IEA/DOE/SNL HYDRIDE DATABASES (Excel Versions)

INTRODUCTION

This is an introduction to the Excel versions of databases on metal-hydrogen systems, their properties, applications and literature sources. Online versions of the databases can be found at http://hydpark.ca.sandia.gov/. However, these Excel versions of the databases are perhaps more convenient to the user for offline searching, sorting, printing and graphing.

The hydride database effort was funded by the **U.S. Department of Energy** as a contribution to the **International Energy Agency Hydrogen Implementing Agreement**. We wish to express our gratitude to the IEA-HIA, U.S. DOE and Sandia National Laboratories for the support and interest provided for this data collection and dissemination effort, as well as to the many users of this information over the last 15 years. The **Databases** are made freely available to anyone interested. There are no copyright restrictions to the lists generated; however, those who use this database are requested to kindly cite it in any resultant reports or publications. All databases must be used with care and in conjunction with the original references cited so you can make your own judgments as to the data reliability before using that data for any purposes. The introductory page for each database used should be carefully read to help understand the nature of the data presented.

We believe the information presented in the original release of these databases is a reasonably accurate representation of the data published; however, the International Energy Agency Hydrogen Implementing Agreement, U.S. DOE and Sandia National Laboratories can offer no warranty, expressed or implied, as to the accuracy, applicability or use of the information for the users' intended purposes. In addition, we cannot be responsible for any changes users may make to the original release.

CAUTION: For maximum usability of the Excel sheets, all cells are unprotected. It is strongly advised that users work on a copy of the Excel file and retain the original file in archival form.

Gary Sandrock
George Thomas
April, 2010

LIST OF THE DATABASES

The following is a list of the databases, as of April, 2010:

List of IEA/DOE/SNL Hydride Databases

Database	Records	Last Update
Hydride Alloy Listings	**2706**	
AB_5 Intermetallic Compounds	477	01/03
AB_2 Intermetallic Compounds	625	01/02
AB Intermetallic Compounds	179	12/01
A_2B Intermetallic Compounds	122	12/01
Misc. Intermetallic Compounds	431	01/02
Solid Solution Alloys	263	04/02
Mg Alloys	375	12/02
Complex Hydrides	234	12/02
Hydride Properties	**47**	1999
Hydride Applications	**373**	09/07
References	**1616**	09/07

Note that some of the databases have not been updated for nearly a decade. In particular, the extensive activities in complex hydrides during recent years have not been captured. In addition, efforts in the areas of H_2-adsorbents and chemical hydrogen carriers are not included.

OVERVIEW OF THE DATABASES

The field of metal-hydrogen systems R&D has been active for more than a century, and especially so since the middle of the 20th Century. Discoveries of easily rechargeable metal hydrides based on alloys and intermetallic compounds started about 1970 and led to a hydride renaissance and several proposed and commercial applications. A commonly used applications example is the nickel metal hydride (NiMH) battery that uses a metal hydride for the negative energy storage electrode. A second important application area is the storage of hydrogen fuel for vehicular propulsion and stationary power generation, e.g., in both cases fuel cells. We are rapidly reaching an era when we must seek alternatives to fossil fuels. A promising alternative is hydrogen and we must continue metal hydride R&D as a potential way of safely, efficiently and economically storing and transporting that hydrogen. These databases were created to aid the researchers and application engineers who are following that quest. We offer a series of databases in varying content and detail:

- **Comprehensive Hydride Materials Listings**
- **Properties Database for selected hydriding materials**
- **Hydride Applications**
- **References**

The Metal-Hydrogen Systems databases are based largely on hydride forming alloys, although some M-H systems that form H solid solutions are also included. Elemental hydrides are generally omitted (except for a few important elements included in the Hydride Properties database). Most of the alloys covered are nominally single phase, although many exceptions probably exist. Amorphous, nanocrystalline and multiphase alloys are generally not included. A brief description of each database is given below. More details of each database are given later.

Hydride Materials Listings

These databases are presented as a series of eight comprehensive historical listings of alloys that have been reported to form simple hydrides, hydride complexes or H solid solutions (currently 2706 records). Each is based on a metallurgical or crystallographic class of alloy or intermetallic compound. Unlike the Hydride Properties Database (below), the Hydride Alloy Listings include only a few representative properties, mainly in the area of hydrogen-capacity and representative PCT (pressure - composition - temperature) thermodynamic properties.

Hydride Properties

This database contains more detailed engineering information on a limited number of alloys (currently 47 records). The alloys represented are those that have been used for applications or have special historical and scientific interest. Properties include composition, detailed PCT, H-capacity, enthalpy and entropy of hydriding, plateau slope and hysteresis, metallurgy and synthesis, activation, kinetics, cyclic stability, morphology, gas impurity effects, commercial suppliers, known applications and selected literature citations.

Applications

This database lists 373 specific hydride applications or application-related studies and reviews in the general areas of H-storage, H-processing, thermal, electrochemical, materials processing and others.

References

The references used in all the hydride databases (more than 1600) are located in a separate database. The Excel version of the Reference Database can also be used in a self-standing mode, i.e., independently of the hydride databases. It is searchable either by using the usual bibliographic fields (author, co-author, year, journal, organization, etc.) or by keywords.

Prudent Use of the Data

The users of these databases should fully understand they represent only a door to the published literature. They are not meant to be used for the design of hydride devices. The user should carefully read the background information associated with each database and the disclaimers. The original reference sources for each datum of interest should be read before it is utilized. As always with the published literature, be wary of erroneous data. In addition to errors in the original publications, occasional errors in reading graphs or converting units are possible. You would be wise to repeat the experiment if it is critical to your application or if any doubt exists. In general, no attempt has been made to filter the data, with the possible exception of the Hydride Properties database where some limited degree of selectivity has been made relative to our own personal experience.

HYDRIDE MATERIALS LISTINGS

These databases are extensive historical retrospectives of materials that are reported to form hydrides or M-H solid solutions. It is intended to aid both the beginning and experienced researcher in surveying past work on rechargeable hydrides and avoiding repetition of prior work. These gas-phase, PCT-based lists represent the largest and most complete compilations of hydriding alloys to date. The present series contain 2706 entries, believed to be several times the size of any survey previously published. They follow in the tradition of other pioneers who started such tabulations in the 1980s, particularly Buschow et al., 82 (Ref. 284) and Goodell, 86 (Ref. 401).

Organization of the Hydride Materials Listings

The primary organization of the Hydride Materials Listings is relative to the metallurgical or crystallographic form of the hydriding material. In addition to random Solid Solution Alloys, there are five classes of Intermetallic Compounds of the form AB_x, where A represents one or more strongly hydride-forming elements and B represents one or more weakly hydride-forming elements. There are also individual databases for Mg-alloys and Complex Hydrides, i.e., those hydrides that form mixed ionic-covalent structures with a charged MH_x complex incorporated. All of the materials in these databases are considered to be predominantly single phase, although this assumption is not always confirmed in the original publications. In fact, many probably contain minor amounts of second phases, and occasionally this fact is noted in the original publications. Those materials that are clearly and predominantly multiphase (by authors' analysis or simple comparison with well-accepted phase diagrams) are not included here.

The listings go well beyond binary alloys into multi-component systems. Many records represent ranges of alloy compositions within a basic family [e.g., $LaNi_{5-y}Al_y$ (y=0.1-1.0)], where the authors investigated several individual alloys. Rather than burden the listing with a large number if such sub-entries, composition and property ranges are often listed, and the browser should go to the original reference for more detail on individual alloys.

Properties

The Hydride Materials Listings tabulate a limited number of gas-phase hydride properties as available: H-Capacity (both maximum H/M and wt.%, the latter usually calculated), enthalpy of hydriding (ΔH) and one selected mid-plateau P-T combination. More complete definitions of these parameters are given in the preface to the separate **Hydride Properties** database. It should be remembered that the H-capacity is usually the value representing the highest pressure and lowest temperature of the study and is almost always greater than the reversible engineering capacity or effective plateau width. Wherever possible, the enthalpy and pressure-temperature values are given for desorption, although some authors do not clearly differentiate. Reported enthalpies are usually as derived by the authors from van't Hoff plateau analysis. To be as comprehensive as possible, any alloy reported to hydride from the gas phase is included, even if only H-capacity is available. In general, electrochemically derived hydriding properties are not included.

Citations

The citations to the original references are based on the family name of the first author, year of publication and (**Reference Database** number). Refer to the **Reference Database** for the complete citation. When searching the Materials Listing by year, use a four-digit date, e.g., 1995, not 95.

Abbreviations

The data is occasionally qualified by the following abbreviations:

(M)	Multiple plateaus reported.
(Dp)	Alloy reported to disproportionate when hydrided.
(Amorp)	Amorphous hydride.
(cal)	Enthalpy determined by calorimetry.
(calc)	Enthalpy calculated by some non-van't Hoff or non-calorimetric means.
(Sloping plateau)	Plateau evident but very sloping. Most plateaus show some slope, but this notation is used for rather severe slope, usually several times pressure change from one end of the plateau to the other.
(No plateau)	No plateau evident, showing a continuous H-solution behavior. Some may prefer to not use the term "hydride" for such a material, but we include them for completeness.
(Absorption)	Data derived from absorption (not desorption) curves.
(Deuterium or Tritium)	Capacity and PCT values for heavy hydrogen isotopes. Wt.% usually not listed, or converted to effective protium weights.

HYDRIDE PROPERTIES DATABASE

This database is a collection of basic and engineering data on 47 reversible metal hydrides of historical and commercial interest. It contains more metal-hydrogen detail than the Hydride Materials Listings database. Following are descriptions of the individual datafields contained in the Hydride Properties Database.

Formula
Elemental composition of the base metal or alloy before incorporation of hydrogen. The formulas are nominal and often represent a single intermetallic phase, but not necessarily so.

Name
Names represent commonly generic usages when available. Included in this category are registered trade names and alloy numbers used by commercial suppliers.

Composition
These fields on the far right of the database represent conversion of the nominal chemical formula into weight percent. The composition is divided into major and minor elements.

Pressure at 25° C , Temperature at 1 atm pressure

Unless otherwise stated, all temperatures are given in degrees C and all pressures in absolute atmospheres. Wherever possible, mid-plateau pressures from actual experimental isotherms are used; however, data are seldom available at exactly this temperature or pressure, so entries usually represent extrapolations or interpolations of the van't Hoff equation. For very stable hydrides, one may obtain immeasurably low pressure at 25° C. The values listed should be used merely as relative indications of room temperature stability.

Hydrogen Capacity

This property is presented in both an atomic ratio, H/M, and weight percent [wt.%=(100)(H)/(H+M)]. Capacity is given as the fully hydrided value, that is, the highest hydrogen concentration measured in the hydride phase limit. It does not necessarily represent the reversible capacity for engineering purposes.

Structures

Crystal lattice structures, when known, are represented by the Strukturbericht Symbols.

PCT Properties

These thermodynamic properties are presented in direct relationship to the van't Hoff equation:

$$\ln P = \Delta H/RT - \Delta S/R,$$

where

$\ln P$ = natural logarithm of pressure (in absolute atmospheres),
T = temperature in K (˚C+273),
ΔH = enthalpy change of hydriding (in kJ/mol H_2),
ΔS = entropy change of hydriding (in kJ/K-mol H_2),
R = gas constant (0.0083145 kJ/K-mol)

The user should not assume that a given batch of material should exactly reproduce the PCT properties tabulated here, since impurities, composition variations, and other metallurgical factors can influence hydride behavior. These data should be used only as a guide.

ΔH, ΔS

Wherever possible, the values published by the investigator(s) are given. However, in some cases the values are derived by us from our van't Hoff plots, generally using desorption data. Thus, it should be understood they do not represent the chemical parameters determined by calorimetry. The values used here effectively include such terms as strain and interface energies. It should also be recognized that test technique (especially desorption vs. absorption), prior sample history and, to some extent, test temperature can influence these results.

Plateau Slope and Hysteresis

These values are determined from published data using the following expressions:

$$\text{Slope} = d\ln P/d(H/M)$$
$$\text{Hysteresis} = \ln[P(\text{absorption})/P(\text{desorption})]$$

The pressures were evaluated near mid-plateau, if possible. They are in logarithmic terms because they relate to energy losses, which should go to zero when slope or hysteresis are zero. It should be realized that the values cited are representative and not necessarily invariant. For example, plateau slope can increase markedly near the critical temperature or if the sample has metallurgical segregation. Hysteresis often decreases at higher temperatures where stress relief (recovery) or recrystallization can occur.

Pressure vs. Temperature Points
Wherever possible, data points are taken from experimental curves. Where few data are available, van't Hoff calculated values are given.

Plateaus
This field gives a brief summary of the plateau behavior (single or multiple) over appropriate H/M ranges and at various temperatures, if applicable.

Metallurgy and Synthesis
A brief summary of the metallurgy of the material is given along with typical alloy synthesis methods. General comments on the formation of the hydride may also be included.

Activation
Basic hydrogen activation procedures described in the literature are briefly summarized. The user should realize that activation techniques are not necessarily unique, but depend on many variables, including particle size, grinding technique, storage time and environment, vacuum pumping system and configuration, and hydrogen purity.

Kinetics
Only qualitative or semiquantitative comments on hydriding and dehydriding kinetics are given, along with occasional references to published studies.

Cyclic Stability
Where known, data on changes in hydride performance with hydriding-dehydriding cycles will be cited.

Morphology
The form of the samples used to obtain PCT data, when known, are given.

Gas Impurity Effects
Certain gaseous impurities are known to deteriorate hydride performance in some materials. Quantitative or qualitative data, when known, are referenced here.

Comments
Items of potential interest not covered elsewhere.

Commercial Suppliers
This section is intended for connecting potential users with suppliers. These data are rather dated; some suppliers may no longer exist. ***The lists of suppliers are given for information***

purposes only and the IEA, the DOE and Sandia National Laboratories offer no endorsement or recommendation of the capabilities of such suppliers. Any contract made between a User of this database and any Supplier listed herein is the sole responsibility of the User and Supplier.

Applications
Examples of typical applications are listed in this section along with citations. This section is not intended to be comprehensive.

Citations and Authors
The sources of the PCT parameters, as well as other references, are included here. See the **Reference Database** for more citation detail.

METAL HYDRIDES APPLICATIONS DATABASE

This is a database on hydride applications with particular emphasis on the gas phase applications, as opposed to electrochemical applications. The principal applications covered in this release include those in the following nonexclusive list:

HYDROGEN STORAGE
- Stationary
- Mobile

HYDROGEN PROCESSING
- Separation
- Purification
- Gettering
- Isotope Separation
- Compression

THERMAL APPLICATIONS
- Heat Storage
- Heat Pumping
- Refrigeration
- Heat Engine/Actuator

ELECTROCHEMICAL
- Battery
- Catalysis

MATERIALS PROCESSING

OTHER

This release does not include many of the following applications:

- **GETTERING**, e.g., vacuum maintenance and inert gas purification
- **ELECTROCHEMICAL** - Batteries, e.g., Ni-MH secondary batteries
- **MATERIALS PROCESSING**, e.g., magnet powder processing

Each Application Record is represented by a primary reference in the Reference Database, and occasionally additional references by the same organization. The application(s) associated with that reference are indicated, along with the hydriding alloy(s) used in the application(s) and the type(s) of study involved, i.e.:

- Theory/Modeling
- Conceptual
- Experimental
- Prototype
- Commercial
- Review

An ORGANIZATION:DESIGN section lists the organization doing the work and a brief description of the hydride container and/or system design. A COMMENTS section gives a brief description of the study and sometimes lists other associated references in addition to the primary one.

The **Applications** and **References Databases** are not meant to be a substitute for direct and complete reading of the references. They are only convenient mechanisms to give you some preliminary indication as to what has been done in the past. You are urged to obtain, read, and interpret the original references for yourself. Although a best effort has been made, the abstracts in the Applications records should not be taken as necessarily correct or complete representations of the original reference. See the general **Prudent Use of the Data** that applies to all the Databases.

REFERENCE DATABASE

The **Reference Database** is an extension and substantial enlargement of the one started in the mid-1980s by Goodell, 86 (Ref. 401). It contains complete citations for all the references used to generate all the M-H databases. In addition to the usual bibliographic form, the complete titles of the articles or reports are included, along with a field for the publishing organization(s) and our own system of key words. The database is sortable and searchable as any Excel file. Reading a few of the reference lines will give the browser a feeling as to the key words typically used.

Because of personnel limitations and copyright restrictions, the IEA-HIA, U.S. DOE, and Sandia National Laboratories all regret that they are not in positions to supply copies of the references listed. Many are articles published in readily available journals that are traditional outlets for hydride R&D results, e.g., the **Journal of Alloys and Compounds** (formerly **Journal of the Less-common Metals**) or the **International Journal of Hydrogen Energy**. Many large national, public, or university libraries subscribe to such journals and also have collections of government reports and conference proceedings. Internet connections to the pertinent societies and publishers often allow easy on-line purchase of individual articles.

The **Reference** Listings are made freely available to anyone interested. There are no copyright restrictions to the lists; however, those who use this database are requested to kindly cite it in any future reports or publications.