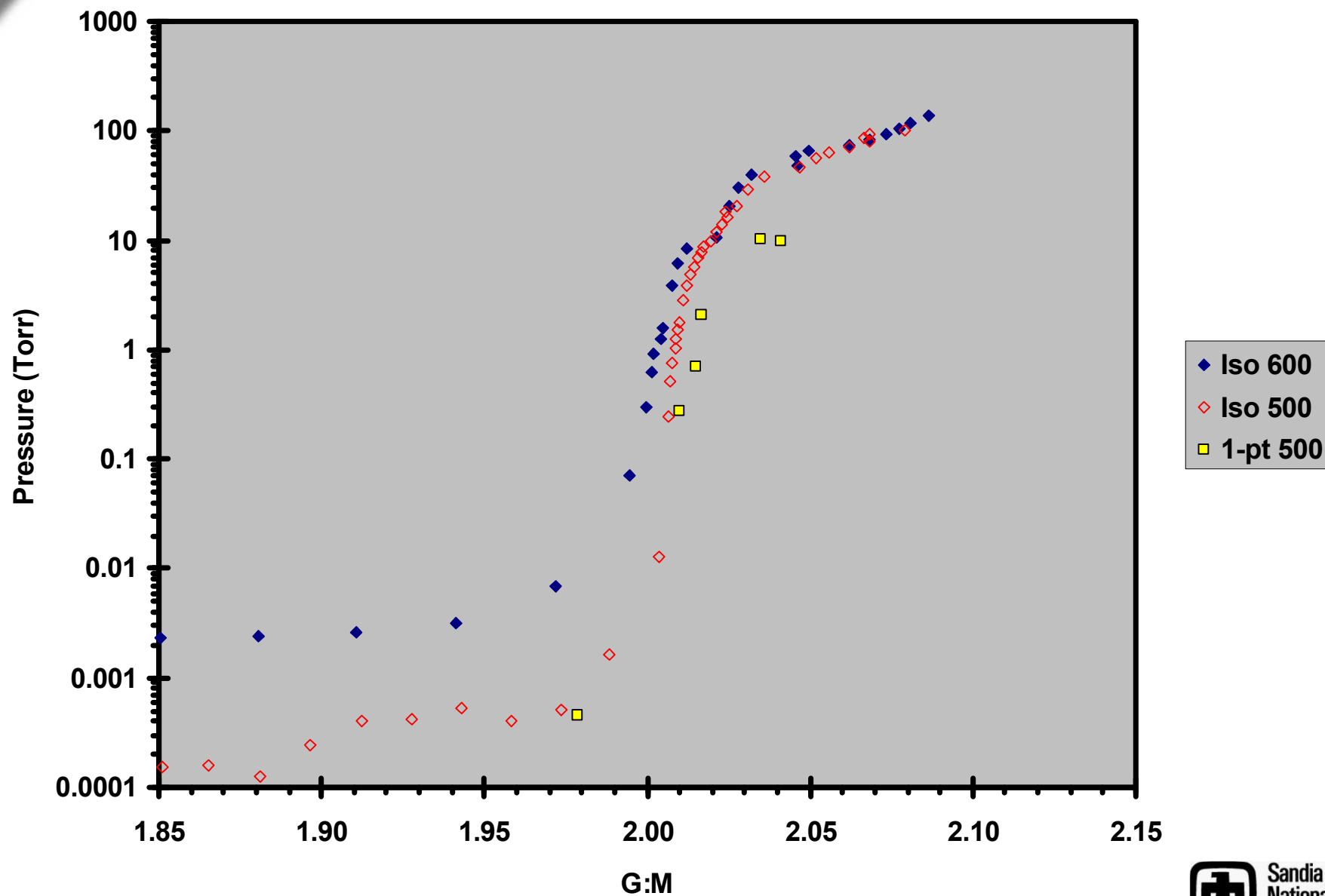
Calculate Total Molar Uptake $n_U = \Sigma n_{A_i} - n_G$

Calculate G:M ratio, $GM = 2 \times n_U \times MW_{Er} / \text{mass}_{Er}$

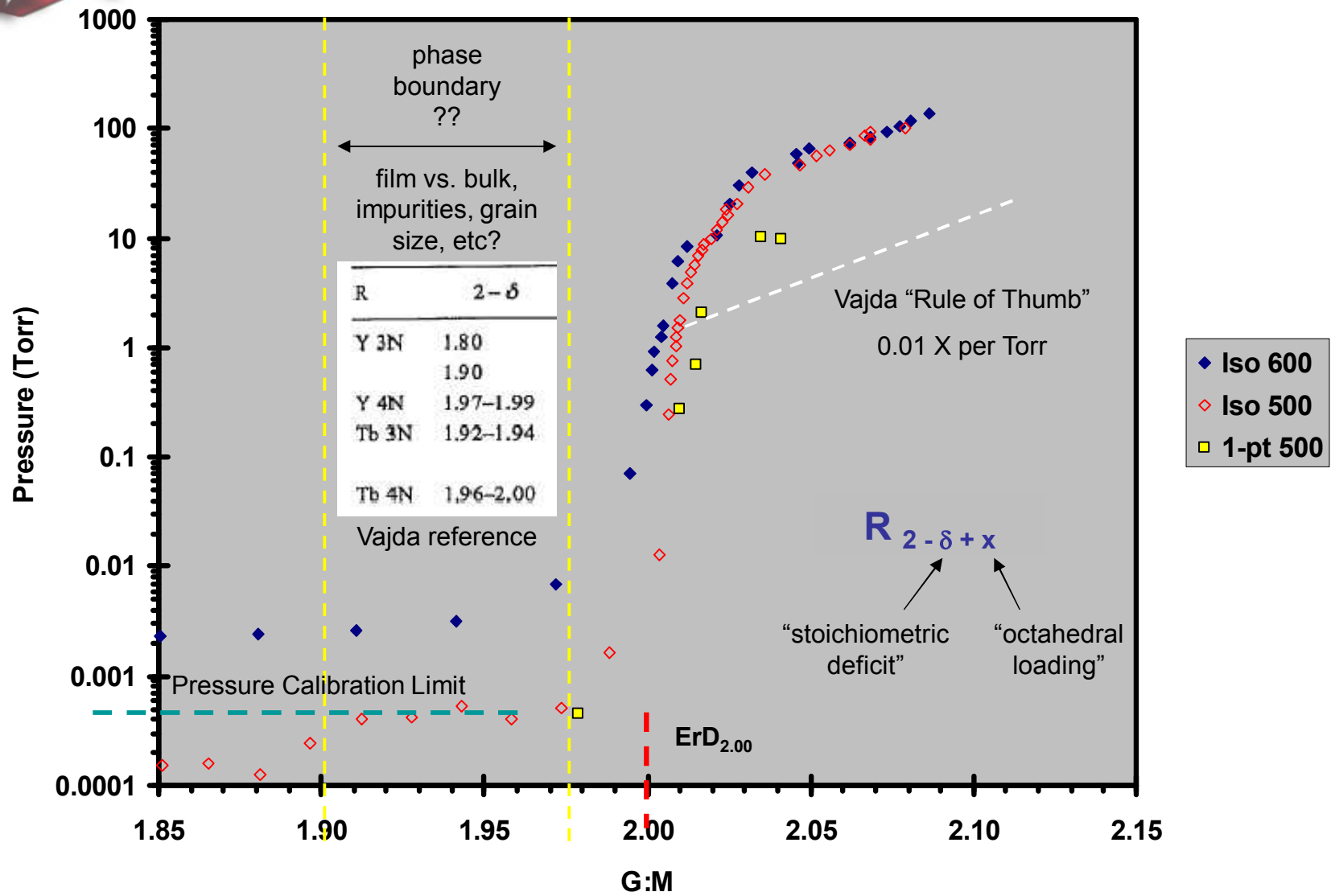
Step 4.) Close Vcal1



500 & 600 C Bulk Er-D Isotherms



500 & 600 C Bulk Er(4N)-D Isotherms

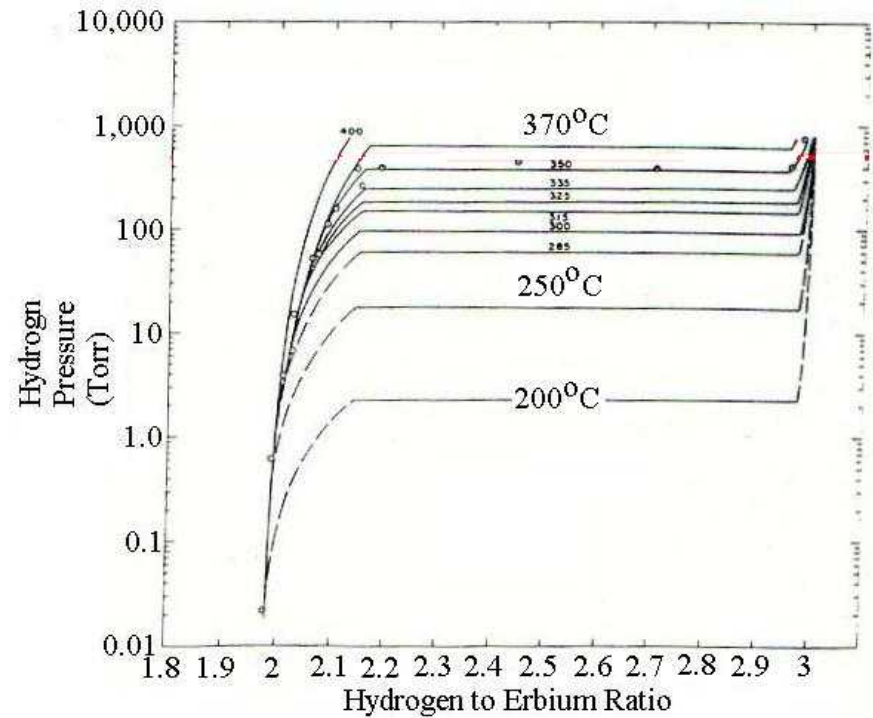
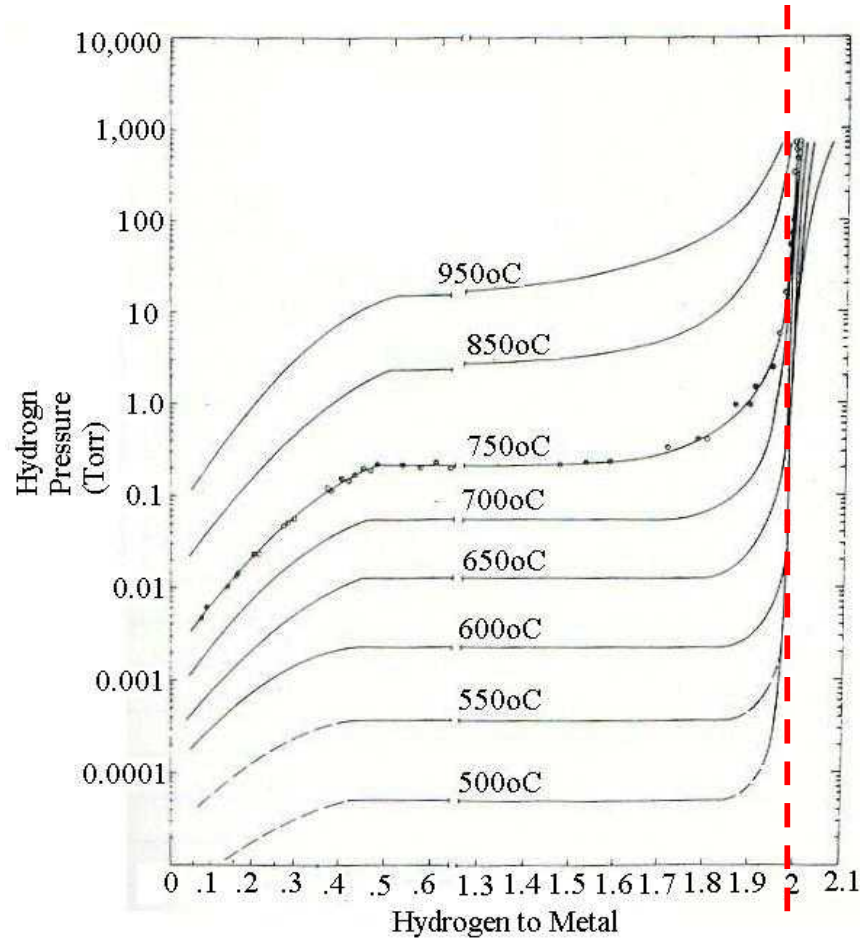


Does β -phase equilibrium data move in G:M space?

Does 10 - 100 Torr region of pressure space dictate % octahedral loading?

Lundin's Isotherms

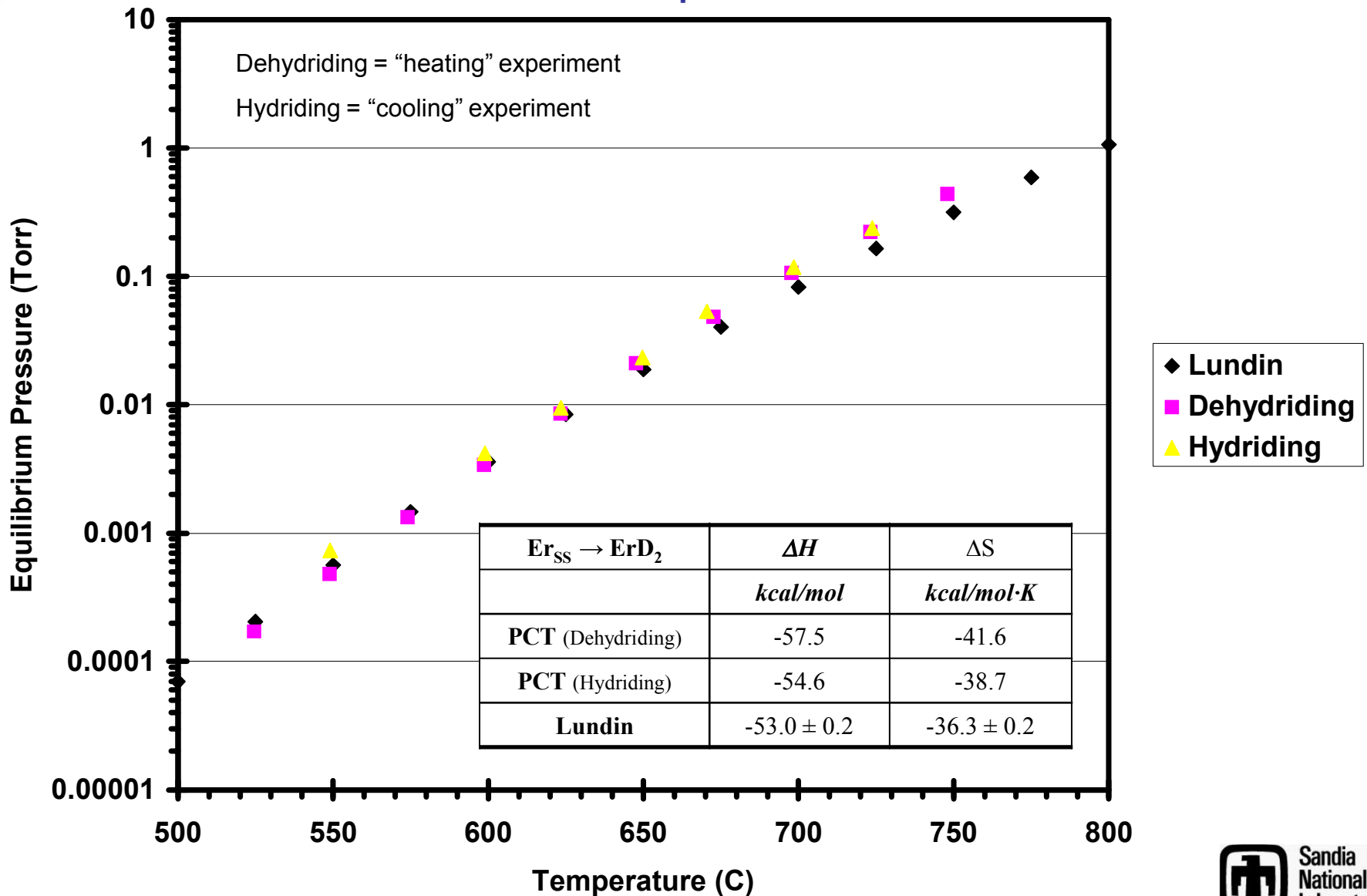
Lundin, C. E. (1968). "The erbium-hydrogen system." Transactions of the Metallurgical Society of AIME 242: 903-907



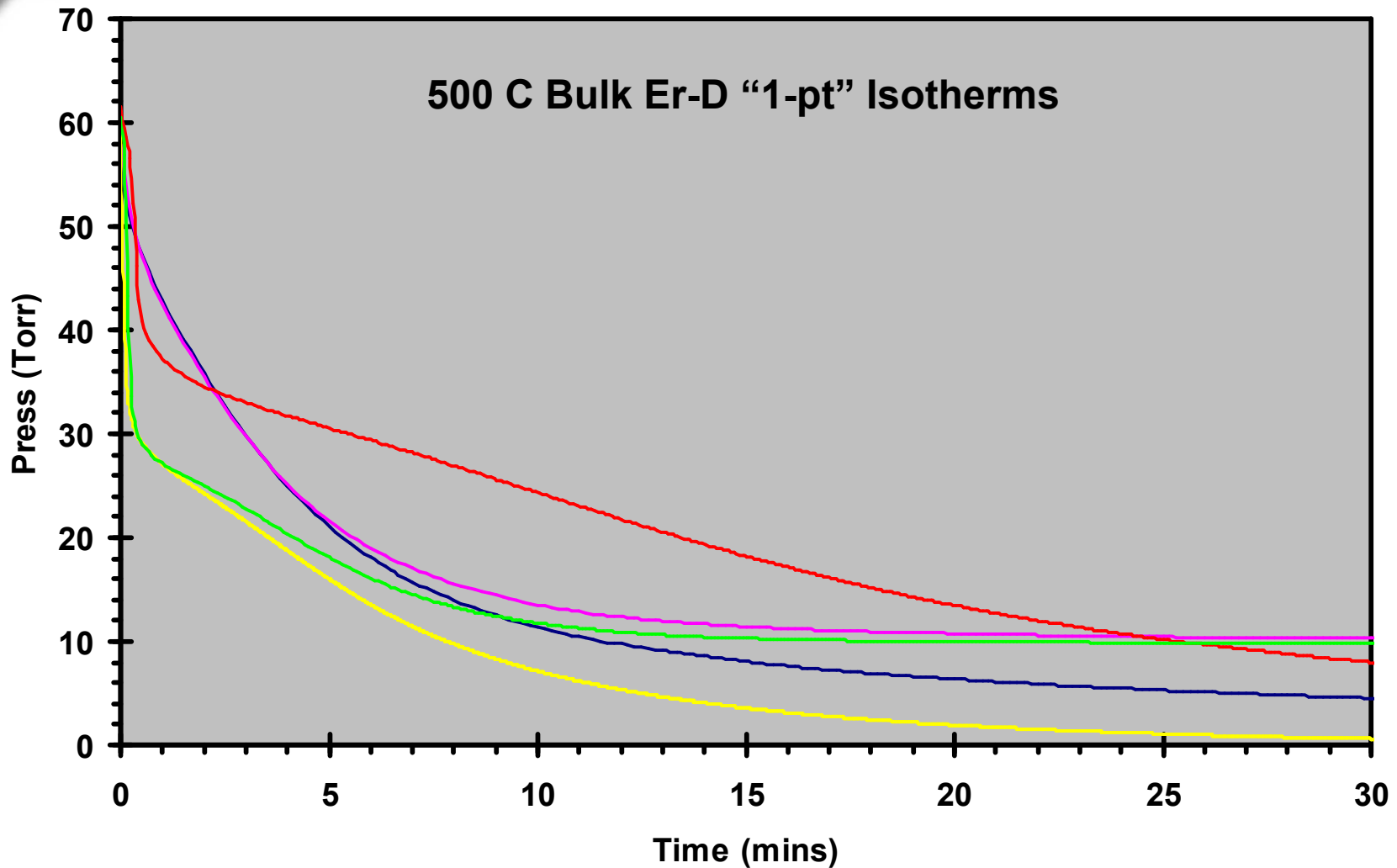
Material: 3N Erbium (99.9+%)

α - β Plateau Pressures

“Van’t Hoff Experiment”



Hydriding Kinetics



Approach:

Bloch, J., Kinetics and mechanisms of metal hydrides formation – a review.
Journal of Alloys and Compounds **253-254**, 529-541 (1997).

Luo, W., Gross, K. J., A kinetics model of hydrogen absorption and desorption in
Ti-doped NaAlH₄. *Journal of Alloys and Compounds* **385**, 224-231 (2004).

% Octahedral & lattice parameter

HYDROGEN IN RARE-EARTH METALS, INCLUDING RH_{2+x} PHASES*

P. VAJDA

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Concept: remove sample from PCT and
measure lattice parameter using XRD ...

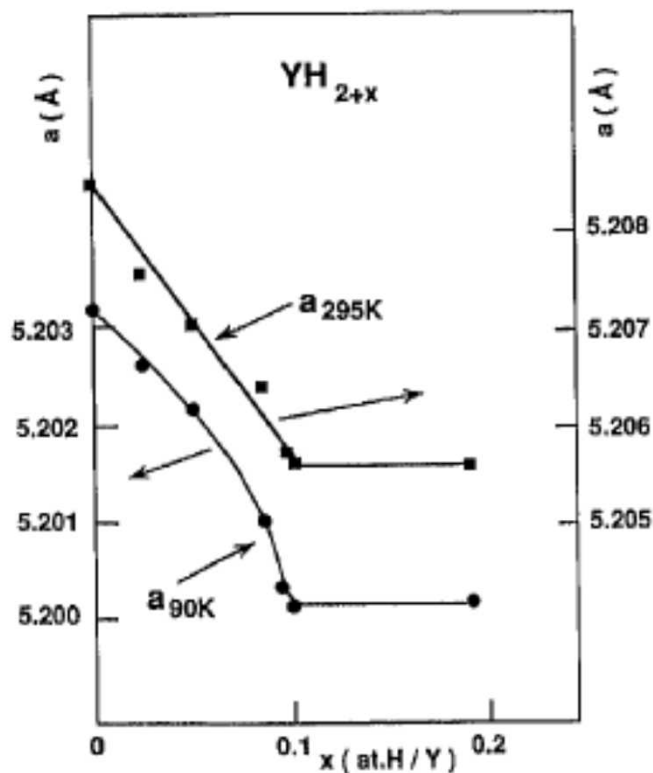
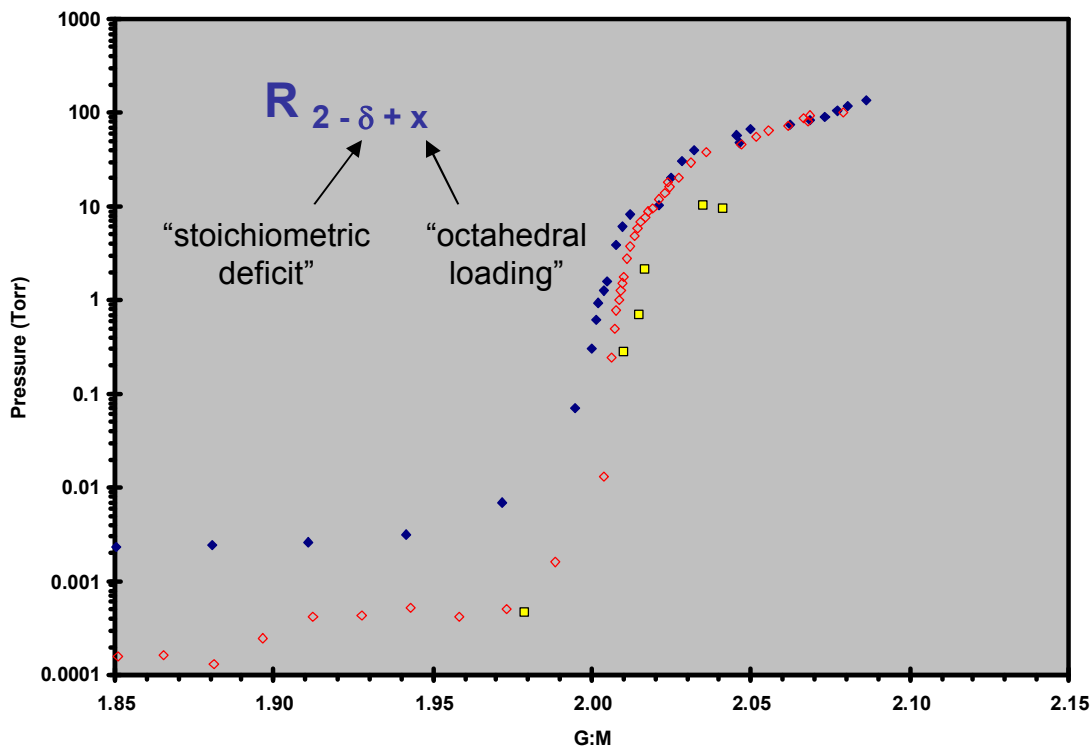


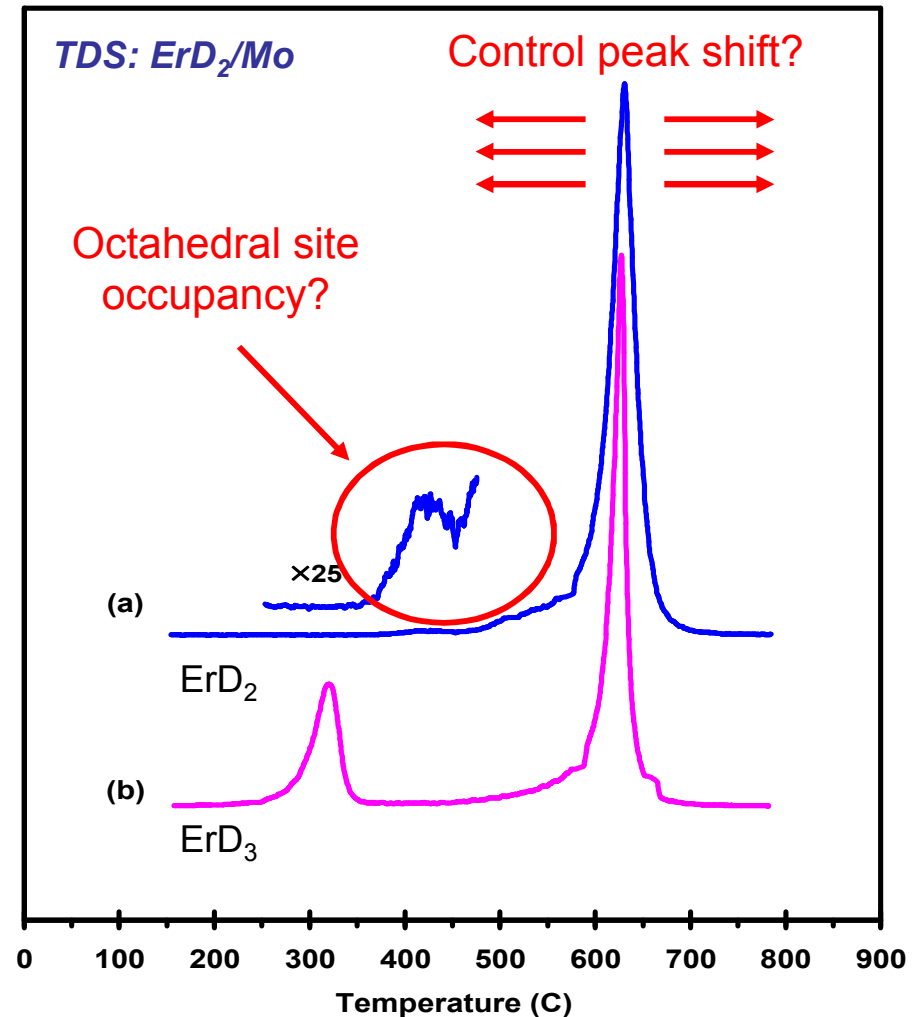
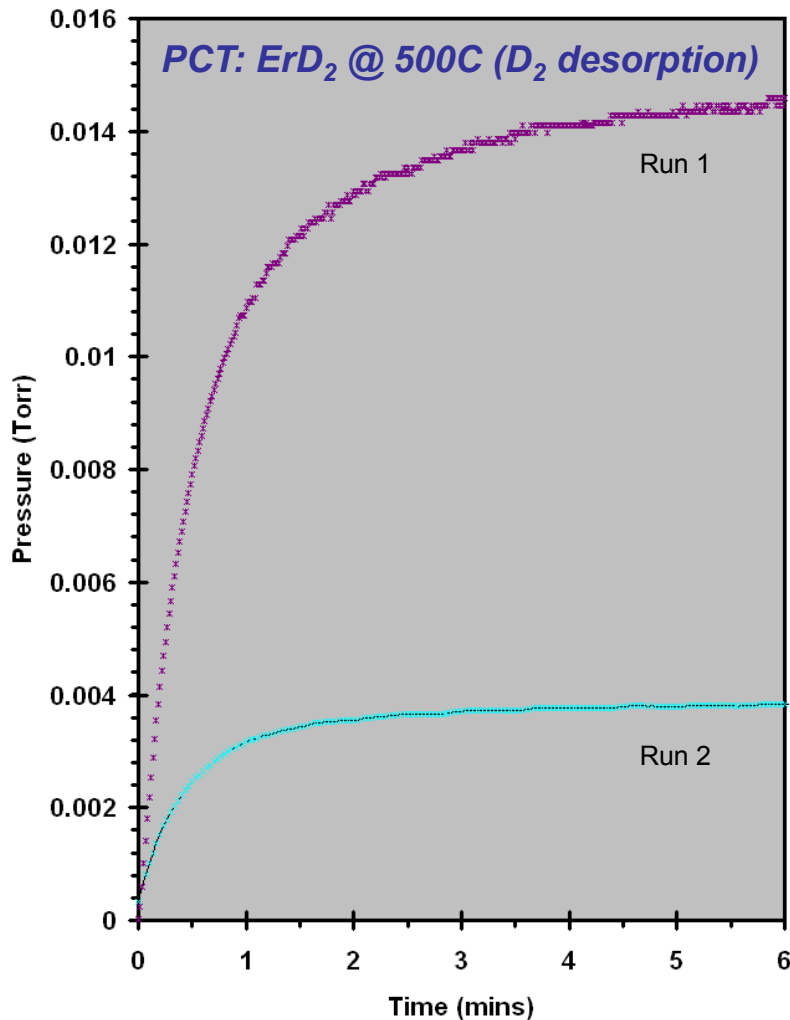
Fig. 9. Lattice parameter of YH_{2+x} as a function of x at room temperature and at 90 K (Daou and Vajda 1992).



... but what about desorption kinetics??

Dehydriding Kinetics

See also: Vajda and “pumping octahedrals”



Kinetics and Thermodynamics Controls Final Composition