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The IEA/DOE/SNL On-Line Hydride Databases

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Abstract

As part of International Energy Agency (IEA) Hydrogen Agreement Task 12, a series of comprehensive hydride databases have been constructed and made freely available on the Internet (URL <http://hydpark.ca.sandia.gov>). They include extensive listings of alloys reported to hydride, detailed engineering properties on selected hydrogen storage elements and alloys and a hydride applications database. These databases and an associated reference database are described, along with other hydride information available on the website. The databases were created under the auspices of the IEA with financial support from the U.S. Department of Energy (DOE) and Internet service support from the Sandia National Laboratories (SNL).

Introduction

Task 12 of the IEA Hydrogen Implementing Agreement was an R&D effort aimed at developing new solid hydrogen storage media, in particular aiming at properties that might be suitable for H₂-fueled vehicles. The prologue to future R&D is past R&D. Most scientists (but not all) carefully review the past literature before undertaking a new project. To make that process easier for the Task 12 scientists, overall hydride community and potential users of hydrides for H₂-storage, as well as to help minimize duplication of past work, we decided in 1995 to create a series of retrospective hydride databases and to make those databases freely available via the growing power and convenience of the Internet (URL <http://hydpark.ca.sandia.gov>). The databases have grown in subject, content and use since 1995. This is a brief introduction to those databases for those who have not yet used them.

The IEA/DOE/SNL Hydride Databases - Today

The databases were created, and are maintained, under Task 12 of the IEA Hydrogen Implementing Agreement with contributory funding from the U.S. DOE. The data is tabulated from the open literature by Sandrock and loaded into Claris FileMaker® Pro databases. Thomas of SNL supplies and maintains the Apple Macintosh Internet Server and associated software to connect the databases to the Internet. The databases are organized in ways we think most useful to hydride scientists and applications engineers. We have chosen an emphasis on hydride PCT (pressure-composition-temperature) properties and hydride applications, but other useful hydride information is also included. The hydride databases themselves are accompanied by a detailed bibliographic database.

The hydride databases presently available are shown in Table 1, along with the number of records as of late 2000. Although rather thorough individual descriptions of the databases can be found in on-line introductory material, a brief summary of each type is given below. All of the

hydride databases are searchable via access query forms. They can also be displayed in their entirety for those so inclined.

Table 1
List of IEA/DOE/SNL Hydride Databases
 (Numbers of records as of late 2000)

<u>Database</u>	<u>Records</u>
Hydride Alloy Listings	1942
AB ₅ Intermetallic Compounds	330
AB ₂ Intermetallic Compounds	509
AB Intermetallic Compounds	156
A ₂ B Intermetallic Compounds	103
Misc. Intermetallic Compounds	287
Solid Solution Alloys	171
Mg Alloys	213
Complex Hydrides	173
Miscellaneous	Planned
Hydride Properties	47
Hydride Applications	271
References	1180
M-H Organizations	22
M-H Meetings Calendar	Varies

Hydride Alloy Listings - These databases are a series of comprehensive historical listings of hydriding alloys. Each is based on a metallurgical or crystallographic class of alloy and intermetallic compound. The Hydride Alloy Listings are designed for a rapid and broad search to see if others have published in one's particular compositional area of interest or to outline areas lacking prior work. They include only a few representative properties, mainly in the area of hydrogen-capacity and representative PCT thermodynamic properties like ΔH and individual reported plateau pressure – temperature combinations. They are searchable as to composition, first author and publication year.

Hydride Properties - This database contains a limited number of hydride-forming alloys, at least in comparison to the Hydride Alloy Listings, but exhibits much more engineering property detail on each. The alloys (and a few elements) represented are those that have been often used for applications or have historical and special 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. This database is searchable as to name, formula, plateau pressure at room temperature, temperature for 1 atmosphere plateau pressure and weight percent H-capacity.

Hydride Applications - This database summarizes many of the publications, reports and patents on hydride applications. Searchable categories (and subcategories) include H-storage (stationary, mobile), H-processing (separation, purification, isotope separation, compression), thermal applications (heat storage, heat pumping, refrigeration, actuator/heat engine), electrochemical (battery, catalysis), material processing and others. Records are categorized as theory/modeling, conceptual, experimental, prototype, commercial and review.

References - The references used in all the above hydride databases are located in this separate database. The Reference database can also be used in a self-standing mode, i.e., independently

of the hydride databases. It is searchable by reference number (from the other hydride databases), first author, coauthors and key words.

M-H Organizations - This database consists of profiles of organizations involved in M-H research, development and commercialization. The information contained in each record is exactly as submitted by the organization itself. The database is searchable as to organization name, principal contact, organization country and specialties. Participation in this database by the hydride community has been disappointing. We urge interested M-H organizations to complete and submit the profile form we have included on the website.

M-H Meetings Calendar - This is a compilation of worldwide conferences and symposia in the field of metal-hydrogen systems. It includes information on the basic parameters of the meetings (date, place, organization, abstract submission, etc.), as well as Internet or other addresses for further information. Anyone interested in having a meeting listed should forward the basic information to Sandrock.

Use of the databases – The use of the databases is free on a worldwide basis. The users of these databases should fully understand they represent only gates to the published literature. Numerical and qualitative data given are not meant to be used *per se* for the design of hydride devices. The user should carefully read the background information and definitions 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. The IEA, DOE, SNL and SunaTech, Inc., make no warranty, express or implied, as to the accuracy and applicability of the database information for users' intended purposes.

The IEA/DOE/SNL Hydride Databases - Future

The main continuing effort will be the updating of the existing databases, adding missing information and periodic updating. Users of the databases can help by informing us (particularly Sandrock) of missing papers, including your own. The papers should be available in the open literature and conform to the existing categories, in particular papers that contain some PCT data (at least H-capacity) or hydride applications.

At present, the metallic, covalent (Mg) and mixed ionic-covalent (complex) hydrides are well represented in the databases. As shown in Table 1, we plan to add a new Hydride Materials Listing under the category Miscellaneous. This is intended to cover papers in the non-traditional categories: nanocrystalline, amorphous, quasicrystalline, multiphase, etc. In addition we have not yet included much on certain application categories such as hydrogen getters and metal hydride batteries. These and others will perhaps be added in due course. Finally, we are closely observing the developing area of carbon hydrogen storage media and will decide during the next year whether it would be helpful to add a database on that category. There are perhaps other categories that will someday deserve consideration, e.g., H-rechargeable liquid and solid organics and liquid solutions of complex hydrides.

Suggestions from users of the databases as to what database additions might be helpful are welcome. Our time and funding is very limited and we must admit the IEA/DOE/SNL hydride databases cannot be all things to all people. One suggestion that is receiving serious consideration is the production of a CD-ROM version of the databases that will allow more rapid off-line use. This has been proposed to IEA/DOE and will probably be implemented in late 2001 or 2002 when the databases are more complete.

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