



Thermodynamic Modeling of Mg-Cu-Y-H System Combined with Key Experiments

Guy-Joël Rocher, Mamoun Medraj, Hoi Dick Ng, Mezbahul Islam
Concordia University, Montréal, Québec, Canada, H3G 1M8

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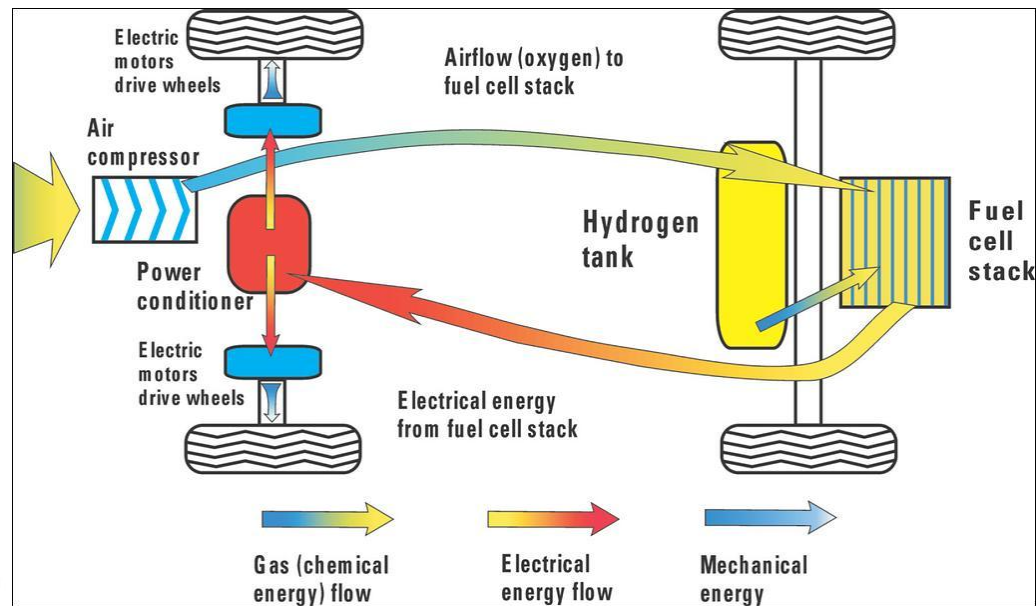


Outline

- Introduction
- Methodology
- Results
- Summary

Introduction

- A key element of a fuel cell system is the H₂ storage tank



Schematic of a Fuel Cell powered car¹

Source: Gerry Nolan, Silicon Chip, Issue 166, July 6 2002

Objectives

- Predict compositions with favourable properties, such as enthalpy of formation, using thermodynamic modelling.
- Synthesize and characterize the composition.
- Test the hydrogen sorption properties of the composition to validate the model.

Research Facilities

Arc Melting Furnace



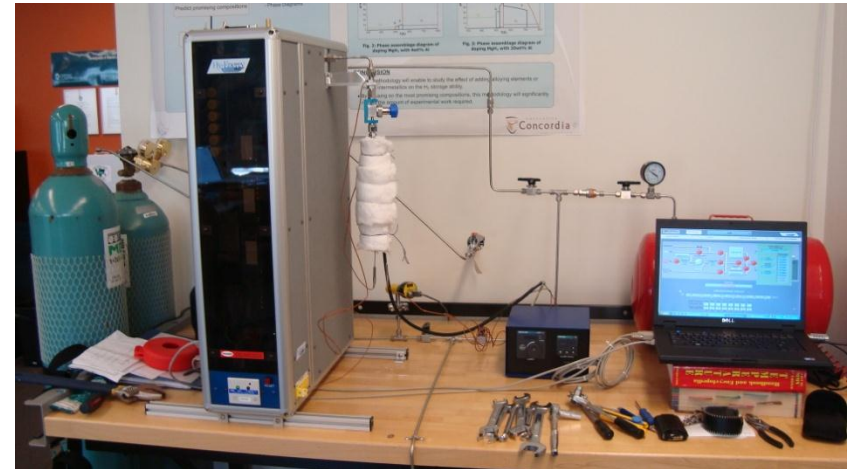
Arc Melting Furnace

XRD



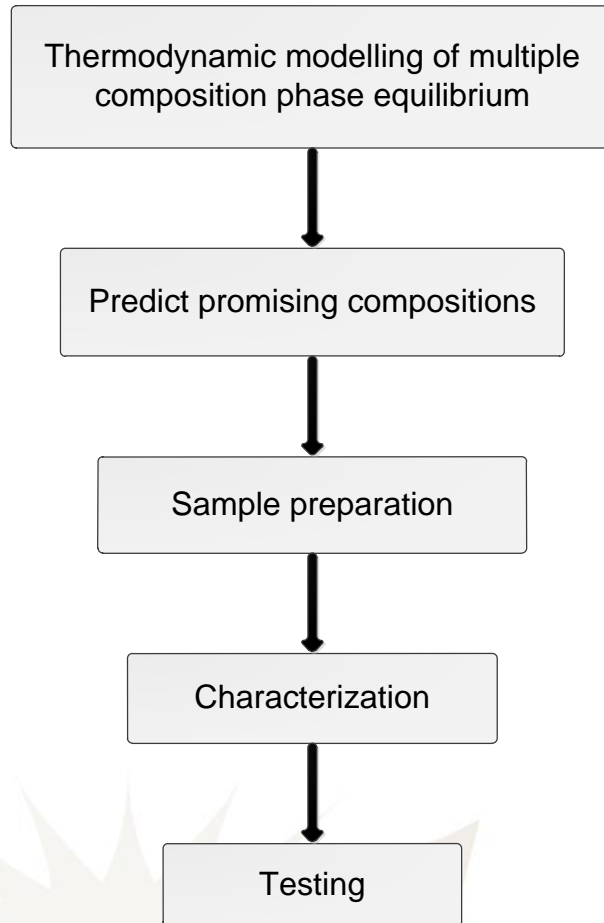
X-Ray Diffraction

Volumetric H₂ Testing PCT-SYS



Hy-Energy PCT-SYS

Methodology



» - FactSage™, CALPHAD

» - Phase Diagrams

» - Melting, Mechanical Alloying

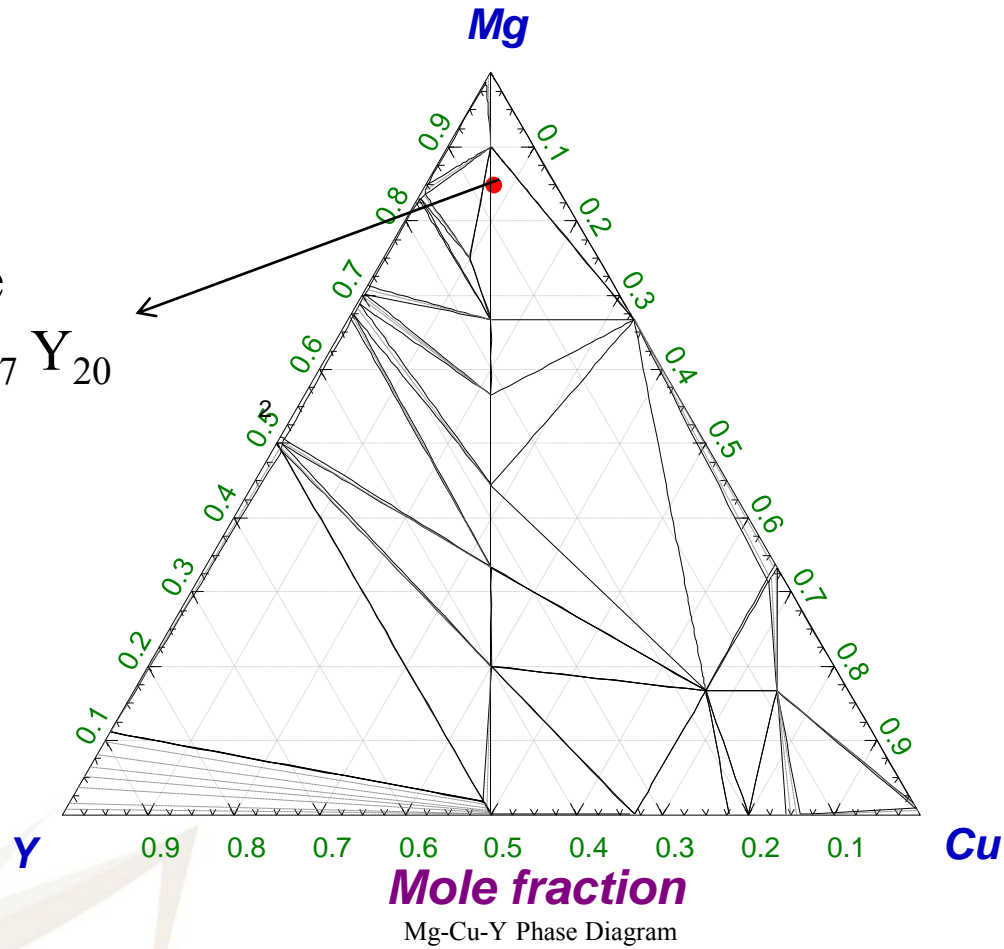
» - XRD, ICP, DSC, SEM/EPMA

» - Volumetric Method

Results

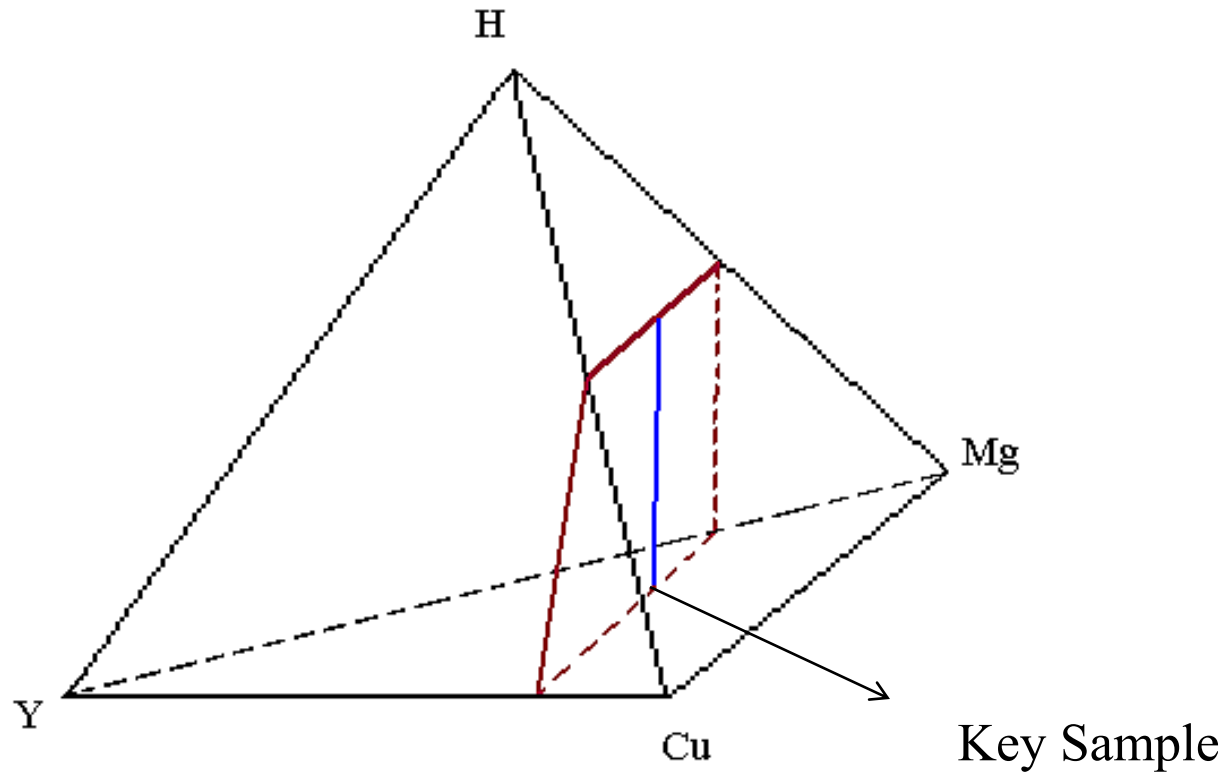
Mg-Cu-Y Ternary System Isothermal Section at 300°C

Key Sample
 $\text{Mg}_{64.3} \text{Cu}_{15.7} \text{Y}_{20}$



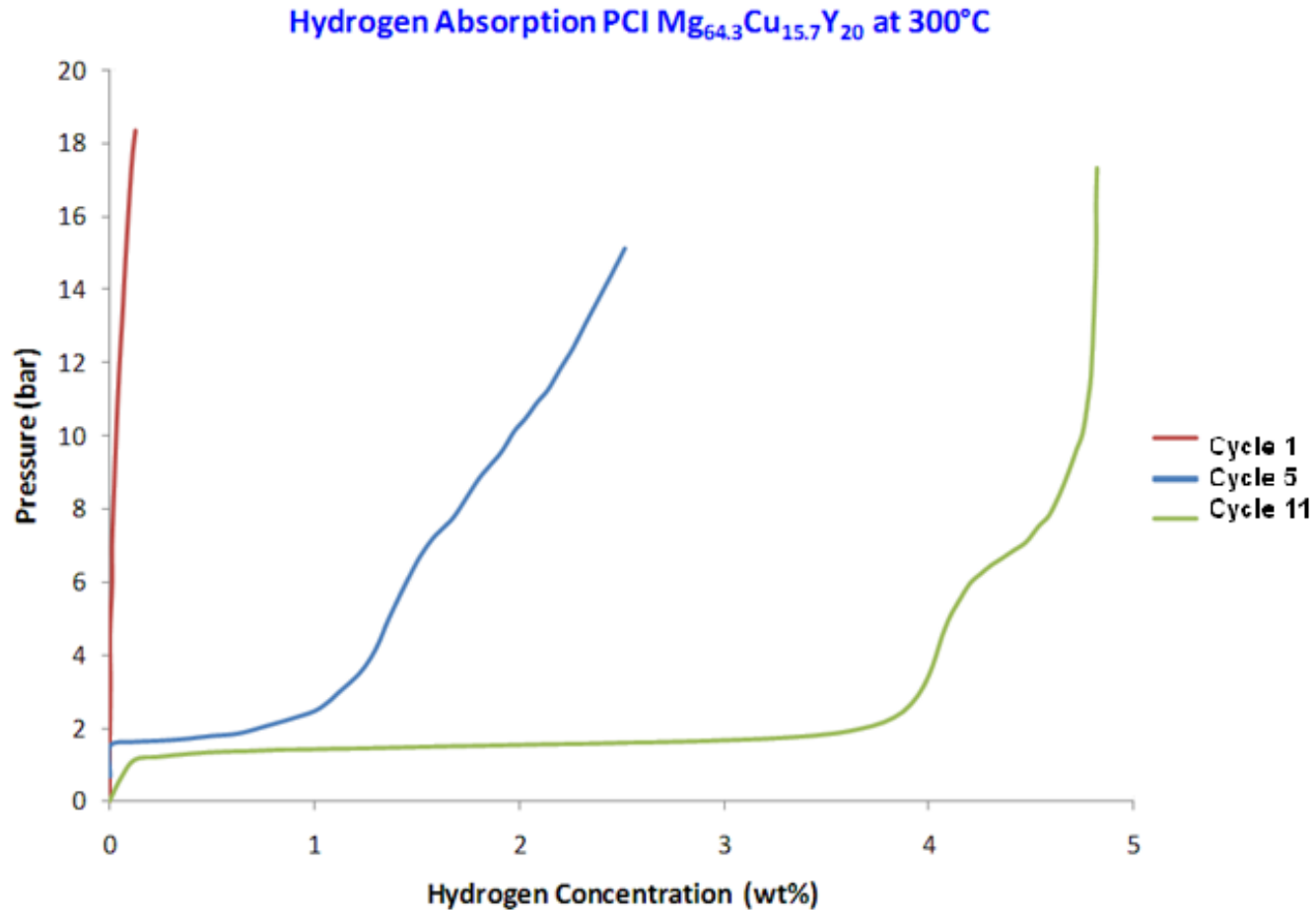
FactSage™

Quaternary Phase Diagram Mg-Cu-Y-H



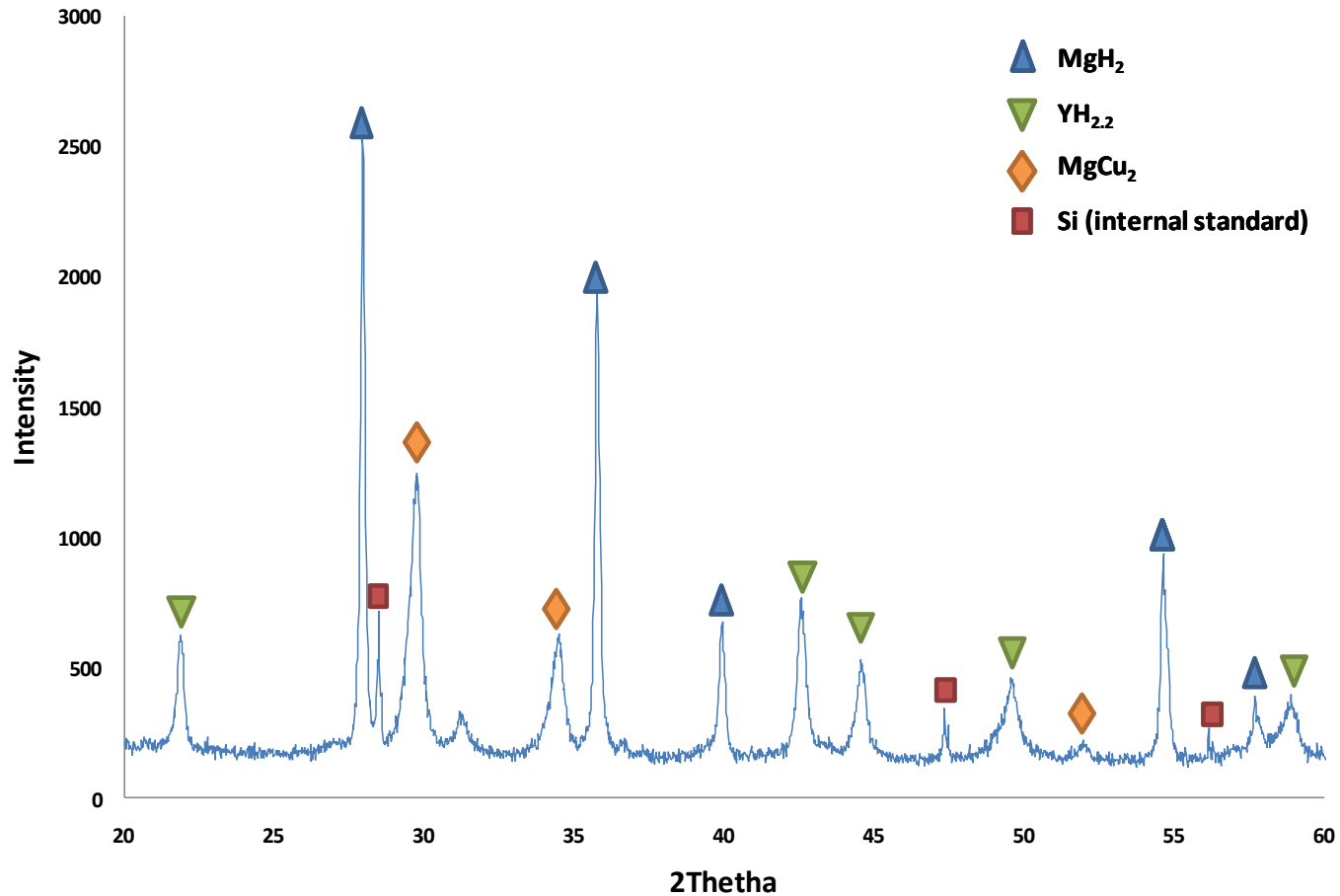
Phase Diagram of the Mg-Cu-Y-H System

Pressure Composition Isotherm (PCI)



XRD Analysis

XRD Pattern $\text{Mg}_{64.3}\text{Cu}_{15.7}\text{Y}_{20}$ after H_2 PCI at 300°C



Summary

- Use thermodynamic modeling of the ternary Mg-Cu-Y system to identify key compositions.
- Synthesize and characterize the promising compositions.
- Perform Hydrogen PCI experiments using volumetric method.
- Develop the quaternary phase diagram for the Mg-Cu-Y-H system using the ternary Mg-Cu-Y database and the key experiments.

Questions?



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